Each problem that I solved became a rule, which served afterwards to solve other problems, Rene Descartes
COUPLED-MODE THEORY FOR RF AND MICROWAVE RESONATORS

by

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ABSTRACT

The case of two dielectric resonators inserted in a cavity is fully analyzed. It is shown that the three uncoupled modes interact to form three coupled ones. Accordingly, Energy Coupled-Mode Theory, a coupled mode formalism where energy is conserved, is developed to study the coupling of RF and microwave resonators. The governing equations are written in the form of an eigenvalue problem where the eigenvalues represent the square of the frequencies and the eigenvectors are the fields’ coefficients. Both external and internal boundary conditions are discussed. The coupled mode formalism is capable of analyzing a system consisting of an arbitrary number of resonators.

Using the proposed equations, the physical origin of the coupling coefficient is found and interpreted based on the energy conservation principle. The interpretation is general and universal and is believed to encompass cases where dielectrics and conductors are present. An important electron paramagnetic resonance probe, namely a cavity with a tiny insert, is studied. It is shown that when the frequency of the cavity is equal to that of the insert, the resulting fields are complete mixes of the two uncoupled modes. This finding, together with others, finds applications in the magnetic resonance and dielectric measurements fields.

Different practical scenarios (large/small cavities, high/moderate relative permittivity values) are discussed in detail. Expressions for field dependent parameters such as coupling coefficients, $Q$ values, filling factors and resonator efficiency are derived. It is shown how these parameters contribute to the probe performance and how, in some circumstances, trade-offs need to be made.
Design procedures for electron paramagnetic resonance probes, verified using finite-element simulations, are proposed. It is found that proper design can indeed enhance the electron paramagnetic resonance signal. Particularly, the shield can help in boosting the resonator efficiency of a lossy dielectric resonator.

The method of images, area commonly used electromagnetic technique, is used together with the coupled mode theory to study cases where resonators are placed close to conducting planes. The aforementioned situations occur in the field of magnetic resonance spectroscopy when dielectric resonators are used as tuners. These situations also exist when conducting planes are used to enhance wireless power transfer using resonant inductive coupling.
DEDICATION

To my parents, son, wife, brother and sisters.
ACKNOWLEDGEMENTS

For their advice and directions from the initial stages of my PhD program to their help with the final draft of this thesis, I owe extreme debt of gratitude to my supervisors Professors Saba Mattar and Richard Tervo. Their help and support were absolutely invaluable.

It gives me great pleasure in acknowledging the support and help of Professor Brent Petersen.

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I owe my deepest gratitude to Shelley, Denise, Karen and all the ECE staff for their keen support and attitude.

For her support, care, infinite patience and understanding, million thanks to my wife Asmaa Ayad.

For their support and love, my parents, sisters, brother, mother and father in law and family.
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<tr>
<td>EPR</td>
<td>Electron Paramagnetic Resonance</td>
</tr>
<tr>
<td>ESR</td>
<td>Electron Spin Resonance</td>
</tr>
<tr>
<td>TE</td>
<td>Transverse Electric</td>
</tr>
<tr>
<td>TM</td>
<td>Transverse Magnetic</td>
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<tr>
<td>CMT</td>
<td>Coupled Mode Theory</td>
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<tr>
<td>WPT</td>
<td>Wireless Power Transfer</td>
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<td>DR</td>
<td>Dielectric Resonator</td>
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<td>CROW</td>
<td>Coupled Resonators Optical Waveguide</td>
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<td>ECMT</td>
<td>Energy Coupled Mode Theory</td>
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<tr>
<td>CW</td>
<td>Continuous-wave</td>
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<td>ENDOR</td>
<td>Electron-nuclear double resonance</td>
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<td>ELDOR</td>
<td>Electron-electron double resonance</td>
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<td>ESEEM</td>
<td>Electron spin echo envelope modulation</td>
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<td>DQC</td>
<td>Double quantum coherence</td>
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<td>DEER</td>
<td>Double electron-electron resonance</td>
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<td>SNR</td>
<td>Signal to noise ratio</td>
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<td>LGR</td>
<td>Loop Gap Resonator</td>
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<td>JD</td>
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<td>$\mu_B$</td>
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<td>Filling factor</td>
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<td>$Q$</td>
<td>Quality factor</td>
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<td>$P(P_i)$</td>
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<td>$C_p$</td>
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<td>$\tilde{H}$</td>
<td>Magnetic field intensity of the coupled system</td>
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<td>$a_i$</td>
<td>The $i^{th}$ coefficient of the electric field</td>
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<td>$b_i$</td>
<td>The $i^{th}$ coefficient of the magnetic field</td>
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<td>$W_E$</td>
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<td>$J$</td>
<td>Current density</td>
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<td>$\kappa$</td>
<td>Coupling coefficient</td>
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<td>$\kappa_e$</td>
<td>Electric component of the coupling coefficient</td>
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<td>$\rho_{ik}$</td>
<td>The $(i,k)$ component of the transferred energy</td>
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<tr>
<td>$\sigma_{ik}$</td>
<td>The $(i,k)$ component of the conduction current energy</td>
</tr>
<tr>
<td>$\psi_{ik}$</td>
<td>The $(i,k)$ component of the polarization current energy</td>
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<td>$Q^{++}$</td>
<td>The quality factor of the symmetric mode</td>
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<tr>
<td>$Q^{+-}$</td>
<td>The quality factor of the anti-symmetric mode</td>
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<td>$L_C$</td>
<td>Lumped inductance of a cavity</td>
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<td>$C_C$</td>
<td>Lumped capacitance of a cavity</td>
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<tr>
<td>$L_D$</td>
<td>Lumped inductance of a dielectric resonator</td>
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<td>Coupling capacitance</td>
<td>$C_{cc}$</td>
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<td>Lambda (Resonator) efficiency</td>
<td>$\Lambda$</td>
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<td>Average electric energy of a resonator</td>
<td>$\langle W_{E_i} \rangle = \frac{1}{4} \int \mu \bar{E} \cdot \bar{H} , dv$</td>
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<td>Average magnetic energy of a resonator</td>
<td>$\langle W_{M_i} \rangle = \frac{1}{4} \int \mu \bar{H} \cdot \bar{H} , dv$</td>
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<td>Average Poynting vector</td>
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<td>Uncoupled overlap electric component</td>
<td>$D_{ik} = \int_V \varepsilon_i \bar{E}_i \cdot \bar{E}_k , dv$</td>
</tr>
<tr>
<td>Uncoupled overlap uncoupled magnetic component</td>
<td>$C_{ik} = \int_V \mu_i \bar{H}_i \cdot \bar{H}_k , dv$</td>
</tr>
<tr>
<td>Coupled overlap electric component</td>
<td>$H_{ik} = \int_V \varepsilon \bar{E}_i \cdot \bar{E}_k , dv$</td>
</tr>
<tr>
<td>Coupled overlap magnetic component</td>
<td>$G_{ik} = \int_V \mu \bar{H}_i \cdot \bar{H}_k , dv$</td>
</tr>
<tr>
<td>ECMT eigenvalue problem</td>
<td>( UVa = \omega^2 a )</td>
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<tr>
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<tr>
<td>Magnetic component of the coupling coefficient</td>
<td>( \kappa_m = \frac{\int \mu \bar{H}_i \cdot \bar{H}_k , dv}{\int \mu \bar{H}_i \cdot \bar{H}_i , dv} )</td>
</tr>
<tr>
<td>Electric component of the coupling coefficient</td>
<td>( \kappa_e = \frac{\int \varepsilon_0 \bar{E}_i \cdot \bar{E}_k , dv}{\int \varepsilon_0 \bar{E}_i \cdot \bar{E}_i , dv} )</td>
</tr>
<tr>
<td>Coupling coefficient</td>
<td>( \kappa = \kappa_m - \kappa_e )</td>
</tr>
<tr>
<td>Electric field of a dielectric resonator (Cohen model)</td>
<td>( \bar{E}_i = \phi A J_1 (k_1 r) \begin{cases} \cos (\beta z) &amp; r \leq \frac{d_1}{2},</td>
</tr>
<tr>
<td>Magnetic field of a dielectric resonator</td>
<td>( \bar{H}_1 = \frac{1}{j \omega \mu} \nabla \times \bar{E}_1 ) (Found using Maple®)</td>
</tr>
<tr>
<td>Electric field of TE(_{011}) cylindrical cavity</td>
<td>( \bar{E}_2 = \phi M J_1 (k_2 r) \cos \left( \frac{\pi z}{d_2} \right) )</td>
</tr>
<tr>
<td>Magnetic field of the TE(_{011}) mode</td>
<td>( \bar{H}_2 = \frac{1}{j \omega_2 \mu} \nabla \times \bar{E}_2 ) (Found using Maple®)</td>
</tr>
<tr>
<td>Lambda (resonator) efficiency</td>
<td>( \Lambda = \frac{B_m}{2 \sqrt{P}} )</td>
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1 Overview

1.1 Introduction

In this work, a coupled-mode formalism is developed to study how microwave resonators interact. The developed system of equations is capable of describing coupled systems using the properties of the simpler uncoupled subsystems. This set of equations is put in an eigenvalue problem form.

One of the main aims of the thesis is to study resonators used in the electron paramagnetic resonance spectroscopy field. However, the developed set of equations can be used to describe many other coupled electromagnetic systems such as filters, wireless power schemes and meta-materials.

The coupling coefficient between resonators is very important in band-pass filter design [1-3]. However, as shall be seen later, there are different formulae for the coupling coefficient found in the literature. One important objective of this work is to find a universal expression for the coupling coefficient which can be successfully applied to different scenarios. Another objective is to physically explain the nature of the coupling coefficient.

Section 1.2 gives a brief introduction to electron paramagnetic resonance and its application. Section 1.3 briefly introduces the theory behind magnetic resonance. The role of the cavity (Probe) is studied in section 1.4. Section 1.5 demonstrates a primitive electron paramagnetic resonator spectroscope. In section 1.6 the history of coupled mode theory is succinctly presented. Finally, section 1.7 gives a brief discussion of the layout of the next chapters.
1.2 Applications of Electron Paramagnetic Resonance (EPR)

Electron Paramagnetic Resonance (EPR), also referred to as Electron Spin Resonance (ESR), is a spectroscopic method which is used in various branches of science to detect, identify and study free radicals and paramagnetic species. Electron Paramagnetic Resonance finds applications in the fields of biology [4-5], chemistry such as the kinetics study of highly reactive radical intermediates [6], and physics for example to measure the magnetic susceptibility [7]. It is also used in industrial research, effects of radiation on biological compounds, archaeological dating, and in many other fields and applications [8-9].

1.3 Basic EPR theory

EPR spectroscopy can only detect samples which have unpaired electrons [9]. Spin is an intrinsic property of an electron. An electron, a Fermion, has a spin quantum number of $1/2$. Spin is a quantum mechanical property which does not have a counterpart in classical mechanics. Particles with spin possess magnetic dipole moments. This is similar to a rotating charged sphere in classical physics. In the absence of external magnetic fields, the magnetic dipoles inside the sample are randomly oriented so the resultant magnetization is zero. However, when an external DC magnetic field is applied, the electrons spins align themselves either parallel or anti parallel to the field. The magnetic moments parallel to the field have lower energy than that of the anti-parallel ones. This split in the energy levels, called Zeeman splitting, is shown in Figure 1-1.
Zeeman splitting $\Delta E$ is equal to

$$\Delta E = g \mu_B B_0,$$

(1.3.1)

where $g$ is the electron’s g factor (approximately equal to 2 for an electron in free space) and $\mu_B$ is the Bohr magneton.

An unpaired electron moves between the two energy levels by absorbing or radiating a photon with energy equal to $\Delta E$. Thus

$$h\nu = \Delta E = g \mu_B B_0,$$

(1.3.2)

where $h$ is Planck’s constant and $\nu$ is the absorbed (radiated) frequency. For practical cases, one deals with an ensemble of electrons rather than with a single electron. Thus, in such cases, we resort to statistical mechanics. At thermal equilibrium the electrons can be described using Maxwell-Boltzmann statistics [10]. Thus the ratio of the number of
electrons in the upper energy level, $N_{Up}$, to the number of electrons in the lower energy levels, $N_{Low}$, is

$$\frac{N_{Up}}{N_{Low}} = \exp\left(-\frac{\Delta E}{KT}\right).$$

(1.3.3)

Here $K$ is Boltzmann’s constant and $T$ is temperature in kelvin. Substituting (1.3.2) in (1.3.3) we arrive at,

$$\frac{N_{Up}}{N_{Low}} = \exp\left(-\frac{\hbar \nu}{KT}\right).$$

(1.3.4)

From equation (1.3.4) it is clear that $N_{Up} < N_{Low}$. Therefore, shining the sample with an electromagnetic wave of a frequency $\nu$, results in a net absorption. This absorption is what EPR spectroscopy detects. When the frequency is equal to $\nu$ we say that the sample is at resonance which corresponds to maximum absorption.

### 1.4 Importance of the resonator

At room temperature ($\approx 300 \text{ K}$), Figure 1-2 shows the plot of the ratio $N_{Up}/N_{Low}$ as a function of frequency. From the figure it is clear that to get a better absorption, due to lower $N_{Up}/N_{Low}$ ratio one may think that it is better to increase the frequency up to the visible light range. Although increasing the frequency will indeed improve the sensitivity, there is a practical limit governed by equation (1.3.2). This can be explained by calculating the magnetic field needed to raise the resonance frequency of the sample into the infrared range ($\approx 100 \text{ THz}$).
At this frequency, the magnetic field value is approximately equal to $3.5 \times 10^7$ gauss.

Comparing this value to that produced by the strongest magnet reported in the literature ($10^6$ gauss) [11], clearly shows that working in the infrared and visible light spectrum is practically unachievable. Therefore, EPR spectrometers work in the microwave and millimeter ranges [12] where magnets can be fabricated and used. However, as Figure 1-2 shows, the ratio of $N_{up}/N_{low}$ at room temperature in the microwave range is slightly less than one. Accordingly one should expect that the absorption of the microwaves is very small. Illuminating the sample with an electromagnetic wave and detecting the signal from the other side, as shown in Figure 1-3, is not practical. One needs the microwave magnetic field to be homogenous and concentrated on the sample and this is exactly why a resonator is crucial in EPR spectroscopy.
Besides having large magnetic field, it is desirable that the electric field is as small as possible at the sample. This is because most samples have non-resonant absorption through the electric field. Some resonators which satisfy the above requirements are the cylindrical $TE_{011}$ cavities, rectangular $TE_{102}$ cavities, cylindrical $TE_{010}$ dielectric resonators, and loop-gap resonators. Figure 1-4 depicts the electric and magnetic fields inside a cylindrical $TE_{011}$ cavity. The subscripts indicate the number of half wavelengths in the azimuthal ($\phi$), radial ($r$) and $z$ directions respectively. The fields of the rectangular $TE_{102}$ cavity are presented in Figure 1-5. Here, the subscripts correspond to the number of half wavelengths in the $x$, $y$ and $z$ directions respectively.
A dielectric resonator, made of a material which has a high dielectric constant, is shown to resonate [13]. It is helpful to think of dielectric resonators as the analog of cavities, where the dielectric-air boundaries can be modeled as magnetic walls [13-14]. The fields of the $TE_{011}$ mode, shown in Figure 1-6, behave in a similar way to the cylindrical $TE_{011}$ mode. However it should be noted that due to the finiteness of the dielectric constant the correspondence with the $TE_{011}$ mode is not complete. This incompleteness is reflected in the subscript $\delta$, which is always less than one.
Figure 1-5. Fields of a TE102 cavity.

Figure 1-6. Fields of a dielectric resonator.
In EPR spectroscopy it is desirable to maximize the microwave magnetic field for a given incident power. Indeed it was found that the signal enhancement is proportional to

\[ \Lambda = \frac{B_m^2}{2P}, \]  

(1.4.1)

where \( B_m \) is the maximum magnetic field at the sample and \( P \) is the incident power [15]; the square root of (1.4.1) is of crucial importance in EPR spectroscopy and given the name lambda efficiency or resonator efficiency \( \Lambda \). Thus one of the main aims for the resonator designer is to maximize the lambda efficiency. This can be done by using dielectric inserts, loop-gaps, or split-rings [16-19].

**Coupling the microwave Power**

To excite the resonator, an iris is usually used as shown in Figure 1-7. The figure illustrates a typical case where the microwave source is coupled to an X-band \( TE_{102} \) mode through a transmitting waveguide and an iris. It is important that the iris is small enough so that the fields inside the cavity are very close to the ideal \( TE_{102} \) fields. Another important application of the iris is to make sure that the cavity is matched to the transmitting waveguide.
Figure 1-7. A system consisting of a TE$_{102}$ cavity excited through an iris and a waveguide operating in the TE$_{10}$ mode.

Usually the system presented in Figure 1-7 can be represented as a lumped circuit model as shown in Figure 1-8 [20]. Here the cavity is modeled as an $LC$ tuning circuit where $R$ represents the cavity losses. The iris is modeled as a matching transformer.

Figure 1-8. Lumped circuit model of a cavity coupled to the microwave circuit through an iris.
The iris dimension is changed by a plastic screw to match the empty resonator to the waveguide and hence improving the power efficiency. The sample absorbance un-matches the cavity, thus results in a reflected signal. The reflected signal is directed by the circulator, as shown in Figure 1-9, to the detection unit.

![Figure 1-9. A basic EPR system, showing the microwave source, cavity, circulator and signal detector.](image)

### 1.5 Coupled Mode Theory (CMT)

Coupled mode theory is used to analyze and predict the behavior of a compound system by using the known properties of its simpler components. In the middle of the last century, Schelkunoff rigorously developed a form of coupled mode theory [21]. He expanded the unknown electromagnetic fields of the coupled system in terms of those of the uncoupled subsystems to derive a set of equations equivalent to Maxwell's equations.
In theory, the expansion is carried out over a complete set of spatial basis functions (modes). Since the number of basis functions in a complete set may be very large, for practical cases, a truncated set is used. In this sense, CMT is considered as an approximate method. In 1958, Haus derived the CMT equations using the variational principle [22]. From the general properties of the variational method, it is well-known that that the solution is stationary. Therefore a first order change (error) in the fields, due to an incomplete basis set, will not dramatically affect the accuracy of the results [23]. Accordingly, taking a truncated basis set leads to reasonably accurate results [23].

Coupled mode theory has been used in electromagnetics since the 1950s. Pierce used it to design and understand the properties of microwave travelling wave tubes [24]. Later, CMT was employed on other microwave systems such as oscillators, amplifiers and frequency converters [25-26]. In the early 1970s, CMT was applied to optical systems for the first time [27].

In conventional CMT, the modes forming the basis set were assumed orthogonal. This is true for modes belonging to the same structure [23, 28]. However for some situations the modes of the uncoupled systems may be chosen as the basis functions and these modes are not necessarily orthogonal. Orthogonal coupled mode theory (OCMT) is not adequate for describing such cases. Therefore, non-orthogonal coupled mode theory (NCMT) was subsequently developed [23, 29].

Recently, a two of research papers were published, where a set of CMT equations were derived based on a quasi-non-orthogonal approach [30-31]. These articles shed light on the nature of the coupling coefficient between resonators. The CMT equations were limited to two resonators but, generalization to an arbitrary number of resonators is
straightforward. In these papers, the coupling was assumed to be weak and whether the fields satisfy the boundary conditions at the interface of different materials was not mentioned.

Generally speaking, CMT can be divided into two main branches [23]. Space-coupled mode theory is useful in studying the properties of transmission systems such as waveguides and fibre optical systems. On the other hand, time-coupled mode theory is crucial in understanding the interaction between multiple resonators and is therefore suitable for the current work [23].

In recent years there has been a growing interest in coupling between resonators. The field of wireless power transfer (WPT) using magnetically coupled resonators emerged in the last decade. Different WPT schemes show promising results in the design of medical implantable devices and wireless sensors [32-35]. Coupling and transferring power using relay coils is a recent research area where CMT is a prominent method of analysis [36-37].

Yariv and his research team introduced CROW (Coupled Resonators Optical Waveguide), a new optical transmission system based on the coupling between resonators [38-42]. This system transfers the optical signal based on the coupling between adjacent resonators.

1.6 Thesis layout

Chapter 2 investigates the behavior of an EPR resonator consisting of two dielectric resonators inserted in a rectangular cavity, DR/TE$_{102}$ for short. This chapter
points out the fact that the three uncoupled structures (the two dielectric resonators and the rectangular cavity) interact to give three coupled modes which depend on the uncoupled fields. The chapter discusses the properties of the DR/TE_{102} resonator in detail from an EPR spectroscopic point of view. One important conclusion that can be inferred from the results of the chapter is that although, the coupling between the cavity and the dielectric resonators can be considered strong (because the dielectrics are inserted inside the cavity), the coupled modes show behaviors similar to those expected from a coupled mode formalism.

Energy Coupled Mode Theory (ECMT) is developed from first principles in chapter 3. The theory lays out the foundations necessary to study coupled systems. Different coupling schemes are studied and the chapter suggests that coupling depends on two cascaded operators and thus leads to chapter 4.

Chapter 4 discusses the physical meaning of the coupling coefficient based on energy conservation. It is shown that using the given interpretation and ECMT, one can explain the coupling mechanism between different resonator types. It also proposes a general closed form expression for the coupling coefficient.

The coupling between a dielectric resonator and a cylindrical cavity is studied in chapter 5. The frequencies and fields are calculated using ECMT and the results were compared to finite element simulations. The coupling between a dielectric resonator and a cylindrical cavity is very important in EPR spectroscopy. It is an example of dielectric-conductor coupling discussed in chapter 4. The solutions of two coupled mode formalisms found in the literature are shown in the appendix of the chapter. It is shown that both methods do not reflect the coupling between the modes.
The results of chapter 5 show that ECMT is successful in explaining the coupled frequencies and the resulting fields. Accordingly, in chapter 6, resonator parameters which strongly depend on the field distributions are calculated using ECMT. Expressions for the coupling coefficient, quality and filling factors are found.

Chapter 7 studies the design of EPR resonators using ECMT. Different practical cases are studied. It is shown that the lambda efficiency, \( \Lambda \), can be improved using suitable design parameters. The chapter also proposes methods for optimizing cavity’s lambda efficiency by selecting the suitable inserts.

The image method is used in electrostatics and antenna theory [43]. Chapter 8 combines the image method and ECMT to study cases where conducting planes exist. This is important in the EPR field when the inserts (loop-gaps, dielectrics, split-rings) are close to the cavity wall. It can be also applied to study wireless power transfer systems in the presence of conductors where it was shown that transfer efficiency significantly increases [35].
References and Notes


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2 Analysis of two stacked cylindrical dielectric resonators in a TE102 microwave cavity for magnetic resonance spectroscopy

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The candidate prepared and processed the computational calculations in this publication and worked in collaboration with Dr. Mattar to interpret and publish the results.

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Abstract

The frequency, field distributions and filling factors of a DR/TE102 probe, consisting of two cylindrical dielectric resonators (DR1 and DR2) in a rectangular TE102 cavity, are simulated and analyzed by finite element methods. The $TE^{+++}$ mode formed by the in-phase coupling of the $TE_{01\delta}(DR1)$, $TE_{01\delta}(DR2)$ and $TE_{102}$ basic modes, is the most appropriate mode for X-band EPR experiments. The corresponding simulated $B^{+++}$ fields of the $TE^{+++}$ mode have significant amplitudes at DR1, DR2 and the cavity’s iris resulting in efficient coupling between the DR/TE102 probe and the microwave bridge. At the experimental configuration, $B^{+++}$ in the vicinity of DR2 is much larger than that around DR1 indicating that DR1 mainly acts as a frequency tuner. In contrast to a simple microwave shield, the resonant cavity is an essential component of the probe that affects its frequency. The two dielectric resonators are always coupled and this is enhanced by the cavity. When DR1 and DR2 are close to the cavity walls, the $TE^{+++}$ frequency and $B^{+++}$ distribution are very similar to that of the empty TE102 cavity. When all the experimental details are taken into account, the agreement between the experimental and simulated $TE^{+++}$ frequencies is excellent. This confirms that the resonating mode of the spectrometer’s DR/TE102 probe is the $TE^{+++}$ mode. Additional proof is obtained from $B_{1x}$, which is the calculated maximum x component of $B^{+++}$. It is predominantly due to DR2 and is approximately 4.4 G. The $B_{1x}$ maximum value of the DR/TE102 probe is found to be slightly larger than that for a single resonator in a cavity because DR1 further concentrates the cavity’s magnetic field along its x axis. Even though DR1 slightly enhances the performance of the DR/TE102 probe its main benefit is
to act as a frequency tuner. A waveguide iris can be used to over-couple the DR/TE102 probe and lower its $Q$ to $\approx 150$. Under these conditions, the probe has a short dead time and a large bandwidth. The DR/TE102 probe’s calculated conversion factor is approximately 3 times that of a regular cavity making it a good candidate for pulsed EPR experiments.
2.1 Introduction

Pulsed and continuous-wave (CW) electron resonance techniques, such as electron paramagnetic resonance (EPR) [1-6], electron-nuclear double resonance (ENDOR) [4, 7-9], electron-electron double resonance (ELDOR) [4, 6, 10-11], electron spin echo envelope modulation (ESEEM) [9, 12-13], double quantum coherence (DQC) [14-16] and double electron-electron resonance (DEER) [12, 17-21], are powerful spectroscopic methods for studying the magneto-structural properties of molecules containing unpaired electrons. They are becoming the experimental methods of choice to determine spin-spin distances, geometry, structures and gyromagnetic, fine, and hyperfine tensors of paramagnetic molecules of biological and medicinal significance. The paramagnetic centers in these large biological molecules are usually dilute and the sample size is mostly small and limited. Consequently, considerable research is spent on increasing spectrometer sensitivity to facilitate their detection.

One of the ways to increase a spectrometer’s sensitivity and signal-to-noise ratio (SNR) is by substituting its resonant cavities by miniature loop-gap (LGR) [22-28] and dielectric (DR) resonators [29-41]. These resonators have several advantages over metal-walled cavities such as small size, low cost, high energy density in the sample vicinity, large magnetic fields ($B_1$) and high filling factors [22-36].

The use of loop gap resonators is more widespread than DRs and they are now commonly used in EPR spectrometers. They have been reviewed, on more than one occasion, by Hyde et al. [42-43].
As early as 1964 Rosenbaum [29], followed by Walsh and Rupp [37], were the first to employ a DR instead of a cavity in an EPR spectrometer. While DRs have comparable performance to LGRs, some have background signals due to paramagnetic impurities [40]. These may become apparent at low temperatures. Their contribution to the overall spectra is eliminated by subtracting the spectrum of the empty resonator from that containing the sample.

The coupling and tuning of a LGR or DR to an EPR spectrometer’s microwave bridge is not an easy task [44]. A theoretical account of this subject has recently been given by Mett et al. [45]. For LGRs and DRs, coupling is typically carried out by means of a wire loop of appropriate diameter and critical coupling is achieved by varying the distance between the resonator and the loop [22, 24, 30, 35, 46]. Waveguide irises [25], Gordon couplers [47] and other antennae [48] have also been used to critically couple LGRs to the spectrometer’s microwave bridge.

Usually a shield is used to house LGRs and confine the microwave radiation. Dielectric resonators have been housed in microwave shields as well [32-36]. For example, DRs placed inside a microwave shield have been used for high pressure [30], stopped flow and rapid scan [33] EPR. The theory of doubly stacked resonators in a microwave shield has been discussed by Jaworski et al. [32].

In addition to the convenient coupling via a waveguide iris, cavities serve the same purpose as a microwave shield and have also been used to house LGRs [49-50] and DRs. A single resonator placed in a TE_{102} cavity was studied by different groups [31, 38, 40, 41]. Nesmalov et al. studied a single ferroelectric resonator in a TM_{110} Cavity [40], while Golovina et al. employed a cylindrical TE_{011} cavity [38].
The DR/TE\(_{102}\) probe used in our laboratory consists of a pair of dielectric resonators, with \(\varepsilon_r = 29.2\), in an unmodified TE\(_{102}\) rectangular cavity. Thus a regular EPR cavity is converted into a dielectric probe with higher SNRs that are at least 24 times larger than the TE\(_{102}\) cavity alone [39]. In addition, the frequency of the resonator can be tuned over an extended range. The frequency of the DR/TE\(_{102}\) probe is coarsely tuned by varying the distance between the two dielectric resonators. Once the appropriate frequency range is determined, it is then fine tuned by keeping that distance constant and changing resonators’ positions along the cavity x axis where the sample tube resides. As a result, the two dielectric resonators are asymmetrically positioned in the TE\(_{102}\) cavity.

In this article one attempts to numerically assess by simulation [51], using the finite integration methods [52], the microwave electric and magnetic field distributions, sensitivity, filling factors and frequency behavior of the DR/TE\(_{102}\) probe used in our EPR spectrometers.

The paper is partitioned as follows. In Section 2.1 the problem and the goals of the work are presented. Section 2.2 provides a theoretical background on the linear combination of the electromagnetic fields for two dielectric resonators in a rectangular cavity. In Section 2.3 a description of the numerical and experimental methods is given while Section 2.4 is divided into three subsections that present and discuss the results. The first subsection deals with the properties of two identical dielectric resonators symmetrically placed in a TE\(_{102}\) cavity while the next section discusses the results of positioning them asymmetrically in the cavity. Section 2.4.3 compares the magnetic field distributions of one and two resonators in a TE\(_{102}\) cavity. Section 2.5 summarizes the results and conclusions of the work.
2.2 Theoretical Background

In the previous analyses of an EPR probe formed by stacking two dielectric resonators the shield was not considered to be a resonator with distinct resonant modes but simply imposed boundary conditions due to its electrical conducting walls [32, 53]. Mett et al. were the first to simulate the effect of a cylindrical cavity as a resonating entity on a single dielectric resonator [54].

In general, two dielectric resonators, DR1 and DR2, in a conducting cavity can be regarded as a combined system of three coupled structures. Consequently, the coupling of any three basic modes arising from DR1, DR2 and the cavity results in three new modes that are approximated as a linear combination of the basic ones. These new coupled modes will differ from one another according to the relative phases and coupling coefficients of their basic modes. Here, the individual DR1, DR2 and cavity basic modes are $TE_{01\delta}$, $TE_{01\delta}$ and $TE_{102}$ respectively. They give rise to the three coupled modes, $TE^{+++}$, $TE^{++-}$ and $TE^{+-+}$. Their corresponding spatial electric and magnetic field components, $E$ and $B$, are

$$E^{+++} = a_1^{+++} E_{01\delta} (DR1) + a_2^{+++} E_{01\delta} (DR2) + a_3^{+++} E_{102}, \quad (2.2.1)$$

$$E^{++-} = a_1^{++-} E_{01\delta} (DR1) + a_2^{++-} E_{01\delta} (DR2) - a_3^{++-} E_{102}, \quad (2.2.2)$$

$$E^{+-+} = a_1^{+-+} E_{01\delta} (DR1) - a_2^{+-+} E_{01\delta} (DR2) - a_3^{+-+} E_{102}, \quad (2.2.3)$$

$$B^{+++} = b_1^{+++} B_{01\delta} (DR1) + b_2^{+++} B_{01\delta} (DR2) + b_3^{+++} B_{102}, \quad (2.2.4)$$

$$B^{++-} = b_1^{++-} B_{01\delta} (DR1) + b_2^{++-} B_{01\delta} (DR2) - b_3^{++-} B_{102} \quad (2.2.5)$$

and
Here $a_i^{++}$ and $b_i^{++}$ are the coupling coefficients where the ± superscripts indicate the relative phase between the modes, which can be either 0 or 180°. The frequency, composition and electromagnetic fields of the new modes will depend on their dimensions and relative positions. As an example, the simulated magnetic field modes, $\textbf{B}^{+++}$, $\textbf{B}^{++++}$ and $\textbf{B}^{+-+-}$, are schematically drawn in Figures 2-1a to 2-1c.
Figure 2-1. Simulated resonant magnetic field modes of two identical dielectric resonators in a cavity. a) Magnetic field, $\vec{B}_{LCBM}^{+++}$ where all three basic modes are in phase. The individual characteristics of the basic TE$_{010}$ and TE$_{102}$ modes are evident. Also shown are the regions of the coupling iris and chimneys (R) where the sample enters the cavity. b) Both resonators are out of phase with the cavity. c) Only one resonator is in phase with the cavity. DR1 and DR2 are out of phase.
The comparison of Figures 2-1a, 2-1b and 2-1c shows that the modes in Figures 2-1a and 2-1b have a larger $TE_{102}$ component than that in Figure 2-1c. The small $TE_{102}$ component of $TE^{--}$, causes its $B^{--}$ fields, shown in Figure 2-1c, to be very small near the cavity walls. Therefore this mode is not suitable for exciting the DR1 and DR2 resonators via the cavity iris.

The further comparison of Figures 2-1a and 2-1b in the vicinity of DR1 and DR2 shows that $B^{++}$ is larger than $B^{+-}$. Consequently, using the $TE^{++}$ mode should result in a spectrometer with a relatively higher SNR and sensitivity.

In general, linear combinations of other $TE_{mnp}$, $TM_{mnp}$ and hybrid modes may also exist. For example the DR1 and DR2 $TE_{01\delta}$ modes may form linear combinations with the cavity’s $TE_{101}$ mode, as will be shown later.

### 2.3 Computational and Experimental Details

A computer employing two Quad-Core Opteron 2350 Processors, with 3 GB of RAM and running Windows XP® was used for the simulations. The DR/TE$_{102}$ properties were calculated using the CST MICROWAVE STUDIO® suite of programs [51]. The dimensions, relative positions in space and dielectric constants of DR1, DR2 and cavity are used as inputs. The program solves Maxwell’s equations, using an eigenvalue formalism, from which the frequencies, filling factors, electric and magnetic field distributions are calculated. The program can use two methods for solving the eigenvalue problem. The first is the Jacobi-Davidson (JD) method [55], while the second is the
Advanced Krylov Subspace (AKS) method [56]. The JD method is computationally expensive and time consuming but is robust when solving degenerate modes. Since, due to its low symmetry, the system under consideration has no degeneracies, the faster AKS method was used. During the solution, the system’s geometry is spatially partitioned into a mesh of grid elements. The equations are then solved using these grid elements by the finite integration technique (FIT) [52].

The EPR spectrum of the Mn$^{2+}$/CaO sample, used as a reference standard, was recorded with a modified Varian E104 spectrometer [39]. The frequency of the DR/TE$_{102}$ resonator was measured with a Hewlet-Packard model HP5340A frequency counter and the microwave power was measured with an HP432C digital power meter equipped with an HP478A thermistor power head. The meter’s output was digitized via a National Instruments ATMIO16E10 data acquisition board. No signals due to paramagnetic impurities from DR1 and DR2 were apparent.

2.4 Results and Discussion

2.4.1 Resonators symmetrically placed within a cavity

In our previous work, the frequency of the DR/TE$_{102}$ probe was coarsely adjusted by changing the distance between DR1 and DR2. In this way, the frequency of the DR/TE$_{102}$ probe could be varied by approximately 2.0 GHz [39]. However it was not known if the frequencies spanning that range were due to one or more resonant modes. To resolve this point, two dielectric resonators placed in a cavity are modeled using the CST program. The dimensions of the resonators correspond to those obtained from
Murata (Model DRT060R020C0227B, \( \varepsilon_r = 29.2 \)). The cavity dimensions were taken from the X-band E-231 Varian TE\(_{102}\) cavity. The cylindrical axes of DR1 and DR2 were aligned with the cavity’s x-direction, as shown in the Figure 2-2.

![Figure 2-2. Two identical dielectric resonators, DR1 and DR2 in a TE\(_{102}\) cavity. The distance between DR1 and DR2 is \( d_{12} \) and the distance of DR1 from the cavity wall is \( s \). The dimensions of the two resonators and the cavity are also shown.](image)

The frequencies of the simulated lowest five modes are shown in Figure 2-3. They were calculated as \( d_{12} \) was increased by symmetrically shifting DR1 and DR2 from the center of the cavity. The inspection of the magnetic field distribution of these modes indicates that the lowest mode, \( TE' \), is a result of the in-phase interaction of the \( TE_{010} \) modes of the dielectric resonators and the \( TE_{101} \) mode of the cavity. Its magnetic field takes the form

\[
B' = c_1 B_{010}^{010} (DR1) - c_2 B_{010}^{010} (DR2) - c_3 B_{101}.
\]  (2.4.1)
Figure 2-3. Frequencies of the $TE'$, $TE^{+++}$, $TE^{++-}$, $TE^{+-+}$ and $TM'$ modes as a function of the separation between the dielectric resonators, $d_{12}$.

The frequency of the $TE'$ mode changes from 6.55 to 7.25 GHz as $d_{12}$ spans the range of 17 mm. It is out of the range of interest (8 to 10 GHz) and will not be considered further.

At any given distance the $TE^{+++}$ frequency is always the lowest of the three remaining $TE^{+++}$, $TE^{++-}$ and $TE^{+-+}$ modes. One of the reasons for coarse tuning the DR/TE$_{102}$ probe by changing the distance between DR1 and DR2 was the linear response of the frequency with $d_{12}$ [39]. The $TE^{+++}$ in Figure 2-3 also displays this desirable feature and changes almost linearly by 850 MHz as $d_{12}$ is varied from 1 to 17 mm. Therefore the lower end of the frequency range obtained experimentally by coarse tuning...
most probably corresponds to the lowest $TE^{+++}$ mode. In contrast, Figure 2-3 indicates that the frequency change of the $TE^{+++}$ and $TE^{++-}$ modes is complicated and nonlinear.

When comparing previous results, it is important to differentiate between a stacked resonator pair in a cavity and those placed in a shield. If the small cylindrical “tight” shield has a radius comparable to those of DR1 and DR2 [32, 35], then it acts only as a microwave shield with very little interaction with the dielectrics. However in the case of a cavity whose internal dimensions exceed $\lambda/4$ and its frequency is comparable to that of the two combined resonators, then significant interactions will occur between DR1, DR2 and the cavity. A similar reasoning was proposed by Mett et al. in the case of one dielectric resonator in a cavity. They found that the interaction was maximum when the frequencies of the dielectric resonator and the cavity were the same [54]. If the shield is considered to be a cylindrical cavity, the frequency of its $TE_{011}$ mode can be calculated using

$$f_c = \frac{c}{2\sqrt{\varepsilon_r}} \left[ \frac{x_{01}}{\pi r_c} \right]^2 + \left( \frac{1}{\ell_c} \right)^2. \quad (2.4.2)$$

Here $x_{01}$ is the first root of $J_0(x)$ Bessel function [54], $r_c$ the radius and $\ell_c$ the length of the cylindrical shield. If the shield is entirely filled with Delrin® ($\varepsilon_r = 2.53$) and has the dimensions given by Sienkiewicz et al. [35] its frequency is approximately 19.8 GHz. On the other hand if the shield is empty ($\varepsilon_r = 1.0$) its frequency jumps to 31.4 GHz.

Therefore in the case where the shield is partially filled with Delrin®, [32, 35] its actual frequency is expected to lie between these two frequencies. Any frequency in that range would be too high for the shield to significantly interact with DR1 and DR2. Thus the
$TE^{++}$ mode has no counterpart in the case of doubly stacked dielectric resonators in a tight shield [32].

To better understand the differences between the frequencies and modes of two DRs in a cavity and a tight shield, the frequency of the symmetric mode resulting from the coupling of two dielectric resonators in free space was calculated [53]. The calculated frequencies were compared to experimental measurements in Table 2 of Jaworski et al. [32]. The results gave an excellent agreement provided that the calculated values were scaled up by a factor of 1.09. This is within the known 10% accuracy of the magnetic wall model used [57]. These results corroborate that the lowest resonant mode of two dielectric resonators in a tight shield are indeed due to the symmetric mode of the doubly stacked resonators [32]. It also indicates that both methods of frequency calculation yield comparable results [32, 53].

In summary, the $TE^{++}$ mode is due to the resonant interaction of the in-phase interaction of the DR1, DR2 and the rectangular $TE_{102}$ cavity. On the other hand, the mode observed by Jaworski et al. [32] is due to the in-phase interaction of the two dielectrics with insignificant interactions with the cylindrical shield.

Figure 2-3 indicates that as $d_{12}$ gets larger DR1 and DR2 approach the cavity walls and the $TE^{++}$ frequency approaches the resonant frequency of an empty $TE_{102}$ cavity. The regions shown as rectangles, R, in Figure 2-1 have very small magnetic fields, $B_{102}$. This leaves the contributions from $B_{010}^{1}\lambda_1^{(DR1)}$ and $B_{010}^{2}\lambda_2^{(DR2)}$. These are also negligible in the R regions due to the following reasons. The surfaces of DR1 and DR2 may be approximated as magnetic walls due to the large difference between their
\( \varepsilon_r = 29.2 \) and that of the cavity interior \( (\varepsilon_r = 1) \). Hence, the tangential components of \( \mathbf{B}_{01\delta} \) (DR1) and \( \mathbf{B}_{01\delta} \) (DR2) in the yz planes are approximately zero. Assuming that the cavity has perfectly conducting walls, then the normal component of \( \mathbf{B}^{+++} \) vanishes at its surface. To maintain the continuity of \( \mathbf{B}^{+++} \) in space then the normal components of \( \mathbf{B}_{01\delta} \) (DR1) and \( \mathbf{B}_{01\delta} \) (DR2) facing the cavity walls in the R regions must also be very small. Only minor perturbations due to \( \mathbf{B}_{01\delta} \) (DR1) and \( \mathbf{B}_{01\delta} \) (DR2) in the parts that face the interior of the cavity will exist. The net result is that in these two R regions \( \mathbf{B}^{+++} \approx 0 \).

Consequently when the two DRs are very far apart, the overall \( \mathbf{B}^{+++} \) distribution in the entire DR/TE\(_{102}\) probe is approximately equal to that of an empty TE\(_{102}\) cavity. The same reasoning also applies to \( \mathbf{E}^{+++} \) and as a result, the frequency of the DR/TE\(_{102}\) probe will also be close to that of a rectangular TE\(_{102}\) cavity.

Jaworski et al. have also determined that, in the case of two resonators placed in a tight shield, the nearest spurious mode to the EPR active mode is approximately 400 MHz higher and is TM in character. They also found that this frequency difference is almost constant over the entire range studied (0 to 4.5 mm) \([32]\). In the present case of DR1, DR2 in a cavity, the first TM mode encountered is labeled as \( TM' \) and shown in Figure 2-3. Its frequency also increases almost linearly and is approximately 2.1 to 2.5 GHz higher in frequency than the \( TE^{+++} \) mode. This relatively large frequency gap is attributed to the additional interaction of the DR1, DR2 with the cavity as compared to the tight microwave shield.
The magnitude of \( B^{+++} \) in the vicinity of the sample is an important parameter since it directly affects the filling factor, sensitivity and the SNR of the spectrometer [22, 32, 54]. For an allowed transition, where \( \Delta M_S = \pm 1 \), the effective component of \( B^{+++} \) must be perpendicular to the external homogenous static magnetic field, \( B_0 \).

Consequently, the x component of \( B^{+++} \) (hereafter referred to as \( B_{1x} \)) was calculated along the cavity x axis, where the sample resides, as a function of \( d_{12} \). Again, \( d_{12} \) was increased by symmetrically shifting DR1 and DR2 from the center of the cavity. Figure 2-4a shows the results of these calculations where the two \( B_{1x} \) maxima, corresponding to the positions of DR1 and DR2, move away as the \( d_{12} \) increases. However between the two maxima is a valley that is always nonzero. This implies that in the DR/TE\(_{102}\) probe, the DR1 and DR2 are never fully decoupled. According to Eq. (2.2.4), \( B_{1x} \) is due to the two dielectric resonators and the cavity. To separate the contributions from the three components, the calculated \( B_{1x} \) for the empty cavity was also drawn in Figure 2-4a.

From this figure, it is obvious that for \( d_{12}=16.0 \) mm, where DR1 and DR2 are farthest from one another, the calculated \( B_{1x} \) is predominantly due to the cavity around its center (7-15 mm) as indicated by the vertical dashed lines.
Figure 2.4. Magnetic field, $B_{1x}$, calculated along the cavity x axis at selected $d_{12}$ distances. Also included is $B_{1x}$ due to the empty TE$_{102}$ cavity. b) Magnetic field, $B_{1x}$, after subtraction of the empty cavity contribution.
To further emphasize this point, the difference between the $B_{1x}$ fields of the DR/TE$_{102}$ probe and the empty cavity were plotted in Figure 2-4b. It shows that when $d_{12} = 16.0$ mm and the two resonators are far apart $B_{1x}$ is very close to zero in the center of the cavity. The minute positive values around $x = 11$ to 12 mm are due to the dielectric resonators’ tails, which fall off exponentially with distance. Thus, one may conclude that even at $d_{12} = 16.0$ mm there is still some small coupling between the two resonators and it is accentuated by the presence of the cavity.

It is worth noting from Figure 2-4a that the values of the $B_{1x}$ maxima when $d_{12} = 2.0$ mm is around 4.0 Gauss (G) while at $d_{12} = 8.0$ mm it is approximately 3.4 G. Therefore one estimates that at $d_{12} = 4.0$ mm it is ~ 3.7 G. This is comparable to the $B_{1x}$ of commercial resonators, such as the Bruker® ER4118X-MD5 dielectric Flexline probe. It is also comparable to our previous experimental calculations of $B_{1x}$ which is 4.4 G [39]. However, one must note that in our experimental setup the two dielectric resonators were not symmetrically placed in the TE$_{102}$ cavity [39]. As will be shown later, this has the effect of further increasing the magnitude of the $B_{1x}$ maximum.

### 2.4.2 Resonators asymmetrically placed within the cavity

As mentioned previously, the main aim of this paper is to understand theoretically and analyze numerically the design, microwave characteristics and sensitivity of the DR/TE$_{102}$ probe [39]. The frequency of the probe was fine tuned by keeping the $d_{12}$ distance constant and varying the distance along the cavity x axis, $s$, shown in Figure 2-2.
This causes the DR1 and DR2 to be in equivalent and asymmetrically positioned in the cavity. To simulate the fine tuning process, \( d_{12} \) was fixed at 4.0 mm and the two resonators were moved along the cavity x axis by varying \( s \) from 0.5 mm to 6.85 mm. At the end of the range when \( s = 6.85 \) mm, DR1 and DR2 are symmetric and equivalent.

The frequency of the \( TE^{+++} \) mode, calculated by the CST program, as a function of \( s \) is depicted in Figure 2-5. It shows that as \( s \) is varied by 6.35 mm, the corresponding frequency change is almost 213 MHz. This is approximately one quarter of the frequency range spanned in Figure 2-3 as a result of changing \( d_{12} \) from 1.0 mm to 17 mm. The frequency change per mm in the former case is 50 MHz/mm while that of the latter is 33.5 MHz/mm. Although these tuning rates are comparable, it is easier to fine tune the resonator by moving DR1 and DR2 in tandem.

![Figure 2-5. Frequency change as a function of the distance, s, for the asymmetric \( TE^{+++} \) mode.](image)
The simulated $B^{+++}$ fields of this mode are depicted in Figure 2-6. The comparison of $B^{+++}$ in this figure and Figure 2-1a indicates that the asymmetric $TE^{+++}$ mode still has a considerable $TE_{102}$ component. In addition the $B^{+++}$ vectors have significant amplitudes at the cavity’s iris, DR1 and DR2. Therefore efficient coupling between the microwave bridge and the dielectric resonators is achieved. The figure also indicates that magnetic field density in the vicinity of DR2 is higher than that near DR1.

Figure 2-6. Simulated $B^{+++}$ mode at $d_{12} = 4.0$ mm and $s = 0.5$ mm showing the in phase relation between the three basic modes. Note the larger $B^{+++}$ values within the central resonator, DR2.

The same boundary condition arguments put forward for the symmetric case when both resonators were close to the cavity walls in the R regions also apply in the
asymmetric case for DR1 only. Thus in this case DR1 only acts as a tuner with little influence on $\mathbf{B}^{++}$ and $\mathbf{E}^{++}$.

When $d_{12} = 4.0$ mm and $s = 0.5$ mm, which corresponds to the original experimental setup, the calculated frequency of the $TE^{++}$ mode is very close to the experimental frequency [39]. Therefore, it is highly likely that the experimental operating mode of the DR/TE$_{102}$ probe is actually the $TE^{++}$ mode.

To prove that the asymmetric $TE^{++}$ mode is the experimental mode in question, a series of additional experiments were performed. The exact experimental conditions were simulated. This involved including a teflon holder for DR1 and DR2. In addition, a quartz tube with an inner diameter of 0.6 mm was used as a sample holder. Finally, CaO with a very small amount of Mn$^{2+}$, as a substitutional impurity, was also included. The complete structure, its dimensions and relative dielectric constants of the materials used in the calculations are shown in Figure 2-7 and Table 1. The top of DR2 was maintained at the center of the cavity and DR1 was allowed to move along the cavity x axis. The distance from the bottom of the cavity to the bottom of DR1, $s$, was varied from 2.0 mm to the limit of 5.0 mm. In this limit DR1 and DR2 almost touch one another.
Figure 2-7. Schematic diagram of the DR/TE$_{102}$ probe used in the recording the CaO/Mn$^{2+}$ spectra.

Table 1 Dimensions and relative dielectric constants of materials used in the simulations.

<table>
<thead>
<tr>
<th>Material</th>
<th>ID (mm)</th>
<th>OD (mm)</th>
<th>$\varepsilon_r$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cavity</td>
<td></td>
<td></td>
<td>1.0</td>
</tr>
<tr>
<td>DR1, DR2</td>
<td>2.0</td>
<td>6.0</td>
<td>29.2</td>
</tr>
<tr>
<td>Teflon</td>
<td>6.0</td>
<td>8.2</td>
<td>2.1</td>
</tr>
<tr>
<td>Quartz</td>
<td>0.6</td>
<td>1.8</td>
<td>3.75</td>
</tr>
<tr>
<td>CaO/Mn$^{2+}$</td>
<td>0.6</td>
<td></td>
<td>11.8</td>
</tr>
</tbody>
</table>

As $s$ was varied, the spectrometer’s frequencies were measured and compared to those calculated by the CST program.
Figure 2-8. Frequency change as a function of the distance, s, for the calculated and experimental asymmetric TE+++ mode.

Figure 2-8 shows that the agreement between the experimental and computed values is excellent. The maximum deviation between them is approximately 0.22 %. Since by taking into consideration all the experimental details the simulator reproduces the experimental frequencies, then this indicates that the method is accurate and reliable. It also proves that the resonating mode used in the spectrometer is indeed the $TE^{+++}$ mode. This gives us confidence to use these types of simulations to design and verify similar dielectric resonator probes and understand how some of the existing ones function. Further confidence in the method arises from the calculation of $B_{lx}$ and filling factors discussed below.
One is now in a position to investigate the behavior of $B_{1x}$ when DR1 and DR2 are moved in space to go from the symmetric configuration to the experimental asymmetric one. The $B_{1x}$ fields for the experimental configuration can also be calculated as was done previously for the symmetric case. In this case $d_{12}$ was fixed at 4.0 mm and both resonators were moved as a single unit along the cavity x axis. Thus $s$ was changed from 0.1 to 6.85 mm. Seven selected $s$ values were chosen and the simulations repeated. For clarity these results are broken up into two Figures 2-9a and 2-9b.
Figure 2-9. a) Magnetic field $B_{1x}$ for $s = 6.85, 5.0$ and $3.0 \text{ mm}$. b) $B_{1x}$ for $s = 3.0, 1.0, 0.5$ and $0.1 \text{ mm}$.

Figure 2-9a shows that when $s = 6.85 \text{ mm}$, which corresponds to the symmetric positioning of DR1 and DR2, the maximum of $B_{1x} \approx 3.77 \text{ G}$. This value is very close to the interpolated value predicted in the previous section. When $s$ is decreased, DR1 and DR2 move towards the bottom wall; become asymmetrically positioned within the cavity and the two maxima of $B_{1x}$ around DR1 and DR2 become different. While $B_{1x}$ of DR1 decreases that of DR2 increases. Figure 2-9b indicates that at the extreme position when $s = 0.1 \text{ mm}$ and DR1 is very close to the cavity wall, its $B_{1x}$ maximum is a shoulder that is barely resolved under that of the DR2 wing.

It is important to note from Figure 2-9b, that at the experimental configuration ($s = 0.5 \text{ mm}$) $B_{1x}$ maximum at DR2 is calculated to be $\approx 4.4 \text{ G}$. This is almost identical to
the experimental $B_{1x}$ value measured previously [39]. This is further proof of the accuracy of the simulations and that the resonating mode of the DR/TE$_{102}$ probe is the $TE^{+++}$ mode. Consequently to get the maximum spectral intensity and filling factors, a small sample should be placed in the DR2 resonator and fill its inner hole.

The next step is to calculate the asymmetric filling factor. It is defined as [32, 58]

$$\eta = \frac{\iint_{V_{\text{Sample}}} |H_{1x}|^2 \, dv}{\iint_{V_{\text{cavity}}} |H|^2 \, dv} \equiv \frac{\iint_{V_{\text{Sample}}} |B_{1x}|^2 \, dv}{\iint_{V_{\text{cavity}}} |B|^2 \, dv},$$  
(2.4.3)

where

$$B_{1x} = \mu_0 H_{1x}$$  
(2.4.4)

and $\mu_0$ is magnetic permeability in free space. However the time averaged magnetic energy stored in the entire DR/TE$_{102}$ probe volume, $V_{\text{cavity}}$, is [59]

$$W_M = \frac{1}{4\mu_0} \iint_{V_{\text{cavity}}} |B|^2 \, dv.$$  
(2.4.5)

Therefore

$$\eta = \frac{\iint_{V_{\text{Sample}}} |B_{1x}|^2 \, dv}{4\mu_0 W_M}.$$  
(2.4.6)

The CST program normalizes, the total energy (algebraic sum of the instantaneous electrical and magnetic energy at any time) to 1.0 joule. Thus Eq. (2.4.6) becomes

$$\eta \approx \frac{1}{2\mu_0} \iint_{V_{\text{Sample}}} |B_{1x}|^2 \, dv$$  
(2.4.7)

or
Here \( \ell \) is the length of the sample and \( r \) is the radius of the DR2 inner hole. It is equal to 1.0 mm. In the case of a sample inside the hole of DR2, hereafter referred to as the “small sample”, with \( s = 6.85 \) mm the calculated \( \eta \) is relatively small. As \( s \) decreases, \( \eta \) increases and starts to saturate at \( s = 0.8 \) mm, as shown in Figure 2-10. The relatively large filling factor at the experimental setting, corresponding to \( s = 0.5 \) mm in Figure 2-10, results in the largest SNR because it is directly proportional to \( \eta \),

\[
SNR \propto \eta \sqrt{Q/P}.
\]  

\((2.4.9)\)

\[
\eta \approx \frac{\pi r^2}{2\mu_0} \int_{0}^{\ell} |B_{1x}|^2 \, dx.
\]  

\((2.4.8)\)

**Figure 2-10.** Filling factor of the small sample in DR1 as a function of the distance \( s \).

The \( \eta \) values when the sample fills the entire tube are also calculated and drawn in Figure 2-11. In this case, the integral limits in Eq. \((2.4.8)\) span the whole cavity x axis.
in contrast to the small sample in Figure 2-10 where one only integrates over the height of DR2. Thus it is not surprising that the comparison of Figures 2-10 and 2-11 indicates that $\eta$ is smaller for the small sample. This simply implies that the larger sample results in a stronger, albeit inhomogeneous, signal. One should warn that for large aqueous samples dissipative losses will decrease the sensitivity by degrading the quality factor.

![Experimental setting](image)

**Figure 2-11.** Filling factor of a long sample tube as a function of the distance $s$.

Figure 2-11 also indicates that $\eta$ increases as $s$ increases and eventually saturates at $s = 6.85$ mm. According to Eq. (2.4.8) $\eta$ is proportional to the area under the curve in Figure 2-12. It shows that the area under the curve for $s = 0.1$ mm is *slightly* less than that for $s = 6.85$ mm and explains the $\sim 21\%$ increase in $\eta$ as $s$ increases in Figure 2-11.
Beyond $s = 6.85$ mm the curve becomes its mirror image. As $s$ increases further the DR2 resonator face ultimately reaches a distance of 0.5 mm from the opposite wall. This is the mirror image of the original experimental setting.

![Plot of $\left| \vec{B}_{1x} \right|^2$ as a function of the cavity x axis for $s = 0.1$ and 6.85 mm.](image)

**Figure 2-12.** Plot of $\left| \vec{B}_{1x} \right|^2$ as a function of the cavity x axis for $s = 0.1$ and 6.85 mm.

One may estimate the EPR signal enhancement (SE) due to the different filling factors of the DR/TE$_{102}$ probe and the TE$_{102}$ empty cavity and compare it with our previous experimental results [39]. According to Nesmelov et al. [40], if one assumes that the quality factor does not change appreciably by the insertion of DR1 and DR2, then the SE (ratio of signal intensities $S_{DR/TE_{102}}$ and $S_{TE_{102}}$) is related to their corresponding filling factors, $\eta_{DR/TE_{102}}$ and $\eta_{TE_{102}}$, by
In reality the EPR signal intensity depends on many parameters besides the filling factor such as temperature, relaxations times, nature of the host lattice, concentration of the paramagnetic species and the degree of its saturation. Consequently, in our previous work [39] the SE of the various samples tested varied from 24 to 35. The calculated SE in this study is approximately 32.5 which is in good agreement with those determined experimentally [39].

2.4.3 Comparison with a Single Resonator in a TE\textscript{102} cavity

The DR/TE\textscript{102} probe is compared to the case when only one resonator is in the cavity. To make the comparison meaningful the single resonator was placed in the exact same position of DR2 of the DR/TE\textscript{102} probe. This was followed by simulating and plotting its $B_{1x}$ in Figure 2-13. It shows that the $B_{1x}$ maximum value due to DR1 and DR2 is slightly larger than the corresponding one for a single resonator. This is because the high dielectric constant of the second resonator (DR1) collimates the magnetic field of the TE\textscript{102} cavity mode along its x axis. This also explains why the calculated filling factor for the doubly stacked resonator at the experimental position ($s=0.5$ mm, $\eta=0.057$) is slightly higher than that for a single resonator calculated to be 0.048. Therefore although the two curves are different, their $B_{1x}$ maxima, shown in Figure 2-13, are close to one another and DR1 mainly acts as a frequency tuner.
Since the second resonator mainly functions as a tuner, it is not necessary to have a hole in it. Recalculating the frequency with DR1 as a solid cylindrical pill caused the probe frequency to decrease by approximately 60 MHz.

From the above arguments, Figure 2-6 and Figure 2-13, one may conclude that the DR/TE\textsubscript{102} probe is very similar to a single resonator in a cavity. This is in agreement with the experimental results of Nesmelov \textit{et al.} [40] where the DR simply redistributes the microwave fields within the cavity, and focuses $B_{1x}$ inside its hole leading to an increase in $\eta$.

Finally a rough estimate of the DR/TE\textsubscript{102} conversion factor, $C_p$, is made. According to Blank \textit{et al.} [41]
where \( P \) is the incident power. From this \( C_p \) is estimated to be \( \approx 4.4 \text{ G/}/\sqrt{\text{W}} \). It is in the same range of loop-gap resonators [24] and other commercial probes, such as the Bruker\textsuperscript{®} ESP380–1052–DLQ–R/N/H. On the other hand, \( C_p \) for a rectangular TE\(_{102}\) cavity alone ranges from 1.1 to 1.4 G/\sqrt{\text{W}} [40-41, 48]. Thus the DR/TE\(_{102}\) probe has a \( C_p \) that is approximately 3 times that of a regular cavity and makes it a viable resonator for a pulsed EPR spectrometer. In addition, the simplicity of over-coupling the DR/TE\(_{102}\) probe, using its regular cavity iris [39], allows one to easily lower its \( Q \) to \( \approx 150 \). Under these conditions, it has a large bandwidth and a relatively short dead time. It is currently being tested in our laboratory for use in pulsed EPR experiments.

### 2.5 Summary and Conclusions

The frequency, filling factors and field distributions of the DR/TE\(_{102}\) probe, made up of two dielectric resonators in a rectangular cavity, are assessed by simulation using the finite integration technique.

The \( TE^{++} \) mode of the DR/TE\(_{102}\) probe, formed by the in-phase coupling of the \( TE_{01\delta} \), \( TE_{01\delta} \) and \( TE_{102} \) basic modes, is found to be the most suitable mode for X-band EPR experiments. It resonates in the right frequency range and can be conveniently coarse tuned because its frequency changes almost linearly by 850 MHz as the distance between DR1 and DR2, \( d_{12} \), changes from 1 to 17 mm. It can be further fine tuned by moving DR1 and DR2 in tandem along the cavity x axis. The frequency change per mm
in the coarse tuning process is 50 MHz/mm while for fine tuning it is 33.5 MHz/mm. However, it is more convenient to fine tune the DR/TE\textsubscript{102} probe frequency by changing \(s\) asymmetrically instead of changing \(d_{12}\).

For the probe to be efficient its \(B\) fields should be significantly large at DR1, DR2 and the cavity’s coupling iris. The simulated \(B^{+++}\) fields of the fine-tuned asymmetric \(TE^{+++}\) mode fulfill this condition. Therefore efficient coupling between the microwave bridge and the dielectric resonators is still maintained. It is also found that \(B^{+++}\) in the vicinity of DR2 is larger than that near DR1 indicating that DR1 merely acts as a tuner with little influence on \(B^{+++}\).

In addition to DR1 and DR2, the cavity is found to be an essential component of the probe and plays an important role in affecting its frequency and properties. For example when \(d_{12}\) is large and the dielectric resonators are close to the cavity walls, the \(TE^{+++}\) frequency and \(B^{+++}\) distribution are very close to that of an empty \(TE_{102}\) cavity. The plot of \(B_{1x}\) versus \(d_{12}\) along the cavity x axis shows that DR1 and DR2 are never fully decoupled. Even at \(d_{12} = 16.0\) mm some coupling still exists and is accentuated by the presence of the cavity.

On the other hand, for a tight shield the EPR active mode is only due to the in-phase interaction of DR1 and DR2 with insignificant interactions with the shield. There is no counterpart for the \(TE^{+++}\) mode of the DR/TE\textsubscript{102} probe in this case. In addition, the frequency of the nearest spurious TM mode in the case of a tight shield is approximately 400 MHz higher than the EPR active mode. However, for a DR1, DR2 and a cavity, the first TM mode is approximately 2.1 to 2.5 GHz higher in frequency than the \(TE^{+++}\) mode.
This larger frequency gap is ascribed to the additional interaction of the cavity with DR1 and DR2 in comparison to the tight microwave shield.

If all the experimental details are taken into consideration, the agreement between the experimental and simulated $TE^{+++}$ frequencies confirms that the resonating mode of the DR/TE$_{102}$ probe used in the spectrometer is the $TE^{+++}$ mode.

At the experimental configuration DR1 is very close to the cavity wall and its $B_{1x}$ is small compared to that of DR2. The calculated $B_{1x}$ maximum due to DR2 is 4.4 G and is almost identical to the measured experimental value. This is additional proof that the DR/TE$_{102}$ mode is $TE^{+++}$ and that the simulations are accurate.

The filling factors, $\eta$, for a small sample and when the sample fills the entire tube are calculated. For the experimental configuration, the small sample $\eta=0.057$ while for the entire sample tube it is larger (0.094) and indicates that a larger sample gives a stronger signal. However the $B_{1x}$ across the sample length is not homogenous.

When the $B_{1x}$ of the DR/TE$_{102}$ probe is compared to that of only one resonator in the cavity, its $B_{1x}$ maximum value is found to be slightly larger than that for a single resonator. This is because the second resonator (DR1) further concentrates the cavity $B_{102}$ along its x axis. Accordingly the filling factor, $\eta$, for the doubly stacked resonator is 0.057 and is somewhat higher than 0.048 for a single resonator. Although DR1 only slightly increases the performance of the DR/TE$_{102}$ probe its main advantage, as mentioned previously, is to act as a frequency tuner.
The DR/TE\textsubscript{102} probe has a $C_p$ that is approximately 3 times that of a regular cavity and can be easily over-coupled, using its regular waveguide iris, to lower its $Q$ to $\approx 150$. Under these conditions, it has a relatively short dead time and a large bandwidth. Therefore it is possible to use it for pulsed EPR experiments.

This work gives us confidence in the finite integration simulations. They can be used in the future to design and verify the properties of LGR and DR probes housed in cavities or microwave shields.

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References and Notes


3 Energy coupled mode theory for an arbitrary number of resonators

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Abstract

A time-coupled mode theory is developed to study the coupling between resonators in the radio frequency (RF) and microwave (MW) regions. The theory fulfills the boundary conditions for different structures. For conducting cavities, the boundary conditions are satisfied at each point. It is also shown that open structure resonators (dielectric, loop-gap, split-ring, etc.) do not significantly alter the boundary conditions across internal interfaces because they are usually small compared to the resonant wavelength. The formalism is in the form of an eigenvalue problem, in which the eigenvalues represent the square of the frequencies of the coupled system while the eigenvectors represent the coefficients of the electromagnetic field components. The theory can be applied to an arbitrary number of resonators and modes. Although originally developed to design new electron paramagnetic resonance (EPR) probes, it can be used to study complex systems used in different application fields. This includes electron-nuclear double resonance (ENDOR), electron-electron double resonance (ELDOR), magnetic resonance imaging (MRI), wireless power transfer (WPT) and the interaction of meta-material elements. The eigenvalue equation is proven to obey the energy conservation principle and hence is named energy coupled mode theory (ECMT). The theory suggests that coupling depends on two cascaded operators: the material operator represented by the polarization matrix and the free space operator represented by the free space matrix. The coupling induced resonance frequency shifts (CIFS) are included in the main diagonal terms of the eigenvalue matrix. In the case of two dielectric resonators in free space, the material operator has the dominant effect while the
free space operator is equal to the identity matrix. Therefore applying ECMT results in a formula for the coupling coefficient similar to the one found in the literature. It gives excellent agreement with the results obtained from the finite element simulations. The eigenvalue formalism is also applied to the case of two conducting resonators and a similar formula to that found in the literature is obtained. In this case the free space operator is the main factor, while the material operator is equal to the identity matrix. These results suggest that, in general, coupling depends on the two operators.
3.1 Introduction

An increasing number of biological molecules of medicinal significance are found to be paramagnetic and contain unpaired electrons. Consequently understanding the magneto-structural properties of these paramagnetic molecules, such as electronic structure, geometry, spin-spin distances and gyromagnetic, fine, and hyperfine tensors is of crucial importance. Accordingly, pulsed and continuous-wave (CW) electron resonance techniques, like electron paramagnetic resonance (EPR) [1], are powerful spectroscopic methods for studying the properties of paramagnetic molecules.

The paramagnetic centers in these large biological molecules are usually quite small in number and dilute. In addition, the sample size is generally small and the supply is limited. As a result, extensive research is spent on increasing the sensitivity of EPR spectrometers to facilitate paramagnetic center detection. To increase a spectrometer’s sensitivity, miniature loop-gap (LGR) [2-4] or dielectric (DR) resonators [5-11] are used as components in their probes. These resonators have small sizes, high energy density in the sample vicinity, large magnetic fields ($B_1$) and large filling factors [3-13].

A probe shield is normally used to house the LGRs or DRs and confine their microwave radiation. Cavities serve the same purpose as microwave shields and have also been used to house LGRs and DRs [14]. A single resonator placed in a TE$_{102}$ cavity was used by different groups [5-7, 10-11, 13]. In our laboratory, the DR/TE$_{102}$ probe consists of two dielectric resonators, DR1 and DR2 with $\varepsilon_r = 29.2$, that are asymmetrically placed in an unmodified TE$_{102}$ rectangular cavity. Its signal to-noise-ratio (SNR) is at least 24 times larger than the TE$_{102}$ cavity alone [8].
Theoretical treatment and numerical simulation of EPR probes are rare. Mett et al. were the first to simulate the effect of a cylindrical cavity as a resonating entity on a single dielectric resonator [15]. The frequency, field distributions and filling factors of the DR/TE\textsubscript{102} probe used in our laboratory, were simulated and analyzed by finite element methods [16].

In summary it is essential to understand theoretically the coupling between the different components such as the cavity, DRs or LGRs, in order to design efficient magnetic resonance probes and microwave filters etc. To accomplish this, we derive from first principles (\textit{ab initio}) a set of coupled mode equations for an arbitrary number of interacting resonators. These equations are based on the fact that the total energy of the system must be conserved. Their derivation, as will be shown, also guarantees that the boundary conditions of the electromagnetic fields are satisfied for most practical cases.

The paper is partitioned as follows: Section 3.2 deals with both the historical and theoretical backgrounds. The historical development of the theory is briefly investigated in subsection 3.2.1. Boundary conditions are thoroughly examined in subsection 3.2.2. In section 3.3 the analytical expressions for the total stored energy (both electrical and magnetic) and for the Poynting vector [17] are derived. In section 3.4 the results are discussed. Finally, a proof that the coupled mode equations obey the law of conservation of energy is explicitly shown.
3.2 Background

3.2.1 Historical Background

In general, coupled mode theory (CMT) is used to analyze and predict the behavior of a compound system by using the known properties of its simpler components. Schelkunoff was amongst the first to rigorously develop a form of coupled mode theory [18]. The unknown electromagnetic fields of the coupled system were expanded in terms of those of the uncoupled subsystems and a set of equations equivalent to Maxwell's equations was derived. In principle, the expansion is carried out in a space of functions using a complete set of spatial basis functions (modes). The dimension of the space may be very large. Accordingly, a truncated set of basis functions is used instead. As an example, in 1958, Haus derived the CMT equations using the variational principle [19]. Pierce applied CMT to study the properties of microwave traveling wave tubes [20], which are high power amplifiers and are presently an essential component of modern pulsed EPR spectrometers [1, 21-28]. Later, CMT was used to study other microwave devices such as oscillators, amplifiers and frequency converters [29-30]. Yariv used CMT for optical systems since the early 1970s [31].

In general, CMT can be divided into two main branches [32]. Space-coupled mode theory is very useful in studying the interaction of propagating modes. On the other hand, time-coupled mode theory is concerned with the interaction between multiple resonators. Hence, time-coupled mode theory is suitable for the current article [32].
Finally, there has recently been a growing interest in the field of wireless power transfer using magnetically coupled resonators which is important in the design of medical implantable devices and wireless sensors [33-36].

### 3.2.2 Theoretical Background

The electric and magnetic fields (eigenmodes) for a single resonator satisfy its own boundary conditions. But once two or more resonators are coupled, care must be taken to ensure that the resulting fields, which are the superposition of the eigenmodes, satisfy the boundary conditions of the new composite structure. In this section the boundary conditions of the coupled modes are discussed. They are divided into two categories, external and internal boundary conditions. The external boundary represents the enclosure of the coupled system. This can be either free space or a conducting surface. On the other hand, internal boundaries are defined as the interfaces between different materials inside the system.

The fields of the coupled system are expanded in terms of an infinite number of fields of the uncoupled eigenmodes. However for practical purposes, the infinite sets can be truncated to a finite value, $N$. Therefore

$$\bar{E} = \sum_{i=1}^{N} a_i \bar{E}_i$$  \hspace{1cm} (3.2.1)$$

$$\bar{H} = \sum_{i=1}^{N} b_i \bar{H}_i.$$  \hspace{1cm} (3.2.2)

Here $a_i$ and $b_i$ are the expansion coefficients of the electric and magnetic components respectively. The $N$ modes can be equal to or greater than the number of resonators. So a
valid coupled mode can be the linear combination of the first mode of resonator one and the first mode of resonator two, or it can be the first mode of resonator one, the second mode of resonator one and the first mode of resonator two, etc. This procedure is very helpful if the frequencies of two modes of one resonator are very close, so a third nearby mode of a different resonator may easily couple with both of them.

Each $i^{th}$ uncoupled mode satisfies the sinusoidal time-varying Maxwell’s equations for isotropic media [37], therefore:

$$\nabla \times \vec{E}_i = -j\omega_i \mu_i \vec{H}_i,$$  \hspace{1cm} (3.2.3)

$$\nabla \cdot \varepsilon_i \vec{E}_i = \rho_i,$$  \hspace{1cm} (3.2.4)

$$\nabla \times \vec{H}_i = j\omega_i \varepsilon_i \vec{E}_i + \vec{J}_i,$$  \hspace{1cm} (3.2.5)

and,

$$\nabla \cdot \mu_i \vec{H}_i = 0.$$  \hspace{1cm} (3.2.6)

Here $\omega_i$, $\mu_i$, $\varepsilon_i$, $\rho_i$ and $\vec{J}_i$ are the frequency, permeability, permittivity, charge density and current density of the $i^{th}$ uncoupled resonator respectively. In general $\varepsilon_i$ and $\mu_i$ vary over space. Similarly, for the coupled system, Maxwell’s equations for isotropic media can be written as:

$$\nabla \times \vec{E} = -j\omega \mu \vec{H},$$ \hspace{1cm} (3.2.7)

$$\nabla \times \vec{H} = j\omega \varepsilon \vec{E} + \vec{J},$$ \hspace{1cm} (3.2.8)

$$\nabla \cdot \varepsilon \vec{E} = \rho,$$ \hspace{1cm} (3.2.9)

and,

$$\nabla \cdot \mu \vec{H} = 0.$$ \hspace{1cm} (3.2.10)
where \( \omega, \mu, \varepsilon \) and \( \vec{J} \) are the corresponding symbols for the coupled system. The resulting fields should satisfy the external and internal boundary conditions of the coupled system. This reasoning applies to cavities, dielectric resonators, loop-gap resonators, split ring resonators or micro-strips. From the above equations, the spatial material distribution is not necessarily the same for each resonator. This requires us to study the boundary conditions of the coupled system in detail.

3.2.2.1  **External boundary conditions**

The external boundary is defined as the enclosure which encompasses the whole coupled structure. Since the external boundary can be either free space or a conducting surface, the external boundary conditions can be modeled as a perfectly electrical wall that satisfies the following equations

\[
\hat{n} \times \vec{E} = 0 \quad (3.2.11)
\]

and

\[
\hat{n} \cdot \vec{H} = 0 . \quad (3.2.12)
\]

Here \( \hat{n} \) is the unit vector normal to the boundary surface.[37]

Substituting equations (3.2.1) and (3.2.2) in (3.2.11) and (3.2.12), shows that such an expansion approximately satisfies the boundary conditions of the coupled system. This is because the individual modes are either cavity modes where they automatically satisfy the external boundary conditions or open structures (the fields in such resonators, for example dielectric, loop-gap, split ring, etc., are not confined inside the resonator volume) and the fields are negligible on the conducting walls. For example, for a general
system composed of dielectric resonators inside a conducting cavity, the fields of the
dielectric resonators decay exponentially outside the dielectric material [38].
Theoretically speaking, once the dielectrics are inserted in a conducting cavity, the
boundary conditions resulting from the linear combinations of the modes at the cavity
walls are not satisfied. But from a practical point of view, the contribution of the
dielectrics, provided that they are far enough from the cavity walls, is negligible.

3.2.2.ii Internal boundary conditions

Internal boundaries are due to the presence of the open structure resonators. In
general, the dimensions of the open structure resonators are much smaller than the
resonant wavelength. This implies that the fields at the vicinity of, and inside the
elements do not significantly change the fields’ distribution in the whole coupled
structure. For example, the presence of the electric field of the \(i^{th}\) resonator inside or at
the boundary of the \(k^{th}\) resonator does not considerably alter the field distribution of the
whole coupled structure since the \(k^{th}\) resonator occupies a region in space much smaller
than the wavelength. It is worth noting that in general the fields at the \(k^{th}\) resonator due to
other resonators are small. This, together with the small size of the resonators compared
to the wavelength mean that the internal boundaries do not alter the fields significantly.
3.3 Analytical Derivation

In this section the rate of change of the total energy, starting from the conservation of energy principle, is derived. The electric and magnetic stored energies \( W_E \) and \( W_M \) of an electromagnetic system are [37]

\[
W_E = \frac{1}{2} \int_V \varepsilon E \cdot E \, dv, \quad (3.3.1)
\]

\[
W_M = \frac{1}{2} \int_V \mu H \cdot H \, dv, \quad (3.3.2)
\]

where \( V \) stands for the volume under consideration. The total energy of the given system, being a scalar, is simply the algebraic sum of equations (3.3.1) and (3.3.2), i.e.

\[
U = W_E + W_M. \quad (3.3.3)
\]

If the system is open (not isolated), in the sense that energy can flow in and out through the system boundary, then one can calculate the energy flow through the system boundary by taking the time derivative of equation (3.3.3). By using the identity

\[
\frac{\partial}{\partial t} (\vec{A} \cdot \vec{A}) = 2 \vec{A} \cdot \frac{\partial \vec{A}}{\partial t},
\]

this gives

\[
\frac{\partial U}{\partial t} = \int_V \vec{E} \cdot \frac{\partial \vec{D}}{\partial t} \, dv + \int_V \vec{H} \cdot \frac{\partial \vec{B}}{\partial t} \, dv. \quad (3.3.4)
\]

Here \( \vec{D} \) is the electric flux density, \( \vec{B} \) is the magnetic flux density and equations (3.2.9) and (3.2.10) were used. Using the time-varying Maxwell’s equations [17], equation (3.3.4) is reduced to

\[
\frac{\partial U}{\partial t} = \int_V \vec{E} \cdot \nabla \times \vec{H} \, dv - \int_V \vec{H} \cdot \nabla \times \vec{E} \, dv - \int_V \vec{E} \cdot \vec{J} \, dv. \quad (3.3.5)
\]
Applying the vector identity [17]

\[ \nabla \cdot (\vec{A} \times \vec{B}) = (\nabla \times \vec{A}) \cdot \vec{B} - (\nabla \times \vec{B}) \cdot \vec{A}, \]  

(3.3.6)

and after some algebraic manipulation, equation (3.3.5) becomes

\[ -\frac{\partial U}{\partial t} = \int_{\partial V} \vec{E} \times \vec{H} \cdot d\vec{S} + \int_{V} \vec{E} \cdot \vec{J} dv, \]

(3.3.7)

\[ = P_{\text{rad}} + \Gamma. \]

where \( \partial V \) is the surface enclosing the volume \( V \)

\[ P_{\text{rad}} = \int_{\partial V} \vec{E} \times \vec{H} \cdot d\vec{S} \]  

(3.3.8)

and

\[ \Gamma = \int_{V} \vec{E} \cdot \vec{J} dv. \]  

(3.3.9)

The left hand side of equation (3.3.7) is the rate of decrease of the total energy, \( U \). The first term on the right hand side is the power flow across the system boundary and \( \vec{E} \times \vec{H} \) is the Poynting vector which is the power flow per unit area [17]. The remaining term in this equation, \( \Gamma \), represents the Ohmic losses and the input power to the system. It can be written as

\[ \int_{V} \vec{E} \cdot \vec{J} dv = \int_{V} \vec{E} \cdot \vec{J}_{\text{loss}} dv - \int_{V} \vec{E} \cdot \vec{J}_{\text{input}} dv \]

(3.3.10)

\[ = P_{\text{loss}} - P_{\text{input}}. \]

Here \( \vec{J}_{\text{loss}} = \sigma \vec{E} \) is the current density inside the system conducting regions where \( \sigma \) is the conductivity, and \( \vec{J}_{\text{input}} \) is the input current density. Consequently equation (3.3.7) takes the form
\[-\frac{\partial U}{\partial t} = P_{\text{rad}} + P_{\text{loss}} - P_{\text{input}}. \tag{3.3.11}\]

If the electromagnetic fields vary purely sinusoidally in time, the real and imaginary components of the time average of equation (3.3.7) are written as \[17\]

\[\text{Re} \left( \frac{1}{2} \int_{\Omega} \vec{E} \times \vec{H}^* \cdot d\vec{S} \right) = -\frac{1}{2} \text{Re} \left( \int_{\Omega} \vec{E} \cdot \vec{J} \cdot dV \right) \tag{3.3.12}\]

and

\[\text{Im} \left( \frac{1}{2} \int_{\Omega} \vec{E} \times \vec{H}^* \cdot d\vec{S} + 2\omega \int_{\Omega} \left( \langle W_M \rangle - \langle W_E \rangle \right) dv \right) = -\frac{1}{2} \text{Im} \left( \int_{\Omega} \vec{E} \cdot \vec{J}^* \cdot dV \right). \tag{3.3.13}\]

Here \(\langle W_M \rangle\) and \(\langle W_E \rangle\) are the time-average stored magnetic and electrical energy

\[\langle W_M \rangle = \frac{1}{4} \int_{\Omega} \mu \vec{H} \cdot \vec{H}^* \cdot dv \tag{3.3.14}\]

and

\[\langle W_E \rangle = \frac{1}{4} \int_{\Omega} \varepsilon \vec{E} \cdot \vec{E}^* \cdot dv. \tag{3.3.15}\]

respectively. From equations (3.3.12) and (3.3.13) the complex Poynting vector, \(\vec{\Lambda}\), is equal to

\[\vec{\Lambda} = \frac{1}{2} \vec{E} \times \vec{H}^* \tag{3.3.16}\]

And the complex power \(\tilde{P}\), is the surface integral of equation (3.3.16)

\[\tilde{P} = \frac{1}{2} \int_{\partial \Omega} \vec{\Lambda} \cdot d\vec{S} \tag{3.3.17}\]

\[= \tilde{P}_{\text{av}} + i\tilde{P}_{\text{react}},\]

where \(\tilde{P}_{\text{av}}\) is the active power and \(\tilde{P}_{\text{react}}\) is the reactive power \[17\].
Having defined the above terms, one formulates an eigenvalue equation which can be used to predict the behavior of the coupled structure and still maintains the conservation of energy. Consequently the Poynting vector can be utilized as the starting quantity used for the derivation. Assuming the system is lossless the real part of the Poynting vector (losses, radiation and input power) vanishes. Hence,

\[ \tilde{P} = i\tilde{P}_{\text{react}}. \]  

(3.3.18)

In practice the losses can be added after the eigenmodes are found and used for computing the quality factor, resonator efficiency, etc. [39].

To derive the coupled mode theory in the form of an eigenvalue problem for resonators, one obviously has to determine the condition at which resonance occurs. At resonance one notes that,

\[ \langle W_M \rangle = \langle W_E \rangle. \]  

(3.3.19)

Therefore using equation (3.13) one can find that

\[ \tilde{P}_{\text{react}} + \frac{1}{2} \text{Im} \int_{V} \vec{E} \cdot \vec{J}^* dv = 0. \]  

(3.3.20)

This condition can be written in matrix form using (3.8) and the expansions of (3.2.1) and (3.2.2),

\[ \tilde{P}_{\text{react}} = \text{Im} \frac{1}{2} \int_{\partial V} \vec{E} \times \vec{H}^* \cdot d\vec{S} = \frac{1}{2} \int_{\partial V} \vec{E} \times \vec{H}^* \cdot d\vec{S} = \frac{1}{2} \sum_{i} \sum_{k} a_i b_i^* \int_{V} \vec{E}_i \times \vec{H}_k^* \cdot d\vec{S}. \]  

(3.3.21)

and

\[ \frac{1}{2} \text{Im} \int_{V} \vec{E} \cdot \vec{J}^* dv = \frac{1}{2} \text{Im} \int_{\text{all Conductors}} \vec{E} \cdot \vec{J}^* dv. \]  

(3.3.22)

For perfect internal conductors [37],

\[ \text{Im} \int_{V} \vec{E} \cdot \vec{J}^* dv = \text{Im} \int_{V} \vec{E} \cdot \vec{J}^* dv. \]
Im \( \int \vec{E} \cdot \vec{J}^* \, dv = \int \vec{E} \cdot \vec{J}^* \, dv = \int \vec{E} \cdot (\hat{n} \times \vec{H}^*) \, dS = - \int \vec{E} \times \vec{H}^* \cdot d\vec{S} \). \hspace{1cm} (3.3.23)

Substituting equation (3.3.23) back in (3.3.22) one gets,

\[
\frac{1}{2} \text{Im} \int \vec{E} \cdot \vec{J}^* \, dv = -\frac{1}{2} \sum_i \sum_k a_i b_k^* \int \vec{E}_i \times \vec{H}_k^* \cdot d\vec{S}.
\]

(3.3.24)

Back substituting (3.3.21) and (3.3.24) in (3.3.20) and taking the complex conjugate, the resonance condition (3.3.19) becomes,

\[\mathbf{a}^\dagger (\mathbf{M} - \mathbf{S}) \mathbf{b} = \mathbf{0}. \hspace{1cm} (3.3.25)\]

Where

\[M_{ik} = \int_{\partial V} \left( \vec{E}_i^* \times \vec{H}_k \right) \cdot d\vec{S}, \hspace{1cm} (3.3.26)\]

and

\[S_{ik} = \int_{\text{all Cond}} \vec{E}_i^* \times \vec{H}_k \cdot d\vec{S}. \hspace{1cm} (3.3.27)\]

Equation (3.3.25) is the resonance condition for lossless resonators. The next step is to find explicit expressions for \( M_{ik} \) and \( S_{ik} \) which constitute the main components in the resonance conditions (3.3.19) and (3.3.25). This is done by expanding \( \nabla \cdot (\vec{E}_i \times \vec{H}_k^*) \) and using identity (3.3.6) to give

\[\nabla \cdot (\vec{E}_i \times \vec{H}_k^*) = (\nabla \times \vec{E}_i) \cdot \vec{H}_k^* - (\nabla \times \vec{H}_k^*) \cdot \vec{E}_i. \hspace{1cm} (3.3.28)\]

Integrating equation (3.3.28) over the whole volume and using the divergence theorem [37] one arrives at

\[
\int_{\partial V} \vec{E}_i \times \vec{H}_k^* \cdot d\vec{S} = \int_{V} \nabla \times \vec{E}_i \cdot \vec{H}_k^* \, dv - \int_{V} (\nabla \times \vec{H}_k^*) \cdot \vec{E}_i \, dv \\
= -j\omega \int_{V} \mu_i \vec{H}_i \cdot \vec{H}_k^* \, dv + j\omega \int_{V} \epsilon_k \vec{E}_k^* \cdot \vec{E}_i \, dv - \int_{V} \vec{J}_k^* \cdot \vec{E}_i \, dv. \hspace{1cm} (3.3.29)\]
In a similar fashion to equation (3.3.23), the integration \( \int_V J_k^* \cdot E_i \, dv \) for perfect conductors can be written as
\[
- \int_{\partial \text{CondK}} \vec{E}_i \times \vec{H}_k^* \cdot d\vec{S}.
\] (3.3.30)

Substituting (3.3.30) in equation (3.3.29); taking the complex conjugate and re-arranging, one gets
\[
M_{ik} - N_{ik} = j\alpha_k C_{ik} - j\alpha_k D_{ki}^*,
\] (3.3.31)
where,
\[
N_{ik} = \int_{\partial \text{CondK}} \vec{E}_i^* \times \vec{H}_k \cdot d\vec{S},
\] (3.3.32)
\[
C_{ik} = \int_{\partial \text{CondK}} \mu_i \vec{H}_i^* \cdot \vec{H}_k \, dv
\] (3.3.33)
and
\[
D_{ik} = \int_{\partial \text{CondK}} \varepsilon_i \vec{E}_i^* \cdot \vec{E}_k \, dv,
\] (3.3.34)
where \( C_{ik} \) and \( D_{ik} \) are the coupled energy matrix elements. Equation (3.3.31) can be written in a matrix form as
\[
\mathbf{M} - \mathbf{N} = j\mathbf{\Omega} \mathbf{C} - j\mathbf{D}^\mathbf{t} \mathbf{\Omega},
\] (3.3.35)
where
\[
\mathbf{\Omega} \equiv \Omega_{nn} = [\omega_1 \omega_2 \cdots \omega_n] \mathbf{I} = \begin{pmatrix} \omega_1 & 0 & \cdots & 0 \\ 0 & \omega_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \omega_n \end{pmatrix}.
\] (3.3.36)

Equations (3.3.31) and (3.3.35) relate the reactive power components \( M_{ik} \) and \( N_{ik} \) to the bulk stored energy components \( C_{ik} \) and \( D_{ik} \).
For the coupled system, the total fields $\vec{E}$ and $\vec{H}$ are projected on the $i^{th}$ field components. Projecting the total magnetic field $\vec{H}$ and on the $i^{th}$ electric field component, $\vec{E}_i$, one can write

$$\nabla \cdot (\vec{E}_i \times \vec{H}) = (\nabla \times \vec{E}_i) \cdot \vec{H} - (\nabla \times \vec{H}) \cdot \vec{E}_i^*.$$

(3.3.37)

Using (3.2.3) and (3.2.8) one gets,

$$\nabla \cdot (\vec{E}_i^* \times \vec{H}) = j\omega \mu \vec{H}_i \cdot \vec{H} - j\omega \varepsilon \vec{E}_i^* \cdot \vec{E} - \vec{J} \cdot \vec{E}_i^*$$

(3.3.38)

Expanding $\vec{E}, \vec{H}$ in terms of the $\vec{E}_i, \vec{H}_i$ of the uncoupled systems using equations (3.2.1) and (3.2.2) results in,

$$\sum_k b_k \nabla \cdot (\vec{E}_k^* \times \vec{H}_k) = j\omega \mu \sum_k b_k \vec{H}_k \cdot \vec{H}_i^* - j\omega \varepsilon \sum_k a_k \vec{E}_k \cdot \vec{E}_i^* - \vec{J} \cdot \vec{E}_i^*$$

(3.3.39)

$$\sum_k b_k \nabla \cdot (\vec{E}_i^* \times \vec{H}_k) = j(\sum_k \omega \mu_b b_k \vec{H}_k \cdot \vec{H}_i^* - \sum_k a_k \omega \varepsilon \vec{E}_k \cdot \vec{E}_i^* - \vec{J} \cdot \vec{E}_i^*)$$

(3.3.40)

Integrating equation (3.3.40) over the whole volume yields

$$\sum_k b_k \int_V \nabla \cdot (\vec{E}_i^* \times \vec{H}_k) \, dv = j(\sum_k \omega b_k \mu \vec{H}_k \cdot \vec{H}_i^* \, dv - \sum_k \omega a_k \varepsilon \vec{E}_k \cdot \vec{E}_i^* \, dv - \int \vec{J} \cdot \vec{E}_i^* \, dv).$$

(3.3.41)

Assuming that:

$$\vec{J} = \vec{J} \delta_m \left( \vec{r} - \vec{r}_{Surface} \right),$$

(3.3.42)

where $\delta_m \left( \vec{r} - \vec{r}_{Surface} \right)$ is the Dirac delta function, $\vec{r}$ is the position vector and $\vec{r}_{Surface}$ is the position vector at the surface of the conductors, one can find that,

$$\int_{all \, Cond} \vec{E}_i^* \cdot \vec{J} \, dS = - \int_{all \, Cond} \vec{E}_i^* \times \vec{H} \cdot d\vec{S}.$$  

(3.3.43)

Using the divergence theorem and equation (3.3.43), equation (3.3.41) can written as

$$\sum_k (\omega \mu_{ik} + jM_{ik} - jS_{ik}) b_k = \omega \mu_{ik} a_k = 0,$$

(3.3.44)

where
\[ H_{ik} = \int_V \mathbf{E}_i \cdot \mathbf{E}_k \, dv. \quad (3.3.45) \]

Relation (3.3.44) relates the \( b \) coefficients to the \( a \) coefficients. One needs to find another relation between the two coefficients and substitute the \( b \) constants in term of the \( a \) constants to find the eigenvalue equation. This can be achieved by projecting the total electric field \( \mathbf{E} \) on the \( i^{th} \) magnetic field component, \( \mathbf{H}_i \) and noting that the electric field is either zero at infinity for open structures or it is normal to the bounding surface if the system is enclosed in a shield or a cavity, \( \int_{\partial V} \mathbf{E} \times \mathbf{H}_k^* \cdot d\mathbf{S} = 0 \). Thus one can arrive at,

\[ \sum_k -\omega G_{ik} b_k + \omega D_{ik} a_k = 0, \quad (3.3.46) \]

where

\[ G_{ik} = \int_V \mu \mathbf{H}_i^* \cdot \mathbf{H}_k \, dv. \quad (3.3.47) \]

Equations (3.3.44) and (3.3.46) can be written in matrix forms as

\[ (\Omega C + j(M - S)) b - \omega Ha = 0, \quad (3.3.48) \]
\[ -\omega Gb + \Omega Da = 0. \quad (3.3.49) \]

These two equations represent the projection of the coupled total fields onto the uncoupled ones. From here, the eigenvalue equation can be derived by noting that from equation (3.3.49)

\[ b = \frac{1}{\omega} G^{-1} \Omega Da. \quad (3.3.50) \]

Substituting (3.3.50) back in (3.3.48) one arrives at,

\[ [(\Omega C + j(M - S)G^{-1} \Omega D - \omega^2 H]a = 0. \quad (3.3.51) \]
Equation (3.3.51) is an eigenvalue equation, where the eigenvalues are the square of the frequency and the eigenvectors are the coefficients of the fields given by equation (3.2.1). Using relation (3.3.35) equation (3.3.51) can be rewritten as,

$$[(\Omega C - \Omega G + D^\dagger \Omega + j\{N - S\})G^{-1}\Omega D - \omega^2 H]a = 0.$$  \hspace{1cm} (3.3.52)

The eigenvalue equation (3.3.52) can be simplified further for the case of non-magnetic materials by noting that \(\mu_i = \mu = \mu_0\) which leads to,

$$C = G.$$  \hspace{1cm} (3.3.53)

This reduces (3.3.52) to

$$[(D^\dagger \Omega + j\{N - S\})G^{-1}\Omega D - \omega^2 H]a = 0.$$  \hspace{1cm} (3.3.54)

Equation (3.3.54) represents the eigenvalue equation for nonmagnetic materials.

It can be further simplified when the components are relatively far away from one another, which is usually the case. Accordingly it is safe to assume that,

$$N \approx S.$$  \hspace{1cm} (3.3.55)

Relation (3.3.55) is true because

$$S_{ik} - N_{ik} = \int_{all\ Cond\ except\ k} \vec{E}_i^* \times \vec{H}_k \cdot d\vec{S}$$

is negligibly small if the resonators are far enough from each other. For systems consisting of \(n\) ceramic (dielectric) resonators, or two conducting resonators

$$N = S.$$  \hspace{1cm} (3.3.56)

Indeed for ceramic resonators no conductors are present in the coupled structure. However, for two conducting resonators, it can be shown that
Therefore, a simplified version of the eigenvalue equation (3.3.54) is written as

$$\mathbf{UVa} = \omega^2 \mathbf{a},$$

(3.3.58)

where

$$\mathbf{U} = (\mathbf{H}^{-1} \mathbf{D}^\dagger \mathbf{\Omega}),$$

(3.3.59)

and

$$\mathbf{V} = (\mathbf{G}^{-1} \mathbf{\Omega} \mathbf{D}).$$

(3.3.60)

Equations (3.3.58), (3.3.59) and (3.3.60) represent the eigenvalue system which are used in the next section.

When the uncoupled resonators have the same resonant frequency $\omega_0$ (known as the synchronous condition) [40], equation (3.3.58) is reduced to

$$\omega_0^2 \mathbf{H}^{-1} \mathbf{D}^\dagger \mathbf{G}^{-1} \mathbf{Da} = \omega^2 \mathbf{a}.$$

(3.3.61)

### 3.4 Results and Discussion

It is interesting to verify that the eigenvalue equations (3.3.58), (3.3.59) and (3.3.60) satisfy the energy conservation principle at resonance (3.3.19) or (3.3.25). This can be done by expanding the energy expressions (3.3.14) and (3.3.15) in $\vec{E}$ and $\vec{H}$ according to (3.2.1) and (3.2.2). After some algebraic manipulation one can find that,

$$\langle W_E \rangle = \frac{1}{4} \mathbf{a}^\dagger \mathbf{Ha}, \quad \langle W_M \rangle = \frac{1}{4} \mathbf{b}^\dagger \mathbf{Gb}.$$

(3.4.1)

Using equation(3.3.50),

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\[
\langle W_M \rangle = b^* G b = \left( \frac{1}{\omega} G^{-1} \Omega D a \right)^* G \left( \frac{1}{\omega} G^{-1} \Omega D a \right)
\]
\[
= a^* \left( \frac{1}{\omega^2} D^* \Omega G^{-1} \Omega D a \right)
\] .

From equation (3.3.58) together with (3.3.59) and (3.3.60),

\[
H a = \frac{1}{\omega^2} D^* \Omega G^{-1} \Omega D a .
\] (3.4.3)

Therefore,

\[
\langle W_M \rangle = a^* H a = \langle W_E \rangle .
\] (3.4.4)

Relation (3.4.4) is identical to the resonance condition (3.3.19). This verifies that the eigenvalues and eigenvectors found using equation (3.3.58) guarantee that the system obeys the law of conservation of energy.

In the next two subsections, the eigenvalue equation (3.3.58) will be applied to two important structures; dielectric resonators and conducting ones. The eigenvalues, coupling coefficient and eigenvectors will be discussed.

3.4.1 Two identical dielectric resonators

The eigenvalue equation (3.3.58) will be applied to the case of two identical dielectric resonators. For this case \( D \approx G \), thus equation (3.3.61) reduces to

\[
\alpha_0^2 H^{-1} D a = \omega^2 a .
\] (3.4.5)

Equation (3.4.5) shows that the coupling is totally electrical, since neither \( H \) nor \( D \) depends on the magnetic field. Since

\[
\frac{1}{H_{11}^2 - H_{12}^2} \approx \frac{1}{H_{11}^2} \left( 1 + \frac{H_{12}^2}{H_{11}^2} \right),
\] (3.4.6)
equation (3.4.5) can be simplified to

\[
\omega_0^2 \left[ 1 - \frac{Y_{11}}{H_{11}} + \frac{H_{12}}{H_{11}} \cdot \frac{Y_{12}}{H_{11}} - \frac{Y_{12}}{H_{11}} + \frac{H_{12}}{H_{11}} \cdot \frac{Y_{11}}{H_{11}} \right] \mathbf{a} = \omega a^2, \quad (3.4.7)
\]

where

\[
Y_{11} = H_{11} - D_{11} = \varepsilon_0 (\varepsilon_{r_2} - 1) \int_{\partial \Omega_2} \hat{E}_1^* \cdot \hat{E}_1 \, dv \quad (3.4.8)
\]

and

\[
Y_{12} = H_{12} - D_{12} = \varepsilon_0 (\varepsilon_{r_2} - 1) \int_{\partial \Omega_2} \hat{E}_1^* \cdot \hat{E}_2 \, dv. \quad (3.4.9)
\]

From equation (3.4.8) one notices that \( Y_{11} << H_{11} \) and in general

\( H_{12}^2 << H_{11}^2 \) therefore one can conclude that,

\[- \frac{Y_{11}}{H_{11}} + \frac{H_{12}}{H_{11}} \cdot \frac{Y_{12}}{H_{11}} << 1. \quad (3.4.10)\]

By similar arguments one finds that,

\[
\left| \frac{Y_{12}}{H_{11}} \right| >> \left| \frac{H_{12}}{H_{11}} \cdot \frac{Y_{11}}{H_{11}} \right|. \quad (3.4.11)
\]

Therefore equation (3.4.7) can be written as

\[
\omega_0^2 \left[ \frac{1}{H_{11}} - \frac{Y_{12}}{H_{11}} \right] \mathbf{a} = \omega a^2. \quad (3.4.12)
\]

Solving the above eigenvalue problem (3.4.12), one finds that

\[
\omega \approx \omega_0 \cdot \sqrt{1 \pm \kappa}, \quad (3.4.13)
\]

where \( \kappa \) is the coupling coefficient and it is equal to
This result is identical to that previously derived in the literature [41] [32].

Solving the eigenvalue problem (3.3.61) numerically and comparing the result with the simulated ones computed by ANSOFT HFSS® are shown in the Figure 3-1.

Figure 3-1. Frequency response as the distance d changes for both the symmetric and the anti-symmetric modes due to the coupling between the $TE_{01\delta}$ modes of two identical dielectric resonators

From Figure 3-1 it is clear that the system of equations (3.3.61) gives very similar results to the simulated ones. It is worth noticing that for $TE_{01\delta}$ the electric field is always tangential to the dielectric-air interface. This means that the internal boundary conditions are satisfied at each point on the interface. It is also interesting to note that although these resonators have a moderate relative permittivity ($\varepsilon_r \approx 30$), the resonator’s diameter ($D$) is a fraction of the free-space wavelength $\lambda/D \approx 5$. This means that for
TM modes, provided that $\lambda$ is still greater than the resonator feature dimension, the eigenvalue equation (3.3.58) still gives reasonable results.

The diagonal terms, $-\frac{Y_{11}}{H_{11}} + \frac{H_{12}}{H_{11}} \frac{Y_{12}}{H_{11}}$, in (3.4.7) can be considered as a Coupling Induced Resonance Frequency Shifts, CIFS, term [42]. Indeed, a better approximation to equation (3.4.7) would be

$$\omega_0^2 \begin{bmatrix} 1 - \frac{Y_{11}}{H_{11}} + \frac{H_{12}}{H_{11}} \frac{Y_{12}}{H_{11}} & -\frac{Y_{12}}{H_{11}} \\ -\frac{Y_{12}}{H_{11}} & 1 - \frac{Y_{11}}{H_{11}} + \frac{H_{12}}{H_{11}} \frac{Y_{12}}{H_{11}} \end{bmatrix} \mathbf{a} = \omega^2 \mathbf{a}. \quad (3.4.15)$$

Solving equation (3.4.15) gives the eigenvalues

$$\omega = \omega_0 \sqrt{1 - \alpha \pm \kappa}, \quad (3.4.16)$$

where $\alpha$ is the CIFS term equal to

$$-\frac{Y_{11}}{H_{11}} + \frac{H_{12}}{H_{11}} \frac{Y_{12}}{H_{11}}. \quad (3.4.17)$$

The effect of the CIFS term appears when the distance between the two resonators gets very small. The error for distances below 1 mm is illustrated in Figure 3-2.
Figure 3-2. Error in the calculated frequencies (compared to the HFSS® results) with and without the CIFS terms.

Figure 3-2 shows that the CIFS term has its major effect on the anti-symmetric mode. Still the CIFS is a secondary effect. The main effect is still due to the cross coupling represented by the off diagonal terms. This can be shown by calculating the eigenvectors for either equation (3.4.5), (3.4.12) or (3.4.15). The eigenvectors calculated using any of the forms are the same. This is because the system is symmetric. Therefore one gets

$$a_1 = \frac{1}{\sqrt{2}}, \quad a_2 = \frac{1}{\sqrt{2}}$$  \hspace{1cm} (3.4.18)

for the symmetric mode and

$$a_1 = \frac{1}{\sqrt{2}}, \quad a_2 = -\frac{1}{\sqrt{2}}$$  \hspace{1cm} (3.4.19)

for the anti-symmetric mode. Thus the total electric field is
\[
\bar{E} = \frac{1}{\sqrt{2}} (\bar{E}_1 + \bar{E}_2),
\]

and

\[
\bar{E} = \frac{1}{\sqrt{2}} (\bar{E}_1 - \bar{E}_2),
\]

for the symmetric and anti-symmetric modes respectively. If one neglects the off diagonal terms the eigenvalue equation will result in an un-coupled system. So it is clear that the off diagonal terms are the main terms responsible for the coupling.

### 3.4.2 Two identical conducting resonators

For the case of two conducting resonators, such as loop-gap resonators, micro-strips, split-ring resonators etc, \( \varepsilon = \varepsilon_i \). This is because for two pure conductors like loop gap resonators, LGR, \( \varepsilon = \varepsilon_i = \varepsilon_0 \). While for micro-strips when they are drawn on the same substrate

\[
\varepsilon = \varepsilon_i = \begin{cases} 
\varepsilon_0 & \text{in air} \\
\varepsilon_{\text{sub}} \varepsilon_0 & \text{in substrate.}
\end{cases}
\]

(3.4.22)

For conductors \( \varepsilon = \varepsilon_i \) and hence \( \mathbf{H} = \mathbf{D} \). Therefore the eigenvalue equation (3.3.58) reduces to

\[
\mathbf{V} \mathbf{a} = \omega^2 \mathbf{a}.
\]

(3.4.23)

Equation (3.4.23) is simplified to

\[
\omega_0^2 \begin{bmatrix}
1 & -G_{12} - D_{12} \\
-G_{12} - D_{12} & H_{11}
\end{bmatrix}
\mathbf{a} = \omega^2 \mathbf{a}.
\]

(3.4.24)

From which, the coupling constant \( \kappa \) is found to be:

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\[ \kappa = \frac{G_{12} - D_{12}}{H_{11}} \]

\[ \kappa = \frac{\int \mu_0 \hat{H}_1^* \cdot \hat{H}_2 dV - \int \varepsilon \hat{E}_1^* \cdot \hat{E}_2 dV}{\int \varepsilon \hat{E}_1^* \cdot \hat{E}_1 dV} \]  \hspace{1cm} (3.4.25)

Equation (3.4.25) is identical to equation (4) derived in [43]. It is interesting to note that for the case of two dielectric resonators \( \mathbf{V} = \mathbf{I} \), while \( \mathbf{U} = \mathbf{I} \) for conducting resonators. This suggests that the \( \mathbf{U} \) matrix can be named the **Electrical Polarization** operator since its effect on the energy is reflected in equation (3.4.12) which adds a polarization term \( \mathbf{Y} \) to the system. While \( \mathbf{V} \) can be called the **Free Space** operator since it adds free-space stored energy, indicated by equation (3.4.25). In a system where the two types of resonators are present, the total cross coupling, the off diagonal terms, will be composed of the two factors shown by equations (3.4.14) and (3.4.25).

### 3.5 Summary and Conclusions

In this work, a time-coupled mode theory is developed for studying the coupling between resonators. It is explicitly shown that the theory guarantees that the boundary conditions for a variety of resonators are satisfied. For conducting cavities, the boundary conditions are satisfied at each point on the conducting wall. It is also shown that open structure resonators (dielectric, loop-gap, split-ring, etc) do not significantly alter the boundary conditions across internal interfaces because open structure resonators are usually small compared to the resonant wavelength. The formalism is in the form of an eigenvalue problem, in which the eigenvalues represent the square of the frequencies of...
the coupled system while the eigenvectors represent the coefficients of the electromagnetic field components.

The theory can deal with complex structures made up of an arbitrary number of resonators and modes. The resulting eigenvalue equation is proven to obey the energy conservation principle when applied to lossless resonating systems. Hence it is called energy coupled mode theory (ECMT). The proposed eigenvalue equation derived from ECMT shows that coupling depends on two cascaded portions: the material part represented by the polarization operator and free space represented by the free space operator.

The ECMT eigenvalue equation is solved for the case of two dielectric resonators in free space. The resulting formula for the coupling coefficient identical to the one found in the literature and gives excellent agreement with results obtained from the finite element simulations. It is also capable of detecting Coupling Induced Resonance Frequency Shifts (CIFS) which are the self terms found in the diagonals of the eigenvalue matrix. It shows that such terms have secondary effects compared to the off-diagonal terms. The main operator which comes into play for dielectric resonators is the polarization operator since the free space operator is close to the identity matrix \( V = I \).

The eigenvalue formalism was applied to the case of two conducting resonators and the results were similar to the ones found in the literature. In this case the coupling is due to the free space operator since \( U = I \). For a general structure where dielectric materials and conductors are present, the two operators\( U \) and \( V \) simultaneously have non-zero off-diagonal terms. Accordingly, the two portions, namely polarization (equation (3.4.14)) and free space (equation (3.4.25)) contribute to the total coupling.
In addition to the design of EPR probes, the proposed theory can be applied to study the coupling between resonating structures used in different areas such as, electron-nuclear double resonance (ENDOR), electron-electron double resonance (ELDOR), magnetic resonance imaging (MRI) or in the emerging fields of wireless power transfer (WPT) and meta-materials (MM) [44].

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References and Notes


4 Understanding the coupling coefficients between resonating structures

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Abstract

Using the energy conservation principle, a unified and general expression for the coupling coefficient of radio frequency (RF) and/or microwave (MW) resonators is derived. When applied to special cases, this general expression reduces to the ones reported in the literature. In addition, using the derived expression, the physical meaning and origin of the coupling coefficients become apparent. This is accomplished by using energy coupled mode theory equations (ECMT) applied to a system consisting of two resonators. For clarity, correspondence with a classical forced mass-spring system is also made. The coupling coefficient is found to be equal to the maximum normalized energy (normalized to the maximum uncoupled energy) due to the interaction of the sources of the $p$\textsuperscript{th} mode with the fields of the $i$\textsuperscript{th} mode. It is always the difference between the magnetic and the electric overlap components rather than their sum. This expression is applicable to various structures such as dielectric-dielectric, conductor-conductor, dielectric-conductor pairs.
### 4.1 Introduction

The paramagnetic centers in large biological molecules usually consist of only a few paramagnetic atoms in comparison with the huge number of diamagnetic ones. As a result the paramagnetic centers are dilute and difficult to detect. Consequently, a lot of research effort and time is spent on optimizing the performance of magnetic resonance spectrometers and increasing their sensitivity to detect these species. In this regard, their probes consist of miniature loop-gap (LGR) [14-16] or dielectric (DR) resonators [17-23]. These resonators have high energy density in the sample vicinity, small sizes leading to large magnetic fields ($B_1$) and filling factors [15-25].

In general, shields are used to house the LGRs or DRs and limit their microwave radiation outside the probe. Cavities may also be considered as microwave shields. They have been used to house LGRs and DRs [26]. Accordingly the coupling between loop-gaps, dielectrics and the cavity is of crucial importance. One important parameter which determines the coupling strength is the coupling coefficient $\kappa$.

Different research groups have placed a single resonator in a $TE_{102}$ cavity [17-19, 22-23, 25]. We have employed a probe, named $DR/TE_{102}$, made of two dielectric resonators, with a relative permittivity $\varepsilon_r$ of 29.2 asymmetrically placed in an unmodified $TE_{102}$ rectangular cavity [20].

The effect of a cylindrical cavity, as a resonating entity, on a single dielectric resonator was first simulated by Mett et al.[27]. The field distributions and filling factors of the $DR/TE_{102}$ probe were analyzed and simulated using the finite element technique [28]. It was shown that the two dielectric modes, $TE_{01\delta}$, interact with the cavity $TE_{102}$.
mode to give three coupled modes, $TE^{++}$, $TE^{+-}$ and $TE^{-+}$. These coupled modes are the result of the phase combinations between the three uncoupled modes [28].

Section 4.2 discusses the main features of energy coupled mode theory (ECMT). The different definitions and forms for the coupling coefficient are also presented. In section 4.3 the theoretical basics needed to understand the proposed physical meaning of coupling are provided with emphasis on the mass-spring mechanical system and how it is related to RF/microwave systems. The mathematical analysis of the coupling coefficient is carried out in section 4.4, and closed form expressions are derived. Section 4.5 proposes a physical meaning for the coupling coefficient and discusses how it is related to internal sources. Different situations and cases are discussed, based on the physical interpretation given, in section 4.6. Finally section 4.7 summarizes and lists the conclusion based on the finding of the previous sections.

4.2 Historical Background

To design efficient magnetic resonance probes and microwave filters etc., it is essential to fully understand theoretically the coupling between its resonant components such as cavities, dielectric, split-rings, microstrips and loop-gap resonators. To accomplish this, we previously derived, from first principles, a set of coupled mode equations for an arbitrary number of interacting resonators. These equations are based on the fact that the energy of total system must be conserved; hence the developed theory was called energy coupled mode theory (ECMT).
The derivation guarantees that both the external and internal boundary conditions of the electromagnetic fields are satisfied [29]. For conducting cavities, the boundary conditions are satisfied at each point on the conducting wall. It is also shown that open structure resonators (dielectric, loop-gap, split-ring, etc.) do not significantly alter the boundary conditions across internal interfaces because open structure resonators are usually small compared to the resonant wavelength.

The formalism is in the form of an eigenvalue problem, in which the eigenvalues represent the square of the frequencies of the coupled system while the eigenvectors represent the coefficients of the field components. An arbitrary number of resonators as well as modes can be taken into consideration which means that complex structures can be studied.

ECMT is capable of detecting Coupling Induced Resonance Frequency Shifts (CIFS) which are the self terms found in the main diagonals of the eigenvalue matrix [30]. It was shown that such terms have secondary effects compared to the off-diagonal terms [29].

The proposed equation shows that coupling depends on two cascaded operators: the material operator represented by the electrical polarization matrix and the free space operator represented by the free space matrix. The eigenvalue equation is solved for the case of two dielectric resonators in free space. The resulting formulae for the coupling coefficient were found to agree with those reported in the literature. They also corroborate the results obtained from the finite element simulations [29].

The main operator in the eigenvalue problem of dielectric resonators is the electrical polarization operator since the free space operator is close to the identity matrix.
The eigenvalue formalism was applied to the case of two conducting resonators and similar results to the one found in the literature were also derived. It was noticed that the coupling is due to the free space operator since \( U = I \) in such cases. For a general structure composed of dielectric resonators and conducting ones, the two operators both play a significant role [29].

To enhance our understanding of how the various resonating structures within a probe interact, it is imperative to understand the coupling coefficients amongst them. This is not only important in the case of magnetic resonance probes but is also useful in the design of band pass filters [31] that are also vital components in the microwave bridges of the EPR spectrometers. Recently, as an aside, there is a growing interest in the field of wireless power transfer using magnetic coupled resonators. Wireless power transfer (WPT) is important in the design of medical implant devices, wireless sensors, mobile and handheld devices [32-36].

One proposed form for the coupling coefficient is that it is equal to the sum of the overlap integrals of both the electric and magnetic fields [37]

\[
\kappa = \kappa_m + \kappa_e, \quad (4.2.1)
\]

where

\[
\kappa_m = \frac{\int_V \mu \tilde{H}_1 \cdot \tilde{H}_2 dV}{\sqrt{\int_V \mu \tilde{H}_1 \cdot \tilde{H}_1 dV \cdot \int_V \mu \tilde{H}_2 \cdot \tilde{H}_2 dV}}, \quad (4.2.2)
\]

and

\[
\kappa_e = \frac{\int_V \varepsilon \tilde{E}_1 \cdot \tilde{E}_2 dV}{\sqrt{\int_V \varepsilon \tilde{E}_1 \cdot \tilde{E}_1 dV \cdot \int_V \varepsilon \tilde{E}_2 \cdot \tilde{E}_2 dV}}. \quad (4.2.3)
\]
Here $\vec{H}_i$ and $\vec{E}_i$, are the magnetic field intensity and the electric field of the $i^{th}$ resonator, while $\varepsilon$ and $\mu$ are the permittivity and permeability respectively of the coupled system. The integration is over the total volume of the coupled system.

Expressions (4.2.1), (4.2.2) and (4.2.3) look intuitive since they link the coupling coefficient to the coupled energy components. However in the case of conducting resonators, the coupling coefficient was found to be the difference between $\kappa_e$ and $\kappa_m$ instead of their sum [38-39]

$$\kappa = \kappa_m - \kappa_e.$$  \hspace{1cm} (4.2.4)

On the other hand, in the case of two dielectric resonators, the total coupling is the sum of the electrical and magnetic components [40]. The current paper provides a new interpretation for the coupling coefficient, other than the ones provided previously [41] [42]. The aim of this article is to show that using the current authors’ energy coupled mode equations [29], a unified general expression for the coupling coefficient is derived which when applied to different structures reconciles equations (4.2.1) and (4.2.4). Based on the energy conservation principle, a physical interpretation of the derived expression is provided.

### 4.3 Theoretical Background

The overlap integrals $\int_V \mu \vec{H}_1 \cdot \vec{H}_2 dV$ and $\int_V \varepsilon \vec{E}_1 \cdot \vec{E}_2 dV$ that appear in the expressions for the coupling coefficient (4.2.2) and (4.2.3), are contributions of the average stored energy previously derived [29].
\[ \langle W_E \rangle = \frac{1}{4} \int_{V} \epsilon \mathbf{E} \cdot \mathbf{E}^* \, dv = \frac{1}{4} \mathbf{a}^* \mathbf{H} \mathbf{a} \]

\[ = \frac{1}{4} \sum_{i} \sum_{k} a_i^* \left( \int_{V} \epsilon \mathbf{E}_i^* \cdot \mathbf{E}_k \, dv \right) a_k^* , \]  

\[ \langle W_M \rangle = \frac{1}{4} \int_{V} \mu \mathbf{H} \cdot \mathbf{H}^* \, dv = \frac{1}{4} \mathbf{b}^* \mathbf{G} \mathbf{b} \]

\[ = \frac{1}{4} \sum_{i} \sum_{k} b_i^* \left( \int_{V} \mu \mathbf{H}_i^* \cdot \mathbf{H}_k \, dv \right) b_k^* , \] 

where

\[ H_{ik} = \int_{V} \epsilon \mathbf{E}_i^* \cdot \mathbf{E}_k \, dv \]  

(4.3.3)

is the \((i,j)\) element of the matrix \( \mathbf{H} \),

\[ G_{ik} = \int_{V} \mu \mathbf{H}_i^* \cdot \mathbf{H}_k \, dv \]  

(4.3.4)

is the \((i,j)\) element of the matrix \( \mathbf{G} \),

\( \mathbf{a} \) and \( \mathbf{b} \) are the coefficients of the fields expansions given by the coupled mode theory

\[ \mathbf{E} = \sum_{i=1}^{N} a_i \mathbf{E}_i \]  

(4.3.5)

\[ \mathbf{H} = \sum_{i=1}^{N} b_i \mathbf{H}_i \]  

(4.3.6)

Therefore, in order to understand coupling one needs to find the physical meaning of the overlap integrals shown by equations (4.3.3) and (4.3.4) as well as the cross terms of the Poynting vector integrals,

\[ M_{ik}^* = \int_{\partial V} \mathbf{E}_i \times \mathbf{H}_k^* \cdot d\mathbf{S} \quad S_{ik}^* = \int_{\text{all Cond}} \mathbf{E}_i \times \mathbf{H}_k^* \cdot d\mathbf{S} . \]  

(4.3.7)
To do so, it is convenient to start from the complex Poynting theorem which for lossless systems can be written as [43]

$$\frac{1}{2} \int \bar{E} \times \bar{H}^* \cdot d\bar{S} - \frac{1}{2} \int \bar{E} \cdot \bar{J}^* \, dv = 2 j \omega \left( \langle W_M \rangle - \langle W_E \rangle \right). \quad (4.3.8)$$

Using the maximum values of the stored energies $\max \left( W_{E/M} \right)$, the above equation is written as,

$$-\frac{T}{4\pi} \int \bar{E} \times \bar{H}^* \cdot d\bar{S} - \frac{T}{4\pi} \int \bar{E} \cdot \bar{J}^* \, dv = j \left\{ \max \left( W_M \right) - \max \left( W_E \right) \right\}. \quad (4.3.9)$$

where $T$ is the period of the sinusoidal field.

The interpretation of equations (4.3.8) and (4.3.9) should be handled with care. Although equation (4.3.8) is correct in the mathematical sense, it is an averaging relation more than a conservation of energy identity [44-45]. To better understand relation (4.3.9), correspondence relations with a frictionless, mass-spring system driven by a sinusoidal force, $F_D = F_0 \sin \omega t$, have been made. A full and detailed discussion of the frictionless mass-spring system is given in Appendix A.

Equation (4.3.9) is similar to the work energy relationship (4.8.4). The term $W_M$ corresponds to the potential energy ($PE$), $W_E$ corresponds to the kinetic energy ($KE$), and the reactive energy $-\frac{T}{4\pi} \int \bar{E} \times \bar{H}^* \cdot d\bar{S} - \frac{T}{4\pi} \int \bar{E} \cdot \bar{J}^* \, dv$ is equivalent to the reactive work exerted by or on the source $\int_{x(t=0)}^{x(t=T)} F_D \, dx$. Therefore one can interpret...
\[-\frac{T}{4\pi} \int_{\partial V} E \times H^* \cdot d\vec{S} \text{ as the energy transferred inside the enclosure } V \text{ in a quarter of a cycle.} \]

and \[-\frac{T}{4\pi} \int_V E \cdot \vec{J} \, dv \text{ is the energy supplied by the source } J \text{ to the system enclosed in} \]

volume \( V \) in a quarter of a cycle.

It should be noted that the energy is exchanging periodically back and forth resulting in zero net flow of energy. To better illustrate this point, one can write the electric and magnetic fields as

\[
E(\vec{r}, t) = \bar{E}(\vec{r}) \cos \omega t \quad (4.3.10)
\]

and

\[
H(\vec{r}, t) = \bar{H}(\vec{r}) \sin \omega t, \quad (4.3.11)
\]

where \( \vec{r} \) is the position vector. The instantaneous power flowing across the volume boundary becomes

\[
\phi_{rad}(t) = -\int_{\partial V} E(\vec{r}, t) \times H(\vec{r}, t) \cdot d\vec{S} \\
= -\frac{\sin 2\omega t}{2} \int_{\partial V} E(\vec{r}) \times H(\vec{r}) \cdot d\vec{S}. \quad (4.3.12)
\]

Therefore the energy transferred to the volume \( V \) in a quarter of a cycle, \( \frac{T}{4} \), is
\[ \rho_{\xi(t)} = -\int_{t=0}^{t=T} \phi_{\text{rad}}(t) \, dt \]
\[ = -\int_{\partial V} \bar{E}(\bar{r}) \times \bar{H}(\bar{r}) \cdot d\bar{S} \int_{t=0}^{t=T} \frac{\sin 2\omega t}{2} \, dt . \quad (4.3.13) \]
\[ = -\frac{T}{4\pi} \text{Im} \left( \int_{\partial V} E \times H^* \cdot d\bar{S} \right) \]

It is important to recall that this transferred energy, \( \rho_{\xi(t)} \), will cross outside the volume \( V \) after a quarter of a cycle. Hence, it is not the same sort of energy discussed when one studies radiation by antenna which once it leaves the enclosure never returns.

The type of energy transfer discussed here still belongs to the near field regime [46]. By similar arguments one can write the instantaneous power exerted by the source \( \bar{J} \) as

\[ \phi_{\text{sup}}(t) = -\frac{\sin 2\omega t}{2} \int_{V} \bar{E}(\bar{r}) \cdot \bar{J}(\bar{r}) \, dv . \quad (4.3.14) \]

It is easy to show that \( \sigma_{\xi(t)} = -\int_{t=0}^{t=T} \phi_{\text{sup}}(t) \, dt = -\frac{T}{4\pi} \text{Im} \left( \int_{V} E \cdot J^* \, dv \right) \) is the stored energy in a quarter of a cycle due to the current source \( \bar{J} \). Consequently, relation (4.3.9) can be written as

\[ W_M \left( t = \frac{T}{4} \right) - W_E \left( t = 0 \right) = -\int_{t=0}^{t=T} \phi_{\text{rad}} \, dt - \int_{t=0}^{t=T} \phi_{\text{sup}} \, dt \]
\[ = \rho_{\xi(t)} + \sigma_{\xi(t)} . \quad (4.3.15) \]

If the enclosure \( V \) contains a dielectric material \( (\varepsilon_r > 1) \) then the complex Poynting theorem equation (4.3.9) can be re-written by separating the dielectric material portion as [47].
\[ \rho - \sigma + \frac{1}{2} \int_{\text{Dielectric}} \bar{P} \cdot \bar{E}^* \, dv = \max(W_M) - \max(W_E^{\text{vacuum}}) \]  

(4.3.16)

Here \( \max(W_E^{\text{vacuum}}) \) is the maximum stored electric energy in vacuum and is equal to

\[ \max(W_E^{\text{vacuum}}) = \frac{1}{2} \int_V \varepsilon_0 \bar{E} \cdot \bar{E}^* \, dv, \]  

(4.3.17)

\[ \bar{P} = (\varepsilon_r - 1) \varepsilon_0 \bar{E}, \]  

(4.3.18)

and

\[ \psi = \frac{1}{2} \int_{\text{Dielectric}} P \cdot E^* \, dv \]  

(4.3.19)

is the maximum energy stored in the polarization vector \( \bar{P} \).

Equation (4.3.16) is the complex Poynting theorem when all sources (currents, dipole moments, etc.) are distinguished and separated from the free-space fields [47]. Here, the stored magnetic energy is transferred into electric energy stored in free space, energy stored in materials (conductors and dielectrics) and radiated energy that crosses that enclosure boundary. Figure 4-1 depicts a hypothetical system which contains dielectric and conducting components.
Figure 4-1. A system which contains dielectric and conducting components. The energy is stored in various components as well as crossing the boundary surface.

Using the expansions (4.3.5) and (4.3.6), the maximum transferred energy across the boundary of volume \( V \) and the maximum work done by or on the current element \( J \) for a quarter of a cycle is written as [48]

\[
\rho_{\psi} = -\int_{t=0}^{T/4} \Psi_{\text{rad}}(t) \, dt = -\frac{T}{4\pi} \text{Im} \left( \sum_{i} \sum_{k} a_i b_k \int_{\partial V} \vec{E}_i \times \vec{H}_k^* \cdot d\vec{S} \right) \\
= -\frac{T}{4\pi} \sum_{i} \sum_{k} \text{Im} \left( a_i M_{ik}^* b_k \right) \\
= \sum_{i} \sum_{k} a_i \rho_{\psi}^{ik} b_k 
\]

and

\[
\sigma_{\psi} = -\int_{t=0}^{T/4} \Psi_{\text{sup}}(t) \, dt = -\frac{T}{4\pi} \sum_{i} \sum_{k} a_i b_k \int_{V} \vec{E}_i \cdot \vec{J}_k^* \, dv \\
= \sum_{i} \sum_{k} a_i \sigma_{\psi}^{ik} b_k 
\]
where

$$\rho_{ik}^T = -\int_{\partial V} \bar{E}_i \times \bar{H}_k \cdot d\vec{S} \int_{t=0}^{T} \frac{\sin 2\omega t}{2} dt = -\frac{T}{4\pi} \int_{\partial V} \bar{E}_i \times \bar{H}_k^* \cdot d\vec{S},$$

(4.3.22)

and

$$\sigma_{ik}^T = -\int_{V} \bar{E}_i \cdot \bar{J}_k^* dv \int_{t=0}^{T} \frac{\sin 2\omega t}{2} dt = -\frac{T}{4\pi V} \int_{V} \bar{E}_i \cdot \bar{J}_k^* dv.$$  

(4.3.23)

Similarly $\psi_{ik}$ can be written as

$$\psi_{ik} = \frac{1}{2} \int_{\text{Dielectric}(k)} \bar{P}_k \cdot \bar{E}_i^* dy$$

(4.3.24)

The terms $\rho_{ik}^T$ and $\sigma_{ik}^T$ given by equations (4.3.22) and (4.3.23) form the components of the transferred energy across the boundary of volume $V$ and the work done by or on the current elements $J_k$ for a quarter of a cycle respectively. Since the physical meaning of the cross terms (4.3.7) and (4.3.24) was clarified, one can investigate the solution of the eigenvalue equation which governs the coupled system [29].

### 4.4 Analysis

In this section a closed form expression for the coupling coefficient, $\kappa$ will be derived. The eigenvalue equation derived in [29] can be written as

$$UVa = \omega^2 a,$$  

(4.4.1)

$$U = (H^{-1}D^t \Omega),$$

(4.4.2)

and

$$V = (G^{-1} \Omega D),$$

(4.4.3)
where

\[ D_{jk} = \int_V e_i E^*_i E_j \, dv , \quad (4.4.4) \]

and

\[
\Omega \equiv \Omega_{nn} = [\omega_1 \omega_2 \cdots \omega_n] \mathbf{I} = \begin{pmatrix}
\omega_1 & 0 & \cdots & 0 \\
0 & \omega_2 & \cdots & 0 \\
& & \ddots & \vdots \\
0 & 0 & \cdots & \omega_n
\end{pmatrix} . \quad (4.4.5)
\]

Subsequently, the system of equations (4.4.1), (4.4.2) and (4.4.3) will be simplified to find closed form expressions for the coupling coefficients (\(\kappa\)). For simplicity, two resonators are used in the analysis. However, the findings can be generalized to more than two structures. In this later case the dimension of the eigenvalues matrix will increase accordingly. For two resonators, \(U\) is approximated by

\[
\begin{pmatrix}
\omega_1 \\
\omega_2 - \frac{D_{12}^* - H_{21}}{H_{22}} \\
\omega_1 \\
\omega_2
\end{pmatrix}
\begin{pmatrix}
\omega_1 \\
\frac{D_{21}^* - H_{12}}{H_{11}} \\
\omega_2 - \frac{D_{12}^* - H_{21}}{H_{22}} \\
\omega_2
\end{pmatrix}, \quad (4.4.6)
\]

where the approximations \(H_{11}H_{22} - H_{12}H_{21} \approx H_{11}H_{22}\) and

\(D_{11}D_{22} - D_{12}D_{21} \approx D_{11}D_{22}\) were used. This is a valid assumption especially when the overlap between the two resonators is small. When the uncoupled modes have the same frequency (\(\omega_1 = \omega_2 = \omega_0\)) the system will be referred to hereafter as “synchronous”. If the two modes are synchronous, the term (4.4.6) reduces to

\[
\omega_0 \begin{pmatrix}
1 \\
D_{12}^* - H_{21} \\
D_{21}^* - H_{12} \\
H_{22}
\end{pmatrix}, \quad (4.4.7)
\]

The off diagonal terms of (4.4.7) are the overlap integral,
Expression (4.4.8) is further simplified to give

\[ \frac{D_{ki}^* - H_{ik}}{H_{ii}} = \frac{\int \varepsilon_k E_i^* \cdot \bar{E}_k \, dv - \int \varepsilon E_i^* \cdot \bar{E}_k \, dv}{\int \varepsilon E_i^* \cdot \bar{E}_k \, dv} \]  

(4.4.8)

where the overlap term

\[ Y_{ik} = \varepsilon_0 (\varepsilon_{ri} - 1) \int_{\Omega_{Di}} \bar{E}_i \cdot \bar{E}_k \, dv. \]  

(4.4.9)

The \( Y_{ik} \) term in equation (4.4.10) is proportional to the stored coupled energy in the polarization vector \( \vec{P}_i = \varepsilon_0 (\varepsilon_{ri} - 1) \bar{E}_i \)[47]. This is true if any of the resonators has dielectric components. Hence \( U \) is named the electric polarization operator [29].

Equation (4.4.10) shows that the effect of the \( k^{th} \) resonator on the \( i^{th} \) resonator, that has a dielectric constant \( \varepsilon_r \varepsilon_0 \), is just the energy lost by \( k \) and gained by \( i \) as a stored potential energy in the polarization vector \( \vec{P}_i = \varepsilon_0 (\varepsilon_{ri} - 1) \bar{E}_i \). When any of the resonators is also magnetic (\( \mu_r \neq \mu \)) equation (4.4.1) can be modified. Indeed this can be done by using the general eigenvalue equation derived in [29].

\[ [(\Omega C - \Omega G + D^* \Omega + j \{N - S\})G^{-1} \Omega D - \omega^2 H]a = 0. \]  

(4.4.11)

By similar arguments to those discussed previously [29], one can assume that \( S \approx N \). Therefore, the resulting eigenvalue equation can be written as

\[ H^{-1}[\Omega C - \Omega G + D^* \Omega]G^{-1} \Omega D]a = \omega^2 a. \]  

(4.4.12)
\[ U = H^T (\Omega C - \Omega G + D^T \Omega). \]  
(4.4.13)

The extra term \( \Omega C - \Omega G \) is approximated as

\[
\omega_b \begin{bmatrix}
0 & \frac{C_{12} - G_{12}}{G_{11}} \\
\frac{C_{21} - G_{21}}{G_{22}} & 0
\end{bmatrix},
\]  
(4.4.14)

where \( C_{ii} = G_{ii} \) was assumed. This is a reasonable and a valid approximation when the resonators are far enough from each other. A similar assumption was made in deriving equation (4.4.6) for the electrical components. Equation (4.4.14) shows that magnetic coupling from one mode to another is the energy stored in the magnetization vector. For simplicity the factor (4.4.14) will be ignored since magnetic materials are rarely used in RF and microwave resonators. However, equations (4.4.12) and (4.4.14) illustrate that extending the results when magnetic materials exist is straightforward.

In a similar fashion \( V \) is simplified to

\[
V = \begin{bmatrix}
\omega_1 & \omega_2 D_{12} - \omega_1 G_{12} \\
\omega_2 D_{21} - \omega_1 G_{21} & D_{11} \\
D_{22} & \omega_2
\end{bmatrix}.
\]  
(4.4.15)

For the synchronous case (\( \omega_1 = \omega_2 = \omega_b \)), equation (4.4.15) is reduced to

\[
V = \omega_b \begin{bmatrix}
1 & \frac{D_{12} - G_{12}}{D_{11}} \\
\frac{D_{21} - G_{21}}{D_{22}} & 1
\end{bmatrix}.
\]  
(4.4.16)

The off diagonal terms in equation (4.4.16) suggest that the coupling is the difference between \( \kappa_m \) and \( \kappa_e \) which is the same result derived by Awai in [41]. For pure conductors (\( \varepsilon = \varepsilon_0 \) everywhere), matrix (4.4.16) is the dominant factor. In this case it does not depend on the material, hence \( V \) is called the \textit{free space operator}. The complete
eigenvalue operator presented by equation (4.4.1) can be obtained by multiplying (4.4.6) by (4.4.15) from the right to get

\[
UV \approx \begin{bmatrix}
\frac{\omega_1^2}{\omega_1 (\omega_1 D_{12} - \omega_2 G_{21}) + \omega_2^2 D_{21} - \omega_2^2 H_{21}} & \frac{\omega_2 (\omega_2 D_{12}^* - \omega_1 G_{12}) + \omega_1^2 D_{21} - \omega_2^2 H_{21}}{H_{11}} \\
H_{22} & \frac{\omega_2^2}{\omega_2^2}
\end{bmatrix}.
\] (4.4.17)

It has been previously shown that [29],

\[
M_{ik} - N_{ik} = j \omega_1 C_{ik} - j \omega_k D_{ki}^*,
\] (4.4.18)

where

\[
N_{ik} = - \int_{\text{Cond}_K} \vec{E}_i^* \cdot \vec{J}_k \, dv.
\] (4.4.19)

For perfect conductors \(N_{ik}\) can be written as [29]

\[
N_{ik} = \int_{\partial \text{Cond}_K} \vec{E}_i^* \times \vec{H}_k \cdot \vec{dS},
\] (4.4.20)

and when \(\mu = \mu_i\), \(C_{ik} = G_{ik}\) follows.

Using relation (4.4.18), equation (4.4.17) simplifies to

\[
UV \approx \begin{bmatrix}
\frac{\omega_1^2}{j \omega_1 (M_{12} - N_{12}) + \omega_2^2 D_{21} - \omega_2^2 H_{21}} & \frac{j \omega_2 (M_{12} - N_{12}) + \omega_1^2 D_{21} - \omega_2^2 H_{21}}{H_{11}} \\
H_{22} & \frac{\omega_2^2}{\omega_2^2}
\end{bmatrix}.
\] (4.4.21)

For the synchronous case, matrix (4.4.21) turns to be

\[
UV \approx \begin{bmatrix}
\frac{\omega_0^2}{j \omega_0 (M_{21} - N_{21}) + \omega_0^2 (D_{21} - H_{21})} & \frac{j \omega_0 (M_{12} - N_{12}) + \omega_0^2 (D_{12} - H_{12})}{H_{11}} \\
H_{22} & \frac{\omega_0^2}{\omega_0^2}
\end{bmatrix}.
\] (4.4.22)

The coupling constant, \(\kappa\), is defined as the negative of the off diagonal term divided by the on diagonal one. In lumped circuits this is equal to
\[ C_m / \sqrt{C_1 C_2} \text{ or } L_m / \sqrt{L_1 L_2} \quad (C_m \text{ and } L_m \text{ are the mutual capacitance and inductance respectively}). \] In the case at hand, \( \kappa \) is equal to
\[
\kappa_{ip} = \frac{j \{ N_{ip} - M_{ip} \} - \{ D_{ip} - H_{ip} \}}{H_{ii}}.
\] (4.4.23)

In a similar fashion to (4.4.9) one can find that
\[
\frac{D_{ip} - H_{ip}}{H_{ii}} = \int \varepsilon E_i^* \cdot E^*_\rho \, dv - \int \varepsilon E_i^* \cdot E_\rho \, dv = - \varepsilon_0 \left( \varepsilon_{ip} - 1 \right) \int_{DR_p} E_i^* \cdot E_\rho \, dv = - \frac{\varepsilon_{ip}^*}{H_{ii}}.
\] (4.4.24)

Here \( DR_p \) is the region of space where the \( p^{th} \) resonator consists of a dielectric material with relative permittivity equal to \( \varepsilon_{ip} \). Therefore the coupling constant given by (4.4.23) is written as
\[
\kappa_{ip} = \frac{j \{ N_{ip} - M_{ip} \} + \varepsilon_{ip}^*}{H_{ii}}.
\] (4.4.25)

Using relation (4.4.18), equation (4.4.23) becomes
\[
\kappa_{ip} = \frac{G_{ip} - D_{ip}^*}{H_{ii}} + \frac{\varepsilon_{ip}^*}{H_{ii}}.
\] (4.4.26)

Equations (4.4.23) and (4.4.26) are the general expression for the coupling coefficient.

The general expression is reduced to the known formulae found in the literature [41], [49]. Indeed, for dielectric resonators in free space \( N_{ip} = M_{ip} = 0 \), therefore the coupling coefficient given by (4.4.25) reduces to
\[
\kappa_{ip} = \frac{\varepsilon_{ip}^*}{H_{ii}},
\] (4.4.27)
or by using (4.4.24)
\[ \kappa_{ip} = \frac{\varepsilon_0 (\varepsilon_{ip} - 1) \int_{D_{ip}} \vec{E}_i \cdot \vec{E}_p \, dv}{\int_{V} \varepsilon \vec{E}_i \cdot \vec{E}_i \, dv}. \] (4.4.28)

For two conductors \( Y_{ip} = 0 \), therefore equation (4.4.26) reduces to

\[ \kappa_{ip} = \frac{G_{ip} - D_{pi}^*}{H_{ii}}, \] (4.4.29)

or

\[ \kappa_{ip} = \frac{\int_{V} \mu H_i^* \cdot H_p \, dv - \int_{V} \varepsilon E_i^* \cdot E_p \, dv}{\int_{V} \varepsilon E_i^* \cdot E_i \, dv}. \] (4.4.30)

In equation (4.4.30) the total permittivity of the system did not change, that is to say, \( \varepsilon_i = \varepsilon_p = \varepsilon \). This is the case when the two resonators are either: loop gap resonators (LGR), or micro-strips drawn on the same substrate. But, if two micro-strip resonators are drawn on two separated substrates, the coupled permittivity, \( \varepsilon \), is different from the un-coupled permittivity, \( \varepsilon_i, \varepsilon_p \). In the latter case the general expression (4.4.26) has to be used.

### 4.5 Physical interpretation of the coupling coefficient

In this section a physical interpretation for the general coupling coefficient is given. It is based on the general equations (4.4.23) and (4.4.26) and the physical meanings of \( \rho_{ip}^t, \sigma_{ip}^t \) and \( \psi_{ip} \). For synchronous resonators, equation (4.4.23) can be re-written in terms of the energy components (4.3.22) and (4.3.23) to give
\[ \kappa_{ip} = \frac{\rho_{ip} + \sigma_{ip} + \psi_{ip}}{\max(W_{E}^i)} . \] (4.5.1)

To better understand the numerator of equation (4.5.1) one needs to return to equation (4.4.18) which can be re-written as

\[ \rho_{ip} + \sigma_{ip} + \psi_{ip} = \max(W_{M}^{ik}) - \max(W_{E_{invac}}^{ik}) \] (4.5.2)

Where

\[ \max(W_{E_{invac}}^{ik}) = \frac{1}{2} \int_{V} \varepsilon_0 \vec{E}_i \cdot \vec{E}_k^* dv. \] (4.5.3)

Therefore, the coupling coefficient is proportional to the energy supplied to the system enclosed inside the volume, \( V \) i.e., the energy transferred into the volume (\( \rho_{ip} \)), energy supplied by materials inside the volume such as conductors (\( \sigma_{ip} \)) and dielectrics (\( \psi_{ip} \)). Usually \( \rho_{ip} = 0 \), since either the resonators are in free space so the fields vanish at infinity (near field components decay at least as \( r^{-2} \)) or they are inserted in a cavity (the cavity is taken as one of the resonators). In the later case, the internal wall of the cavity is considered as the internal conductor and the outer enclosure can be taken inside the conductor material itself (deep inside by at least the skin depth \( \delta_s \)) where the fields vanish. This is illustrated in Figure 4-2.
Figure 4-2. A top view of a cylindrical cavity showing how the boundary can be chosen so that $\rho_{ip}^4$ vanishes.

Taking the above arguments into consideration equation (4.5.2) can be re-written as

$$\kappa_{ip} = \frac{\sigma_{ip}^4 + \psi_{ip}}{\max(W_{ii}^E) - \max(W_{ii}^{E_{invac}})} = \frac{\max(W_{ik}^M) - \max(W_{ii}^{E_{invac}})}{\max(W_{ii}^E)}. \quad (4.5.4)$$

The two terms $\sigma_{ip}^4$ and $\psi_{ip}$ show that the coupling coefficient is proportional to the energy exerted on the $i^{th}$ mode by the materials (conductors and/or dielectrics) of the $p^{th}$ mode. This means that the coupling coefficient $\kappa_{ip}$ is the maximum normalized energy (normalized to the maximum uncoupled energy) that the sources of the $p^{th}$ mode ($\bar{J}_p$ and $\bar{P}_p$) exert on the $i^{th}$ mode. In another words, from the $i^{th}$ mode point of view, the fields of the $p^{th}$ mode can be replaced by its sources.
The right hand side of equation (4.5.2) vanishes when there is no coupling. This indicates that the coupling coefficient is also proportional to the deviation from the resonance condition since as indicated previously at resonance [29]

$$\max(W_E) = \max(W_M).$$

Using relation (4.5.2) one can write the coupling coefficient as

$$\kappa_{ip} = \frac{\int \mu \vec{H}_p^* \cdot \vec{H}_i \, dv - \int \varepsilon_0 \vec{E}_i^* \cdot \vec{E}_p \, dv}{\int \varepsilon \vec{E}_i^* \cdot \vec{E}_i \, dv}. \quad (4.5.6)$$

The above equation is the general expression for coupling. This confirms that the coupling coefficient is proportional to the difference between $\kappa_m$ and $\kappa_e$ rather than their sum. The above formula also works for the case of dielectric resonators by setting

$$\kappa_m = \frac{\int \mu \vec{H}_p^* \cdot \vec{H}_i \, dv}{\int \varepsilon \vec{E}_i^* \cdot \vec{E}_i \, dv}, \quad (4.5.7)$$

and

$$\kappa_e = \frac{\int \varepsilon_0 \vec{E}_i^* \cdot \vec{E}_p \, dv}{\int \varepsilon \vec{E}_i^* \cdot \vec{E}_i \, dv}. \quad (4.5.8)$$

The numerator of $\kappa_e$ given by (4.5.8) is different from the one given by (4.2.3) since it does not depend on the relative permittivity of the dielectric material. This difference is what makes formula (4.5.6) applicable to dielectric resonators as well as conductors.
4.6 Results and Discussion

In this section the coupling coefficient will be calculated, using the physical meanings discussed in the previous section, for four different structures, namely Conductor-Conductor, Dielectric-Dielectric, Conductor-Dielectric resonator pairs and finally a general pair where the resonators have a dielectric component as well as a conducting one. Expressions were mathematically derived for the first two cases (equations (4.4.28) and (4.4.30)). However, the focus in this section is on the physical meaning as well as the mathematical form given by equations (4.5.4) and (4.5.6).

4.6.1 Dielectric-Dielectric Coupling

Two dielectric resonators in free space are shown in Figure 4-3. Since no conductor presents \( \sigma_{\parallel}^{12} = 0 \), therefore,

\[
\kappa_{12} = \frac{\psi_{12}}{\max\left(W_{11}^E\right)}. \tag{4.6.1}
\]
This result points out the fact that the increase of magnetic energy (equivalent to the potential energy of the mass-spring system in appendix A) is due to the energy stored in the dielectric material.

### 4.6.2 Conductor-Conductor Coupling

If the coupling is between two conducting resonators ($\varepsilon = \varepsilon_0$ everywhere), then $\psi_{12} = 0$. This is true for resonators that are solely made up from conductors for example loop-gaps and split rings as shown in Figure 4-4.
Figure 4-4. Split-ring and Loop-gap resonators as examples for pure conducting resonators.

The coupling coefficient in this case is

$$
\kappa_{12} = \frac{\sigma_{12} J_s H^E_2}{\max \left(W_{11}^E\right)}. \quad (4.6.2)
$$

The above expression is equivalent to the one previously shown by equation (4.4.30) by taking relation (4.4.18) into consideration. It is clear that the coupling coefficient is proportional to the maximum energy supplied by the surface current source $J_s = \hat{n} \times \vec{H}_2$ on resonator 1.
4.6.3 Conductor-Dielectric Coupling

In this subsection, the coupling coefficient between a conducting resonator and a dielectric one is discussed. The conductor is labeled “resonator one” while the dielectric is labeled “resonator two” as shown in Figure 4-5.

![Diagram of dielectric and loop-gap resonators](image)

Figure 4-5. Coupling between a dielectric resonator and a loop-gap one.

The coupling coefficient $\kappa_{12}$, the influence of resonator two (dielectric) on resonator one (loop-gap), can be written as follows

$$\kappa_{12} = \frac{\psi_{12}}{\max(W_{11})}$$

(4.6.3)

since the dielectric material is a non conductor $\sigma_{t}^{12} = 0$. Similarly the coupling $\kappa_{21}$ is equal to
\[ \kappa_{21} = \frac{\sigma_2^{21}}{\max\left(W_{22}^E\right)}. \]  

Usually the uncoupled fields are normalized such as

\[ \max\left(W_{11}^E\right) = \max\left(W_{22}^E\right). \]

It may seem that, even when the uncoupled fields are normalized, the coupling coefficient is not Hermitian (\( \kappa_{12} \neq \kappa_{21}^* \)). However this is not true. Using the general overlap formula (4.5.6), it can be proven that both coefficients are equal. Indeed the coupling between resonators one and two is always equal to [50]

\[ \kappa_{12} = \frac{\int_V \mu \vec{H}_2^* \cdot \vec{H}_1 \, dv - \int_V \varepsilon_0 \vec{E}_1^* \cdot \vec{E}_2 \, dv}{\int_V \varepsilon \vec{E}_1^* \cdot \vec{E}_1 \, dv} = \kappa_{21}^* \]

### 4.6.4 Coupling between general resonators

In this subsection two resonators which have both conducting and dielectric components are considered, for example, a wireless energy transfer system using resonant magnetic coupling [32]. In this case, each resonator is a coil loaded with a dielectric material to form a resonating structure as shown in Figure 4-6.
Figure 4-6. General resonators which have both dielectric and conducting components.

Usually for wireless energy transfer, the capacitively-loaded coils shown in Figure 4-6 operate when the separation distance is large enough so that the coupling is dominant by the magnetic field. This arrangement is desirable because at moderately large separation distances, the electric field is small and thus its interaction with the human tissues is negligible [33]. However, when the coils are close enough, the electric fields of the two coils overlap and hence one gets a general coupling scheme which is described by the coupled mode equations (4.4.1), (4.4.2) and (4.4.3). For this situation the general coupling coefficient expression (4.5.1) has to be used. When the enclosing volume is taken to be all space, the coupling coefficient (4.5.1) reduces to

\[ \kappa_{ip} = \frac{\sigma_{ji} + \psi_{ji}}{\max(W_{ii}^E)} . \]  

(4.6.7)
Equation (4.6.7) illustrates the fact that coupling depends on both the maximum energy stored due to the interaction with the loop surface currents and on the maximum energy stored in the dielectric capacitor.

### 4.7 Summary and Conclusions

To design efficient magnetic resonance probes used in EPR, ESEEM, ENDOR, ELDOR and DEER, it is essential to fully understand theoretically the coupling between their resonant components such as cavities, shields, dielectric, split-ring and loop-gap resonators. One important parameter which determines the coupling strength is the coupling coefficient $\kappa$. In this article, using the energy conservation principle, a unified and general expression for $\kappa$ is derived as shown by equation (4.5.1). This general expression reduces to previously known special ones [38-39, 41] found in the literature. In addition, from this expression the physical meaning and origin, of the coupling coefficient becomes apparent.

To facilitate this interpretation, the analogous classical frictionless mass-spring system driven by a sinusoidal force $F_D = F_0 \sin \omega t$ is presented in appendix A. In particular, the energy change over its oscillation cycle is illustrated. The correspondence between the component RF/MW resonators and the mass-spring system is made where the potential energy corresponds to the stored magnetic energy while the kinetic energy corresponds to the stored electric energy. The driving source is equivalent to three electromagnetic components: Energy transferred to the system volume $V$, energy supplied by current sources and dielectric inserts found within the volume. The energy
coupled mode theory equations (ECMT) are solved and the general expression for the coupling coefficient is derived.

The coupling coefficient is calculated for different structures and results identical to those in the literature are found. In general for a pair of resonators, the coupling coefficient, $\kappa_{ip}$, is the maximum normalized energy (normalized to the maximum uncoupled energy) that the sources of the $p^{th}$ mode ($\vec{J}_p$ and $\vec{P}_p$) exert on the $i^{th}$ mode.

The derived expression for $\kappa$ suggests that coupling will always be the difference between the magnetic and electric field components rather than their sum. This expression is applicable to various structures. It is clear that the coupling is not the overlap integral as was previously suggested [37]. However $\kappa_p$ is the boost in the maximum energy of the $i^{th}$ resonator due to the $p^{th}$ resonator.

The conductor-dielectric pair, discussed in subsection 4.6.3, gives a symmetric formula, $\kappa_{12} = \kappa_{21}^*$, for the coupling. Based on the physical interpretation proposed, the coupling is due to internal sources (currents on the conducting resonator and the polarization vector inside the dielectric material). It was proven that although the two coupling coefficients, $\kappa_{ip}$ and $\kappa_{pi}$ are the results of two different sources they are the complex conjugate of one another. Practical configurations of a conductor-dielectric pair can arise in the fields of EPR spectroscopy, for example a dielectric resonator with a loop-gap resonator or a dielectric resonator with an enclosing cavity [18, 27-28, 51].
4.8 Appendix A

The energy conversation of a frictionless, mass-spring system driven by a sinusoidal force, \( F_D = F_0 \sin \omega t \), shown in Figure 4-7, is studied in detail. For the mass-spring system one can write the governing equation as

\[
\frac{d^2x}{dt^2} + \omega_0^2 x = \frac{F_D}{m} = \frac{F_0}{m} \sin \omega t, \tag{4.8.1}
\]

where \( x \) is the elongation of the spring, \( m \) is the mass, \( F_0 \) is the amplitude of the driving force and \( \omega_0 \) is the natural frequency and is equal to \( \sqrt{k/m} \) where \( k \) is the spring constant.

Figure 4-7. Frictionless mass spring system driven by a sinusoidal force.

Taking \( x = 0 \) when \( t = 0 \) as the reference point, the forced response of equation (4.8.1) is found to be
The work-energy equation for the lossless mass-spring system can be written as

\[ \int_{x(t=0)}^{x(t=T/4)} F_D dx = (KE_2 + PE_2) - (KE_1 + PE_1). \] 

(4.8.3)

\[ = \Phi_2 - \Phi_1 \]

The right hand side of equation (4.8.3) is the difference in total energy, \( \Phi = KE + PE \), between point (2) and point (1), while the left hand side is the work done by or on the driving source. Taking point (2) to be the point where the potential energy is maximum, \( (t = T/4, dx/dt = 0) \), and point (1) to be the point where the kinetic energy is maximum, \( (t = 0, x = 0) \), one can re-write the work-energy equation (4.8.3) as

\[ \int_{x(t=0)}^{x(t=T/4)} F_D dx = \max(PE) - \max(KE) = \frac{F_0^2}{2m(\omega_0^2 - \omega^2)}. \] 

(4.8.4)

The work term \( \int_{x(t=0)}^{x(t=T/4)} F_D dx \) is reactive in nature. This means that the energy supplied by the source for quarter of a cycle returns back to it in the next quarter cycle. Indeed, this can be understood by examining the instantaneous power

\[ p(t) = F_D \frac{dx}{dt} = \frac{F_0^2 \omega}{2m(\omega_0^2 - \omega^2)} \sin 2\omega t. \] 

(4.8.5)

The instantaneous power is continuously changing from positive to negative.

The sequence of events and how energy is bouncing between the driving source and the mass-spring system is shown in Figure 4-8. For the first quarter of a cycle, \( t \in [0, T/4] \),
the maximum kinetic energy together with the work exerted by the source is converted to the maximum potential energy at the end of the period. Then the potential energy will release its energy in two forms: kinetic energy to the mass and work back to the source. So at \( t = T/2 \) all the work supplied by the source will return back to it. Then once the mass passes the equilibrium point (\( x = 0 \)), where its kinetic energy is maximum, the source will supply the mass with energy so when the spring is full stretched at \( t = 3T/4 \), the potential energy will return to its maximum value this process will repeat indefinitely as long as the force is applied.

\[
\begin{align*}
&x = 0 \\
&x(t) \quad F_s \sin \omega t \\
&KE \downarrow \\
&PE \uparrow \\
&t \in \left[0, \frac{T}{4}\right] \\
\end{align*}
\[
\begin{align*}
&x(t) \quad F_s \sin \omega t \\
&KE \uparrow \\
&PE \downarrow \\
&t \in \left[\frac{T}{4} \div \frac{3T}{4}\right] \\
\end{align*}
\[
\begin{align*}
&x(t) \quad F_s \sin \omega t \\
&KE \downarrow \\
&PE \uparrow \\
&t \in \left[\frac{3T}{4}, T\right] \\
\end{align*}
\]

**Figure 4-8.** The energy is bouncing between the mass and the source. When the driving force is pointing in the same direction as the displacement then work is supplied to the mass. This results in an increase in its potential energy. After quarter of a cycle, this work is returned back to the source.

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[48] \(a_i\) and \(b_k\) are real when the uncoupled modes oscillate at the same frequency. This is true for near field coupling since the retardation is negligibly small. However
the $M_{ik}$ coefficients are imaginary because the electric and magnetic fields are out of phase in the near field.


[50] For near field coupling it is safe to say that $\kappa_{12} = \kappa_{21}$ since the field overlap integrals are real. However, the conjugation was shown in the equations to keep the discussion as general as possible.

5 Coupling between a Dielectric resonator and a Cavity

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The candidate made the mathematical derivations and processed the computational and numerical calculations in this publication, worked in collaboration with Dr. Mattar to interpret the results and with Dr. Mattar and Dr. Tervo to publish the manuscript.

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Abstract

A system consisting of a dielectric resonator inserted in a cylindrical cavity finds many practical applications in the fields of electron paramagnetic resonance and dielectric material measurements. Thus the current article studies the behavior of this system based on the coupling between the dielectric and cavity modes. Accordingly, energy coupled mode theory (ECMT) is applied to determine the eigenfrequencies and fields of the coupled system. It is found that the coupling is due to the standing wave fields rather than the evanescent ones as in the case of two coupled dielectric resonators in free space. Consequently, the coupling is considered strong. General expressions for the frequencies and eigenvectors are obtained for both the symmetric and anti-symmetric modes. Large and small cavities are studied in detail. It is shown that although the frequency difference between a small cavity and the dielectric insert is large, the coupling between the two is significant. In this situation the coupling coefficient $\kappa$ can be as high as 0.4. The case when the two resonators have the same frequency (synchronous) is examined where it is shown that the coupled fields contain equal contributions of the fields of the two uncoupled modes. To verify and validate the results, finite element simulations are carried out. This was achieved by simulating the coupling between a cylindrical cavity’s $TE_{011}$ and the insert’s $TE_{01\delta}$ modes. Coupling between higher order modes is investigated and discussed. Based on ECMT, a closed form expression for the electric field of the coupled system is proposed. Finally, comparisons are made to other coupled mode theory models found in the literature.
5.1 Introduction

The coupling between a dielectric resonator and a conducting cavity is of interest in the field of Electron Paramagnetic Resonance (EPR) because of the signal to noise ratio enhancement afforded by the arrangement [1-4]. If both resonators are resonating at the same frequency, the size of the dielectric resonator is much smaller compared to that of a cavity. This means that the magnetic field of the dielectric resonator is more concentrated in a much smaller region and hence the resonator’s filling factor increases [1]. Usually the frequency of the dielectric $TE_{01\delta}$ mode and that of the rectangular cavity $TE_{102}$ mode ($TE_{011}$ mode for cylindrical cavities) are close. Two dielectric resonators inserted in a cavity allow the user to tune the frequency of the cavity along with enhancing the signal to noise ratio [3, 5-6].

The coupling between the $TE_{01\delta}$ dielectric resonator mode and the cavity $TE_{011}$ mode was studied by R. Mett, J. Sidabras, et al. [7]. It was shown that the coupling can be modeled by lumped circuit elements. Using the lumped circuit model, crucial probe parameters such as frequencies, quality factors and resonator efficiencies were determined. The interaction of both modes results in two modes, i.e. symmetric (parallel) and anti-symmetric (anti parallel or anti-mode for short) modes [7]. A symmetric mode is the mode formed when the two fields add constructively with a phase shift of zero degree, while the anti-mode has a 180 degree phase shift between the two uncoupled modes.

The current authors showed that the interaction between the $TE_{01\delta}$ modes of two dielectric resonators and a $TE_{102}$ cavity mode results in three coupled modes, where the
most appropriate mode for X-band EPR experiments was found to be the $TE^{+++}$ mode [6]. This mode is the result of the in-phase coupling of the three uncoupled ones (the two $TE_{01\delta}$ dielectric modes and the $TE_{10\delta}$ cavity mode). In fact, it was illustrated that indeed, the fields of the $TE^{+++}$ mode is the linear superposition of the three uncoupled ones [6].

The above observation together with the results of [7] inspired the current authors to formulate a coupled mode theory capable of finding the frequencies and the fields for general coupled resonators [8]. The derived equation was shown to be in the form of an eigenvalue problem, where the eigenvalues represent the square of the frequencies and the eigenvectors are the coefficients of the field components [8]. The eigenvalue equation satisfies the energy conservation principle and hence is called the energy coupled mode theory (ECMT) [8].

Using ECMT, the physical origin of the coupling coefficient, $\kappa$, was given. This conclusion is universal in the sense that it works for both dielectric and conducting resonators [9]. The coupling coefficient $\kappa_i$, was shown to be the maximum normalized energy (normalized to the maximum uncoupled energy) which is due to the interaction of the sources of the $p^{th}$ mode (conducting current $J_p$ and polarization vector $P_p$) with the fields of the $i^{th}$ mode [9]. Generally, the boundary is taken at infinity for open structures (micro-strips, loop-gaps, dielectrics and split-rings) or inside the material of the enclosing conductor for resonators held in a cavity or in a shield. So the energy flowing into the system enclosure due to coupling vanishes, thus reducing the coupling to be dependent on internal sources only. The coupling coefficient was calculated for different cases. One
situation which was predicted in [9] is the interaction between a dielectric resonator and a conducting one.

A dielectric resonator inserted in a cavity is an example of dielectric-conductor coupling. Therefore, the aim of this paper is to study the coupling between a dielectric insert and a cavity using ECMT. General expressions for the eigenvalues (frequencies) and the eigenvectors (fields) will be calculated. The case when both resonators have the same frequency (hereafter called the synchronous condition) will be studied in detail. Other situations such as large and small cavities will be investigated thoroughly. The results predicted by the coupled mode theory will then be compared to those of an EM full-wave simulator as well as to those found in the literature [7, 10-11].

Section 5.2 defines the system and problem in a concise sense where properties derived from ECMT and the electric fields are illustrated. The eigenvalues and eigenvectors are found in section 5.3. This constitutes the main core needed to study the coupled system. Section 5.4 investigates the results obtained for different scenarios. The results are verified using finite element simulation. Conclusions and discussion are done in section 5.5. Appendix A compares the results of ECMT to other coupled mode formalisms found in the literature.

5.2 Problem description

ECMT is formulated as an eigenvalue problem to describe the coupled system behavior based on the uncoupled systems. The ECMT eigenvalue equation can be written as [8]
\[ \mathbf{U} \mathbf{V} \mathbf{a} = \omega^2 \mathbf{a}, \quad (5.2.1) \]

\[ \mathbf{U} = (\mathbf{H}^{-1} \mathbf{D}^t \mathbf{\Omega}) \] is the polarization operator, \( (5.2.2) \)

and

\[ \mathbf{V} = (\mathbf{G}^{-1} \mathbf{D}) \] is the free-space operator, \( (5.2.3) \)

where

\[ H_{ik} = \int_{\mathcal{V}} \varepsilon \tilde{E}_i^* \cdot \tilde{E}_k dv, \quad (5.2.4) \]

\[ G_{ik} = \int_{\mathcal{V}} \mu \tilde{H}_i^* \cdot \tilde{H}_k dv, \quad (5.2.5) \]

\[ D_{ik} = \int_{\mathcal{V}} \varepsilon_i \tilde{E}_i^* \cdot \tilde{E}_k dv, \quad (5.2.6) \]

and

\[ \mathbf{\Omega} \equiv \mathbf{\Omega}_{nn} = [\omega_1 \omega_2 \cdots \omega_n] \mathbf{I} = \begin{pmatrix} \omega_1 & 0 & \cdots & 0 \\ 0 & \omega_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \omega_n \end{pmatrix}. \quad (5.2.7) \]

A general expression for the coupling coefficient was found to be [9]

\[ \kappa_{ik} = \frac{\int_{\mathcal{V}} \mu \tilde{H}_k^* \cdot \tilde{H}_i dv - \int_{\mathcal{V}} \varepsilon_0 \tilde{E}_i^* \cdot \tilde{E}_k dv}{\int_{\mathcal{V}} \varepsilon \tilde{E}_i^* \cdot \tilde{E}_i dv} = \kappa_{21}, \quad (5.2.8) \]

where \( \tilde{H}_i \) and \( \tilde{E}_i \) are the magnetic field and electric field of the \( i \)th resonator respectively.

Before digging into the mathematical details, one needs to describe the coupled structure in a rigorous way. The system studied in this paper is shown in Figure 5-1. It consists of a dielectric resonator, referred to by the subscript “1”, inserted in the center of a cylindrical cavity, referred to by subscript “2”. The holder, not shown in the figure, is of a low loss / low permittivity material so its effect is negligible. Two types of dielectric
resonators are used, namely types A and B with specifications:

\[ \varepsilon_r = 29.2, \quad d_1 = 6 \text{ mm}, \quad l_1 = 2.65 \text{ mm}, \quad f \approx 9.7 \text{ GHz} \text{ and } \varepsilon_r = 261, \quad d_1 = 1.75 \text{ mm}, \quad l_1 = 1.75 \text{ mm}, \]

and \( f = 9.5 \text{ GHz} \) respectively. The cavity has an aspect ratio of \( d_2/l_2 = 1 \). The terms \( d \) and \( l \) are the resonators’ diameter and height respectively.

![Diagram of a dielectric resonator inserted in a conducting cavity.](image)

**Figure 5-1.** System structure of a dielectric resonator inserted in a conducting cavity. The dielectric insert is held inside a hollow low loss/low permittivity holder (not shown).

Some basic and useful properties of the system can be deduced. Using the same notations in [8], one can deduce that

\[ \varepsilon_1 = \varepsilon, \]  \hspace{1cm} (5.2.9)
\[ \varepsilon_2 = \varepsilon_0, \]  \hspace{1cm} (5.2.10)
\[ D_{ik}^* = D_{ik}, \]  \hspace{1cm} (5.2.11)
\[ G_{ik} = G_{ki}^*, \]  \hspace{1cm} (5.2.12)
\[ D_{lk} = H_{lk}. \]  \hspace{1cm} (5.2.13)
\[ \omega_1 D_{12} = \omega_2 G_{21}. \] (5.2.14)

Here \( \varepsilon_1 \) is the permittivity distribution of the dielectric resonator which is equal to \( \varepsilon \), the permittivity distribution of the coupled system. Since, originally the cavity is empty, then (5.2.10) follows. Equations (5.2.11) and (5.2.12) state that the fields of the two uncoupled systems were taken to be in phase. Relation (5.2.14) can be proven by using the identity [8]

\[ M_{ik} - N_{ik} = j\omega_k C_{ik} - j\omega_k D_{kl}^*, \] (5.2.15)

where \( M_{21} = \int_{\partial V} E^*_2 \times H_1 \cdot d\vec{S} = 0 \) since \( \vec{E}_2 = 0 \) inside perfect conductors, and

\[ N_{21} = - \int_{\text{Cond}_K} \vec{E}^*_2 \cdot J_1 d\nu = 0, \text{ since } \vec{E}_2 \text{ is perpendicular to the cavity wall}. \]

The two modes of interest are the dielectric \( TE_{01\delta} \) mode and the cavity \( TE_{011} \) mode. The electric field of each mode can be written as [12-13],

\[ E_{\phi 1} = J_1(k_d r) \begin{cases} \cos(\beta z) & r \leq \frac{d_1}{2}, |z| \leq \frac{l_1}{2} \\ \frac{a_l}{e^{\frac{a_l}{2}}} \cos \left( \frac{\beta l_1}{2} \right) e^{-a_l|z|} & r < \frac{d_1}{2}, |z| > \frac{l_1}{2} \end{cases}, \] (5.2.16)

\[ E_{\phi 2} = J_1(k_c r) \cos \left( \frac{\pi z}{d_2} \right). \] (5.2.17)

Here \( k_d, k_c \) are the dielectric, cavity radial wave numbers respectively, \( \beta \) is the wave number inside the dielectric in the \( z \) direction and \( E_{\phi i} \) is the azimuthal electric field component. In equation (5.2.16) a perfectly magnetic waveguide was assumed [13], equivalently

\[ k_d = \frac{2.405}{d_1/2}. \] (5.2.18)
5.3 Analysis

Equipped with the properties (5.2.9)-(5.2.14), one can start by simplifying the eigenvalue equation (5.2.1) as was done in [9] to arrive at

\[ UV \approx \begin{bmatrix} \omega_1^2 & \omega_2^2 (D_{21}^* - H_{12}) \\ \frac{\omega_1 (\omega_1 D_{12}^* - \omega_2 G_{21}) + \omega_2^2 D_{21} - \omega_4 H_{21}}{H_{22}} & H_{11} \\ & \omega_2^2 \end{bmatrix} . \] (5.3.1)

Using equations (5.2.14) and (5.2.13) and the relation \( G_{12} = G_{21}^* \), equation (5.3.1) is reduced to

\[ UV \approx \begin{bmatrix} \omega_1^2 & \omega_2^2 (D_{21}^* - H_{12}) \\ \frac{\omega_2 D_{21}^* - \omega_4 H_{21}}{H_{22}} & H_{11} \\ & \omega_2^2 \end{bmatrix} . \] (5.3.2)

Or,

\[ UV \approx \begin{bmatrix} \omega_1^2 & -\omega_2^2 Y_{12} \\ \frac{-\omega_2^2 Y_{12}^2 + (\omega_2^2 - \omega_1^2) D_{21}}{H_{22}} & H_{11} \\ & \omega_2^2 \end{bmatrix} . \] (5.3.3)

Where

\[ Y_{12} = \varepsilon_0 (\varepsilon_r - 1) \int_{DR} E_1^* E_2 dv. \] (5.3.4)

For the synchronous case equation (5.3.3) is reduced to,

\[ UV \approx \begin{bmatrix} \omega_0^2 & -\omega_0^2 Y_{12} \\ -\omega_0^2 Y_{12} & H_{11} \\ H_{22} & \omega_0^2 \end{bmatrix} . \] (5.3.5)

In this case the complete eigenvalue equation is written as

\[ \begin{bmatrix} \omega_0^2 & -\omega_0^2 Y_{12} \\ -\omega_0^2 Y_{12} & H_{11} \\ H_{22} & \omega_0^2 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} = \omega^2 \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} . \] (5.3.6)
By solving equation (5.3.6) the eigenvalues can be found to be

$$\omega^2 = \omega_0^2 \left( 1 \pm \frac{Y_{12}}{\sqrt{H_{11}H_{22}}} \right).$$  \hspace{1cm} (5.3.7)

Therefore the coupling coefficient is given by (the subscript is dropped because of the symmetry)

$$\kappa = \frac{Y_{12}}{\sqrt{H_{11}H_{22}}}.$$  \hspace{1cm} (5.3.8)

Equation (5.3.8) illustrates that the coupling coefficient depends on the overlap integral, a result which was derived for other cases [11, 14]. However, the coupled mode equations proposed in [11, 14-15] do not include the off-diagonal coupling term found in equation (5.3.6). The coupled mode formalisms [11, 14] are discussed in more detail in appendix A.

Although the coupling coefficient shown by equation (5.3.8) is expressed in terms of the overlap integral, $Y_{12}$, the cavity still affects the dielectric resonator by the surface current flowing on its wall. Indeed using identity (5.2.15) and property (5.2.14) one can deduce that (taking into account the system is assumed to be lossless)

$$Y_{12} = \frac{T}{2\pi} \int_{wall} \hat{E}_1^* \cdot \hat{J}_2 \; dv.$$  \hspace{1cm} (5.3.9)

Therefore the coupling coefficient, $\kappa_{12}$, is equal to the normalized maximum energy supplied to the dielectric mode by the cavity surface current and it is equal to

$$\frac{T}{4\pi} \int_{wall} \hat{E}_1 \cdot \hat{J}_2^* \; dv \cdot \frac{1}{\sqrt{W_{11}^L W_{22}^L}}.$$  \hspace{1cm} Similarly, the coupling coefficient, $\kappa_{21}$, is equal to the normalized maximum energy supplied by to the dielectric mode through its the polarization vector.
This is equal to \( 0.5 \gamma_{12} / \sqrt{W_{11} W_{22}} \). As shown by equation (5.3.9) both coefficients are equal.

For the general case, \( \omega_1 \neq \omega_2 \), and assuming that the two frequencies are close enough such that \((\omega_2^2 - \omega_1^2)D_{21} \ll \omega_1^2 \gamma_{12}\), the eigen-frequencies are found to be

\[
\omega^2 = \frac{\omega_1^2 + \omega_2^2}{2} \pm \sqrt{\left(\frac{\omega_1^2 - \omega_2^2}{2}\right)^2 + \omega_1^2 \omega_2^2 \gamma^2}.
\]

The above result is equivalent to formulae derived in the literature [11, 16-17]. It is worthwhile to mention that equation (5.3.10) depicts a situation similar to that produced by perturbation theory in quantum mechanics [11].

Solving the eigenvalue equation (5.3.3) for the eigenvectors \( a \), one can find that

\[
a^{++}_2 = \left( \frac{1}{2 \gamma^2} \right) \left( \gamma^2 - 1 \right) + \sqrt{\frac{1}{4 \gamma^2} \left( \gamma^2 - 1 \right)^2 + \gamma^2} a^{++}_1
\]

for the symmetric mode and

\[
a^{+-}_2 = \left( \frac{1}{2 \gamma^2} \right) \left( \gamma^2 - 1 \right) - \sqrt{\frac{1}{4 \gamma^2} \left( \gamma^2 - 1 \right)^2 + \gamma^2} a^{-+}_1
\]

for the anti-symmetric mode. Here \( \gamma^2 \) is equal to,

\[
\gamma^2 = \left( \frac{\omega_1}{\omega_2} \right)^2.
\]

### 5.4 Results and Discussions

The eigenvalue equation (5.2.1) is solved for a dielectric resonator of type A. The diameter of the cavity is allowed to change from 2.5 to 5.5 cm with a step of 1 mm,
where \( d_2 \) is kept equal to \( l_2 \). The results are plotted and compared to the simulated ones using HFSS© as shown in Figure 5-2.

![Figure 5-2. Frequency of the symmetric and anti-symmetric modes due to the interaction of the dielectric resonator (\( \varepsilon_r = 29.2, \ d_1 = 6 \text{ mm}, \ l_1 = 2.65 \text{ mm} \)) with the cavity (\( d_2 = l_2 \)).](attachment:figure_5_2.png)

Since the coupling coefficient is the normalized overlap integral, as suggested by equation (5.3.8), one can conclude that as the cavity diameter decreases, the overlap integral and consequently the coupling coefficient increase. This means that for small cavities, the term \( \omega_1 \omega_2 \kappa \) is comparable to the term \( (\omega_1^2 - \omega_2^2)/2 \) and thus cannot be ignored. Hence the eigen-frequencies are different from the uncoupled frequencies, \( \omega_1 \) and \( \omega_2 \). For example for a cavity with \( d_2 = 2.5 \text{ cm}, \ f_{TE_{011}} \approx 15.9 \text{ GHz} \), the anti-mode has a frequency of approximately 16.4 GHz. This 500 MHz shift is due to the increase in \( \kappa \).
The behavior of the eigenvectors can be determined using equations (5.3.11) and (5.3.12). For the synchronous case; \( \gamma^2 = 1 \) and the eigenvectors are

\[ a_1 = a_2, \]  
(5.4.1)

for the symmetric mode, and

\[ a_1 = -a_2 \]  
(5.4.2)

for the anti-symmetric one. Equations (5.4.1) and (5.4.2) illustrate that the coupled modes are complete mixes of the two uncoupled ones, unlike that predicted by the coupled mode equations derived in [10-11] and explained in appendix A. These results are also different from what perturbation theory predicts [12]. In perturbation theory, the fields of the coupled modes were assumed to be slightly perturbed from the uncoupled ones. As seen from the above discussion this is not true especially when the resonant frequency of the dielectric material is equal to that of the cavity. To verify the results (5.4.1) and (5.4.2), one should expect that if the electric field for the coupled system is the vector sum of the electric fields of the uncoupled system then the radial variation of the magnitude of the electrical field will be the sum of the two Bessel functions presented in equations (5.2.16) and (5.2.17). Therefore, using HFSS as a 3D finite element solver, the magnitude of the electric fields for both the symmetric and anti-symmetric modes are obtained and plotted along the cavity radius as shown in Figure 5-3. Here the dielectric resonator of type B is used, while the cavity’s diameter is equal to 4.1598 cm. These dimensions guarantee that the two resonators have the same resonant uncoupled frequencies \( f = 9.5 \text{ GHz} \).
Figure 5-3. The magnitude of the electric field of the coupled system plotted against the cavity radius.

As observed from Figure 5-3, the two modes have two peaks which correspond to the two Bessel functions. Each peak corresponds to the peak of one of the Bessel functions presented in equations (5.2.16) and (5.2.17). This confirms that when the two modes have the same uncoupled frequencies, the coupled system will be a perfect mix of both of them. This should be taken into account when one is designing probes for electron paramagnetic spectroscopy.

When the cavity is large, the limiting condition: \( \gamma^2 \to \infty \) and consequently \( \kappa \to 0 \) (overlap integral decreases) give

\[
\begin{align*}
    a_2^{++} &= 1, & a_1^{++} &= 0, \\
    a_1^{+-} &= 1, & a_2^{+-} &= 0,
\end{align*}
\]  

(5.4.3) (5.4.4)
Here the eigenvectors are normalized. The above results mean that the two modes tend to
decouple when the cavity’s dimensions increase. This is of no surprise since the coupled
energy due to \( \vec{J}_2 \) and \( \vec{P}_1 \) has lesser influence when the cavity dimensions increase.

However when the cavity shrinks, things get more involved. Indeed in this case \( \gamma^2 \to 0 \)
and \( \kappa \) increases. Equations (5.3.11) and (5.3.12) are then reduced to,

\[
\begin{align*}
a_2^{++} &= 0, \quad a_1^{++} = 1, \\
\frac{a_1^{-}}{\sqrt{1+\kappa^2}} &= \frac{1}{\sqrt{1+\kappa^2}} \quad \text{(5.4.5)}
\end{align*}
\]

Equation (5.4.5) suggests that for small cavities, the symmetric mode tends to the
dielectric mode, thus the cavity is considered as a shield and the frequency changes due
to the coupling coefficient \( \kappa \) and the coupled induced frequency shifts [16]. However for
the anti-symmetric mode the two field components (cavity and dielectric) are present.
This means that even though the two modes have different frequencies, the coupled
system is still a mix of the two because \( \kappa \) is considerably large. A typical value for the
coupling constant in such cases is between 0.4 – 0.5. To verify the findings (5.4.6), the
dielectric resonator of type A is inserted in a cavity with a frequency of 16.5 GHz
(\( \gamma^2 \approx \frac{1}{3} \)) and the electric field is simulated using HFSS as shown in Figure 5-4.
Figure 5-4 clearly shows that for small cavities, the anti-symmetric mode is a mix of the two fields. It is interesting to show that for such a case, the eigenvalue equation (5.2.1) predicts that the coupled anti-mode is equal to

$$\vec{E} = 0.41\vec{E}_{DR} - 0.92\vec{E}_{Cav}.$$  \hfill (5.4.7)

Figure 5-5 depicts the ratio $a_2/a_1$ for a range of cavity diameters ($D = 2.5-5.4$ cm).
Figure 5-5. The ratio $|a_2/a_1|$ which is an indication of how the fields decouple. When it is small this means that the mode is more like a dielectric mode and when it is large this indicates that the fields are cavity-like.

As shown in Figure 5-5, the symmetric mode asymptotically decouples, while the anti-mode is a mix of the two components when the cavity is small.

For small cavities, the coupling between the cavity $TE_{011}$ mode and the other dielectric higher modes, for example the $TE_{02δ}$, is usually small. In this case; $γ^2 \to \infty$, thus relations (5.4.3) and (5.4.4) apply. Furthermore, approximating the radial component of cavity fields given by equation (5.2.17) inside the dielectric material gives [18]

$$J_1(k_r r) \approx \frac{k_r r}{2}, \quad \text{(5.4.8)}$$
which is accurate for small values of $r$. The radial component of the overlap integral is proportional to

$$\int_0^{r_d} J_1(k_e r) J_1(k_d r) dr \approx \int_0^{r_d} \frac{k_e r}{2} J_1(k_d r) dr.$$  \hspace{1cm} (5.4.9)

Since for higher order dielectric modes, $J_1(k_d r)$ changes sign over the dielectric insert radius, the integration (5.4.9) is small. However if the cavity dimension is decreased further to the limit where the frequency of one of the higher dielectric modes (For example the $TE_{02,\delta}$ mode) is close to the cavity $TE_{011}$ mode, coupling is observed. Indeed if the cavity’s diameter is decreased down to 2.0 cm, its $TE_{011}$ frequency, $f_{TE_{011}} \approx 20$ GHz, which is close to the $TE_{02,\delta}$ frequency, estimated to be $\approx 22$ GHz.

Therefore, the resulting anti-mode has a $TE_{02,\delta}$ component as shown in Figure 5-6.

![Figure 5-6. A small cavity (2.0 cm x 2.0 cm) where the dielectric $TE_{02,\delta}$ mode couples with the cavity $TE_{011}$ mode.](image-url)
For any dimensions, an approximate closed form expression for the electric field can be obtained. If the dielectric $TE_{01\delta}$ mode fields is calculated using the Cohn model (5.2.16) [13], the electric field can be written as,

$$E_\phi = a_1 J_1 (k_d r) \left\{ \begin{array}{ll} \cos(\beta z) & r \leq \frac{d_1}{2}, \vert z \vert \leq \frac{l_1}{2} \\ \frac{a_i}{e^2} \cos \left( \frac{\beta l_i}{2} \right) e^{-\alpha \vert z \vert} & r < \frac{d_1}{2}, \vert z \vert > \frac{l_1}{2} + a_2 J_1 (k_c r) \cos \left( \frac{\pi z}{d_2} \right) \end{array} \right. \right. (5.4.10)$$

For type A resonators: $\beta = 657 \text{ m}^{-1}$, $\alpha = 778 \text{ m}^{-1}$ while for type B: $\beta = 1293 \text{ m}^{-1}$ and $\alpha = 2742 \text{ m}^{-1}$.

Finally, the frequencies of both the symmetric and anti-symmetric modes, calculated using ECMT, are compared to those determined by the lumped circuit model [7]. In [7], the cavity dimension was held constant $d_2 = l_2 = 4.1598 \text{ cm}$ and the dielectric resonator was of type B where the diameter was allowed to vary from 1.3 mm to 2.1 mm. Using the lumped circuit proposed in [7], the frequencies of both the symmetric and anti-symmetric modes were found after the values of the capacitances and inductances were calculated. In the current paper the same circuit model in [7] was solved for type A resonator and the cavity’s diameter was allowed to change from 2.5 cm to 5.5 cm. The errors in the frequencies (HFSS simulations are taken as the reference) are shown in Figure 5-7.
Figure 5-7. The error in frequencies for the symmetric and anti-symmetric modes using both the lumped circuit model and ECMT.

Although the lumped circuit model in [7] was originally applied to very high epsilon resonators ($\varepsilon_r \approx 261$), the error in frequency for moderately high epsilon inserts ($\varepsilon_r \approx 30$) is below 5%. Energy coupled mode theory gives errors below 1.5%. For the symmetric mode; as the cavity size increases the errors of both methods are reduced. This is opposite to the errors curve of the anti-mode.

5.5 Summary and Conclusions

The frequencies and fields for a cavity with a high dielectric insert were studied using ECMT. It was shown that the coupling coefficient is the normalized overlap
integral. Physically, the dielectric insert affects the cavity by its polarization vector while the cavity injects energy into the dielectric mode through its surface current. Both effects were proven to be equal and thus the coupling is Hermitian. General expressions for the frequencies and eigenvectors, both for the symmetric and anti-symmetric modes, were obtained.

It was shown that for large cavities ($\omega_2 \ll \omega_1$) the two modes tend to decouple. For small cavities ($\omega_1 \ll \omega_2$) the coupling coefficient is large. This means that the frequencies of the coupled system will deviate from those of the uncoupled modes. From the eigenvectors point of view, the symmetric mode tends to be dominantly dielectric which means that the cavity acts as a shield. However, the anti-symmetric mode is always a mix of the two uncoupled modes. This observation was verified using HFSS eigenmodes solver. Here the coupling between the cavity’s $TE_{011}$ and the insert’s $TE_{018}$ modes were examined. It was observed that the anti-mode has a dielectric insert component. It was then argued that the coupling between the cavity $TE_{011}$ mode and other dielectric insert higher modes is small. However when the cavity shrinks to a level where the frequency of one of the higher order modes (for instance the dielectric $TE_{020}$ mode) gets closer to the cavity $TE_{011}$ mode coupling occurs. This was verified using HFSS eigenmodes solver.

Energy coupled mode theory predicts that when the two resonators are synchronously tuned ($\omega_1 = \omega_2$) the coupled modes are perfect mixes of the two uncoupled ones. Finite element simulations showed that the magnitude of the electric field along the cavity radius has two peaks. This verifies that the coupled modes are
composed of the two uncoupled ones. Based on ECMT a closed form expression for the electric field of the coupled system was proposed.

Finally, the frequencies of both the symmetric and anti-symmetric modes, calculated using ECMT, were compared to those determined by the lumped circuit model [7]. Lumped circuit model shows that the error in frequency for moderately high epsilon inserts ($\varepsilon_r \approx 30$) is below 5% while ECMT gives a maximum error bound of 1.5%.

The findings of the current paper raise important scientific questions about the performance of a cavity with a dielectric resonator inserted in its center. The performance is usually measured using known parameters such as the Quality factor, filling factor and resonator efficiency (conversion factor) [2, 19-20]. It was shown that at the synchronous condition, the coupled modes will always be a mix of the two uncoupled ones, therefore one can expect that the cavity mode deteriorates the filling factor compared to the case of a dielectric resonator in free space or in a shield.

5.6 Appendix A

In this section the two different coupled mode schemes proposed in [11, 21], are solved to find expressions for the eigen-frequencies and the eigenvectors.

5.6.1 Coupled Mode Equations: System One

The coupling between resonators studied by H. A. Haus et al [11] is re-written here using the current authors’ notation [8]

$$H^4 \Omega^2 Da = \omega^2 a . \quad (5.6.1)$$
The above equation when applied to the case of a dielectric resonator inside a cavity shows that the resulting modes are as follows:

\[ \omega = \omega_1, \]  
\[ \omega = \omega_2 \sqrt{1 - \alpha}, \]  

where \( \alpha \) is equal to \( \int_{\text{cavity}} \left| \frac{\partial E_{\text{cavity}}}{\partial t} \right|^2 dv \). Since \( \alpha \ll 1 \) a Taylor expansion of equation (5.6.3) yields

\[ \omega \approx \omega_2 \left[ 1 - \frac{1}{2} \int_{\text{cavity}} \left| \frac{\partial E_{\text{cavity}}}{\partial t} \right|^2 dv \right]. \]  

This result is identical to the one derived using the material perturbation technique [12]. In this case the dielectric insert is assumed to be small enough such that the resultant fields can be approximated by the cavity fields alone.

### 5.6.2 Coupled Mode Equations: System Two

The system of equations [15] is re-written here using a different notation compatible with the current authors' notation [8] as,

\[
\frac{da_i}{dt} = \frac{j}{\det(H)} \left[ \omega_i \left( D_{11} H_{22} - D_{12}^* H_{12} \right) + j \sum_{i=1}^{2} \left( D_{i1}^* H_{22} - D_{i2}^* H_{12} \right) \frac{M_{i1}}{D_{11}} \right] b_1 + \\
\left[ \omega_2 \left( D_{21}^* H_{22} - D_{22}^* H_{12} \right) + j \sum_{i=1}^{2} \left( D_{i1}^* H_{22} - D_{i2}^* H_{12} \right) \frac{M_{i2}}{D_{22}} \right] b_2 \right],
\]  

(5.6.5)
\[
\frac{da_2}{dt} = \frac{j}{\det(H)} \left[ \omega_1 \left( D_{12}^* H_{11} - D_{11}^* H_{21} \right) + j \sum_{i=1}^{2} \left( D_{i2}^* H_{i1} - D_{i1}^* H_{i2} \right) \frac{M_{1i}}{D_{1i}} \right] b_1 + \left( \omega_2 \left( D_{22}^* H_{11} - D_{21}^* H_{21} \right) + j \sum_{i=1}^{2} \left( D_{i2}^* H_{i1} - D_{i1}^* H_{i2} \right) \frac{M_{1i}}{D_{2i}} \right] b_2 \right], \quad (5.6.6)
\]

\[
\frac{db_1}{dt} = j \omega_1 a_1, \quad (5.6.7)
\]

\[
\frac{db_2}{dt} = j \omega_2 a_2. \quad (5.6.8)
\]

At steady state

\[
a_1 = \bar{a}_1 e^{j \omega t}, \quad a_2 = \bar{a}_2 e^{j \omega t}, \quad b_1 = \bar{b}_1 e^{j \omega t}, \quad b_2 = \bar{b}_2 e^{j \omega t}. \quad (5.6.9)
\]

Taking advantage of the harmonic dependence represented by equation (5.6.9), it is easy to find that \( \omega \bar{b}_2 = \omega_2 \bar{a}_2 \), \( \omega \bar{b}_1 = \omega_1 \bar{a}_1 \) therefore, equations (5.6.5) and (5.6.6) can be written as an eigenvalue equation

\[
\begin{bmatrix}
\omega_1 \left( \omega_1 + j \frac{M_{11}}{D_{11}} \right) & \omega_2 \left( D_{21}^* H_{22} - D_{22}^* H_{12} \right) + j \omega_2 \frac{M_{12}}{D_{22}} \\
0 & - \frac{\omega_2}{\det(H)} \left( D_{22}^* H_{11} - D_{21}^* H_{12} \right)
\end{bmatrix}
\begin{bmatrix}
\bar{a}_1 \\
\bar{a}_2
\end{bmatrix}
= \omega^2
\begin{bmatrix}
\bar{a}_1 \\
\bar{a}_2
\end{bmatrix}. \quad (5.6.10)
\]

Since the \((2,1)\) element in (5.6.10) is zero, the two eigen-states are decoupled. Therefore one can find the eigen-frequencies to be

\[
\omega^2 = \omega_1 \left( \omega_1 + j \frac{M_{11}}{D_{11}} \right), \quad (5.6.11)
\]

\[
\omega^2 = \omega_2^2 \frac{D_{22}^* H_{11} - D_{21}^* H_{12}}{\det(H)}. \quad (5.6.12)
\]

Using the Poynting vector theorem [22] equation (5.6.11) can be written as
\[ \omega^2 = \omega_1^2 \left( 1 - \frac{\int_{\text{cavity}} \mu |\vec{H}_1|^2 \, dv - \int_{\text{cavity}} \epsilon_1 |\vec{E}_1|^2 \, dv}{\int_{\text{cavity}} \epsilon_1 |\vec{E}_1|^2 \, dv} \right). \] (5.6.13)

When \( \int_{\text{cavity}} \mu |\vec{H}_1|^2 \, dv - \int_{\text{cavity}} \epsilon_1 |\vec{E}_1|^2 \, dv \ll 1 \) the eigen-frequency can be approximated to

\[ \omega \approx \omega_1 \left( 1 - \frac{\int_{\text{cavity}} \mu |\vec{H}_1|^2 \, dv - \int_{\text{cavity}} \epsilon_1 |\vec{E}_1|^2 \, dv}{2\int_{\text{cavity}} \epsilon_1 |\vec{E}_1|^2 \, dv} \right). \] (5.6.14)

Equation (5.6.14) is identical to that derived using the shape perturbation technique [12].

Similarly the other eigen-frequency, shown by equation (5.6.12), can be simplified further. By noting that \( D_{22} H_{11} >> D_{21} H_{12} \), \( \det(H) \approx H_{11} H_{22} \), the eigen-frequency is approximated to

\[ \omega \approx \omega_2 \left( 1 - \frac{Y_{22}}{2H_{22}} \right), \] (5.6.15)

and \( Y_{22} = \epsilon_0 (\epsilon_r - 1) \int_{\partial R} |\vec{E}_2|^2 \, dv \).

This means that one gets two separate modes, one which is similar to the dielectric mode but perturbed slightly by the cavity geometry hence called the “dielectric-like” mode. The other is similar to the cavity mode; however, it is slightly perturbed by the dielectric material, hence called the “cavity-like” mode. It is worth to mention that according to perturbation theory, the fields are assumed not to change much from the unperturbed (uncoupled) structures. As shown in previous sections, this is not true especially if the frequencies of the two uncoupled modes are close in value. The “dielectric-like” mode has its \( \vec{a}_2 = 0 \), which implies that the mode is purely dielectric.
from the fields point of view. However for the “cavity-like” mode, one can see that the resultant eigenvector is a mix of the two fields (cavity and dielectric ones);

\[
\left( \omega_1^2 - \omega_2^2 \right) a_1 \approx \left( \frac{\omega_1^2 \gamma_{12}}{H_{11}} + \frac{\omega_2^2 \gamma_{12}}{H_{22}} \right) a_2. \tag{5.6.16}
\]

Relation (5.6.16) shows that this mode switches from being symmetric, \(a_1a_2 > 0\) when \(\omega_1 > \omega_2\) to anti symmetric \(a_1a_2 < 0\) when \(\omega_1 < \omega_2\), where at the switching point (the synchronous case, \(\omega_1 = \omega_2\)) the mode is completely dielectric.

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6 General expressions for the Coupling Coefficient, Quality and Filling factors for a Cavity with an insert using energy coupled mode theory

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The candidate made the mathematical derivations and processed the computational and numerical calculations in this publication, worked in collaboration with Dr. Mattar to interpret the results and with Dr. Mattar and Dr. Tervo to publish the manuscript.

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Abstract

A system consisting of a cavity with a dielectric insert finds applications in the fields of electron paramagnetic resonance and dielectric constant measurements. Accordingly, this article uses energy coupled mode theory (ECMT) to find general expressions for the coupling coefficient $\kappa$, the quality factors $Q$, and the filling factors $\eta$ for a cavity with a dielectric insert. These parameters are vital in assessing systems’ performance. The coupling coefficient calculated using ECMT is shown to be proportional to the square root of the dielectric constant and to the ratio of the cross sectional areas. Since the quality factor of the coupled system is an important resonator parameter, it is calculated for different coupling scenarios and comparisons to finite elements simulations are carried out to provide corroborative evidence. It is shown that when the frequencies of the uncoupled systems are equal, the quality factor of the coupled system is approximately double the minimum quality factor of the uncoupled resonators. This conclusion is significant for electron paramagnetic probe design. Similarly a simple expression for the coupled filling factor, which has an important role in the performance of EPR probes, is derived. Equipped with the quality and filling factors, expressions for the signal enhancement of the electron paramagnetic resonance signal are obtained. Finally, the separation between the coupled modes compared to the average bandwidth is calculated for different structures. It is shown that for practical dielectric resonators it is possible to excite one of the coupled modes without exciting the other.
6.1 Introduction

A cavity with a loop-gap or a dielectric insert shows a significant enhancement in the signal intensity for electron paramagnetic resonance (EPR) spectroscopy [1-4]. Qualitatively given a certain resonance frequency, the sizes of the dielectric or the loop-gap are much smaller than conducting cavities. Accordingly, the filling factor of the composed structure increases due to the compactness of the magnetic fields inside and in the vicinity of the insert [1]. When the frequencies of the dielectric $TE_{01\delta}$ mode and that of the rectangular cavity $TE_{10\delta}$ mode ($TE_{011}$ mode for cylindrical cavities) are close, the energy exchange between the two modes is at a maximum [5]. It was shown that this situation (hereafter called the synchronous condition) is very helpful if one needs to enhance the signal intensity of a standard conventional cavity without modifying the coupling to the microwave bridge [1]. However if signal enhancement is of a higher priority, a dielectric material inserted in a shield would have a better signal enhancement [2, 6]. In the latter case, coupling to the microwave bridge through an iris on the shield surface may be unachievable due to the diminishing fields’ values [6]. Two dielectric resonators inserted in a cavity gives the user the ability to tune the frequency of the cavity beside the signal intensity improvement [3, 7-8].

The coupling between the $TE_{01\delta}$ dielectric mode and the $TE_{011}$ cavity mode was thoroughly studied in [6] using a lumped circuit model and in [5] using energy coupled mode theory (ECMT) [9]. The lumped circuit model was used to calculate different probe parameters such as coupled frequencies, quality factors and resonator efficiencies. The interaction of both modes results in two coupled ones: symmetric (parallel) and anti-
symmetric (anti parallel or anti-mode for short) modes. The symmetric mode is the one formed when the two fields add constructively with a phase shift of zero degree, while the anti-symmetric has a 180 degrees phase shift between the two uncoupled modes. Energy Coupled Mode theory when applied, was able to determine the coupled fields beside calculating the eigen-frequencies. Coupling is understood to be the result of the interaction between the source elements (polarization vector in the dielectric material and the surface current density on the cavity wall) [5, 10]. These results and observations suggest that probe parameters such as the coupling coefficient, quality factor, filling factor and resonator efficiency can be studied and evaluated based on ECMT. It was illustrated that for moderate relative permittivity values ($\varepsilon_r \approx 20–50$) the coupling coefficient is significantly high especially when the cavity’s dimensions shrink [5]. This means that the modes are still coupled even though the frequency difference between them is large [5]. In contrast, for high values of $\varepsilon_r \approx 100–300$ it is observed that the modes tend to decouple. This was reflected in the quality factor curves presented in [6]. Therefore one important scientific question is raised about how the coupling coefficient depends on the permittivity and the geometric dimensions. One of the aims of the current paper is to answer this question in a mathematical sense. Calculating the coupling coefficient is crucial in determining whether exciting one coupled mode will probably excite the other one or not. To excite a particular mode, the frequency of the driving source should be within $\pm 5(f/Q)$ of the eigen-frequency [6]. Therefore to avoid exciting other spurious modes their frequencies should be at least five times the bandwidth away
from the desired mode. Thus the ratio of the difference of the two coupled modes and the average bandwidth of both modes, \( \Phi = \left( f_{\text{inn}} - f_{\text{sym}} \right) / BW_{\text{avg}} \), needs to be examined.

The coupling coefficient is proportional to the difference between the resulting coupled modes frequencies (numerator of \( \Phi \)). Similarly the bandwidth is inversely proportional to the quality factor [11]. It was shown that depending on the frequency difference between the two uncoupled modes, the quality factor changes tremendously [6]. Consequently it is crucial that one is able to predict beforehand the behavior of the quality factor of the coupled system.

On the other hand, the signal intensity for EPR probes is proportional to the resonator’s parameters [1, 12-13]

\[
S \propto \eta Q P^{1/2},
\]  

(6.1.1)

where \( S \) is the signal intensity, \( \eta \) is the resonator filling factor [13], \( Q \) is the resonator quality factor and \( P \) is the incident power. Although a dielectric insert or a loop-gap may increase the filling factor, the quality factor may decrease in such a way that the signal intensity is deteriorated rather than improved [1, 6]. How the filling factor changes with coupling is another important concept that needs to be investigated.

For the above reasons, it is the aim of this paper to find expressions for the coupling coefficient, quality factor and the filling factor for a system consisting of a dielectric resonator inserted in a cavity. It is also conjectured that the findings here can be directly applied to the case of a loop-gap inserted in a cavity.

Section 6.2 defines the system in a concise sense where properties previously derived from ECMT such as the eigen-frequencies, eigenvectors and the electric fields, are presented. Using ECMT, expressions for the coupling coefficient, the quality and the
filling factors are derived in section 6.3. Hence this section forms the main core needed to study the system in hand. Section 6.4 investigates the numerical results obtained for different scenarios. The results are verified using finite element simulations. Conclusions and discussion are provided in section 6.5.

6.2 Problem description

The system studied in this article, is depicted in Figure 6-1. It consists of a dielectric resonator inserted in the center of a cavity. The holder, not shown in the figure, is of a material with low loss and low permittivity so its effect is negligible. Two types of dielectric resonators are used, namely types A and B with specifications

\[ \varepsilon_r = 29.2, \quad d_D = 2r_D = 6 \text{ mm}, \quad l_D = 2.65 \text{ mm}, \quad f \approx 9.7 \text{ GHz} \quad \text{and} \quad \varepsilon_r = 261, \quad d_D/l_D = 1 \]

respectively. The cavity has an aspect ratio of \( d_C/l_C = 1 \). The terms \( d \) and \( l \) are the resonators’ diameters and heights respectively. It should be noted that the dielectric resonator and the cavity are labeled resonator 1 and resonator 2 respectively.
Figure 6-1. System structure of a dielectric resonator inserted in a conducting cavity. The dielectric insert is held inside a hollow low loss/low permittivity holder (not shown).

The two modes of interest are the dielectric $TE_{010}$ mode and the cavity $TE_{011}$ mode. The electric field of each mode can be written as [11],

$$
E_{\varphi 1} = J_1(k_D r) \begin{cases} 
\cos(\beta z) & r \leq \frac{d_D}{2}, |z| \leq \frac{l_D}{2} \\
\frac{a_{Dp}}{e^{\frac{eta l_D}{2}}} \cos\left(\frac{\beta l_D}{2}\right) e^{-a|z|} & r < \frac{d_D}{2}, |z| > \frac{l_D}{2} 
\end{cases},
$$

(6.2.1)

$$
E_{\varphi 2} = J_1(k_C r) \cos\left(\frac{\pi z}{l_C}\right).
$$

(6.2.2)

Here $k_D, k_C$ are the dielectric, cavity radial wave numbers respectively and $E_{\varphi l}$ is the azimuthal electric field component. In equation (6.2.1) the fields were assumed to be confined within a perfect magnetic wall tube with a diameter equals to the dielectric diameter[14], equivalently

$$
k_D = \frac{2.405}{r_D}
$$

and

$$
E_{\varphi 1} = J_1(k_D r) \begin{cases} 
\cos(\beta z) & r \leq \frac{d_D}{2}, |z| \leq \frac{l_D}{2} \\
\frac{a_{Dp}}{e^{\frac{eta l_D}{2}}} \cos\left(\frac{\beta l_D}{2}\right) e^{-a|z|} & r < \frac{d_D}{2}, |z| > \frac{l_D}{2} 
\end{cases}.
$$

(6.2.1)
\[
\beta = \sqrt{\varepsilon, k_0^2 - \left(\frac{2.405}{r_D}\right)^2}, \text{ where } k_0 \text{ is the free space wave number.} \quad (6.2.4)
\]

Energy Coupled Mode theory is an eigenvalue equation and can be written as [9]

\[
\mathbf{U} \mathbf{V} \mathbf{a} = \omega^2 \mathbf{a}, \quad (6.2.5)
\]

\[
\mathbf{U} = (\mathbf{H}^{-1} \mathbf{D}^T \mathbf{\Omega}) \text{ is the Polarization Operator,} \quad (6.2.6)
\]

\[
\mathbf{V} = (\mathbf{G}^{-1} \mathbf{\Omega} \mathbf{D}) \text{ is the free-space Operator,} \quad (6.2.7)
\]

where

\[
H_{ik} = \int_{V} \varepsilon E_i^* \cdot \bar{E}_k \, dv, \quad (6.2.8)
\]

\[
G_{ik} = \int_{V} \mu \bar{H}_i^* \cdot \bar{H}_k \, dv, \quad (6.2.9)
\]

\[
D_{ik} = \int_{V} \varepsilon_i \bar{E}_i^* \cdot \bar{E}_k \, dv, \quad (6.2.10)
\]

and

\[
\mathbf{\Omega} \equiv \Omega_{nn} = [\omega_1 \omega_2 \cdots \omega_n] \mathbf{I} = \begin{pmatrix}
\omega_1 & 0 & \cdots & 0 \\
0 & \omega_2 & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & \omega_n
\end{pmatrix}. \quad (6.2.11)
\]

Here $\bar{H}_i$ and $\bar{E}_i$ are the magnetic and electric fields of the $i^{th}$ resonator respectively.

The system of equations (6.2.5), (6.2.6) and (6.2.7) were solved for the case in hand where the coupling coefficient ($\kappa$), eigenvalues ($\omega$) and the eigenvectors ($a_i^{++}, a_i^{--}$) were found to be [5]

\[
\kappa = \frac{Y_{12}}{\sqrt{H_{11}H_{22}}}, \quad (6.2.12)
\]
\[ Y_{12} = \varepsilon_0 (\varepsilon_r - 1) \int_{\partial\Omega} \vec{E}_1^* \cdot \vec{E}_2 \, dv, \]

\[ \omega^2 = \frac{\omega_1^2 + \omega_2^2}{2} \pm \sqrt{\left( \frac{\omega_1^2 - \omega_2^2}{2} \right)^2 + \omega_1^2 \omega_2^2 \kappa^2}, \quad (6.2.13) \]

\[ a_{2+} = \left( \frac{1}{2\kappa} (\gamma^2 - 1) + \sqrt{\frac{1}{4\kappa^2} (\gamma^2 - 1)^2 + \gamma^2} \right) a_{1+}, \quad (6.2.14) \]

for the symmetric mode and

\[ a_{2-} = \left( \frac{1}{2\kappa} (\gamma^2 - 1) - \sqrt{\frac{1}{4\kappa^2} (\gamma^2 - 1)^2 + \gamma^2} \right) a_{1-} \quad (6.2.15) \]

for the anti-symmetric mode. Here \( \gamma^2 \) is equal to

\[ \gamma^2 = \left( \frac{\omega_1}{\omega_2} \right)^2. \quad (6.2.16) \]

### 6.3 Analysis

Equipped with the findings (6.2.12), (6.2.13), (6.2.14), and (6.2.15) one can start finding expressions for the resonator parameters such as the coupling coefficient \( \kappa \), the quality factor \( Q \) and the filling factor \( \eta \).

#### 6.3.1 Coupling Coefficient

The coupling coefficient is calculated using the general expression (6.2.12) and the fields represented by formulae (6.2.1) and (6.2.2). Consequently an approximate analytical expression is derived. Accordingly \( H_{22} \) can be written as follows [11]

\[ H_{22} = \frac{\varepsilon_0 c^2 l_c \pi J_0^2 (p'_{01}) M^2}{2}, \quad (6.3.1) \]
where \( r_c \) is the cavity radius, \( p_{01}' \) is the first root of \( J_0'(x) \) and \( M \) is the amplitude of the electric field. The overlap integral is found to be

\[
\gamma_{12} = 2\pi AM \varepsilon_0 (\varepsilon_r - 1) \frac{p_{01}'}{p_{01}} \frac{r_D^3}{r_c^3} J_2(k_D r_D) \frac{1}{\beta} \sin \frac{\beta l_D}{2}.
\]  
(6.3.2)

Here the expressions \( J_1(k_c r) \approx \frac{1}{2} k_c r \), \( \frac{d}{dx} x^2 J_2(x) = x^2 J_1(x) \) [15] and relations

\( l_D \ll l_c \) and \( \beta >> \pi/l_c \) were used. Similarly \( H_{11} \) is found to be

\[
H_{11} = \frac{1}{2} A^2 \pi \varepsilon_0 \varepsilon_r r_D^2 J_1^2(k_D r_D) \left( \frac{\sin \beta l_D}{\beta} + l_D \right).
\]  
(6.3.3)

Consequently, the coupling coefficient given by (6.2.12) can be written as,

\[
\kappa = 13.16 \frac{(\varepsilon_r - 1) \left( \frac{r_D}{r_c} \right)^2}{\sqrt{2\varepsilon_r \beta l_c}} \sqrt{\frac{1 - \cos \beta l_D}{\beta l_D + \sin \beta l_D}}
\]  
(6.3.4)

\[
= 13.16 \frac{(\varepsilon_r - 1) A_D}{\sqrt{2\varepsilon_r \beta l_c} A_C} \sqrt{\frac{1 - \cos \beta l_D}{\beta l_D + \sin \beta l_D}},
\]

where \( A_D \) and \( A_C \) are the dielectric and cavity cross sectional areas respectively. The above equation shows that as long as the dielectric constant is large, the dependence of the coupling coefficient on \( \varepsilon_r \) is moderate compared to its dependence on the ratio of the two areas (area overlap, \( A_D/A_C \)). This explains why the modes (especially the anti-mode) tend to slowly decouple for type A resonators [5].
6.3.2 Quality Factor

To calculate the quality factor of the coupled system, the fields must be used. Accordingly, the total fields of the coupled system are linearly expressed in terms of the uncoupled ones as [9]

\[ \vec{E} = \sum_{i=1}^{N} a_i \vec{E}_i, \quad (6.3.5) \]

\[ \vec{H} = \sum_{i=1}^{N} b_i \vec{H}_i, \quad (6.3.6) \]

where \( \vec{E} \) and \( \vec{H} \) are the electric and magnetic fields respectively. The quality factor of a resonator is defined as [11]

\[ Q = \frac{2\omega W_E}{P_i}, \quad (6.3.7) \]

where \( \omega \) is the resonant frequency, \( W_E \) is the average stored electrical energy (at resonance it is equal to the average stored magnetic energy) and \( P_i \) is the average power loss. Expressing the energy [9] in terms of the eigenvectors and using Dirac notation, one can arrive at

\[ W_E = \frac{1}{4} \langle a | \mathbf{H} | a \rangle. \quad (6.3.8) \]

Similarly the power loss is the sum of the losses inside the dielectric material and the loss on the conductor walls

\[ P_i = P_{ld} + P_{lc}. \quad (6.3.9) \]

Where \( P_i \) is the total loss, \( P_{ld} \), \( P_{lc} \) are the dielectric and conductor losses respectively and they are equal to
\[
P_{ld} = \frac{\sigma}{2} \int_{DR} |E|^2 \, dV ,
\]

\[
P_{lc} = \frac{R_s}{2} \int_{Cavity} |H|^2 \, dS .
\]

Here \(\sigma\) is the dielectric conductivity and \(R_s\) is the cavity surface resistance.

Using expansions (6.3.5) and (6.3.6), equations (6.3.8), (6.3.9), (6.3.10) and (6.3.11), can be re-written as

\[
W_E = \frac{\sum_{i,j} a_i^* a_j \int \mathbf{E}_i \cdot \mathbf{E}_j \, dv}{4} ,
\]

(6.3.12)

\[
P_{ld} = \sum_{i,j} a_i^* a_j \frac{\sigma}{2} \int_{DR} \mathbf{E}_i \cdot \mathbf{E}_j \, dV , \text{ and}
\]

(6.3.13)

\[
P_{lc} = \frac{R_s}{2} \sum_{i,j} b_i^* b_j \int_{\partial V} \mathbf{H}_i \cdot \mathbf{H}_j \, dS .
\]

(6.3.14)

When the coupling is small (overlap area \(A_D / A_c\) is small), the above relations can be approximated by

\[
W_E \approx \frac{a_1^2 \int_{V} \varepsilon |E_1|^2 \, dv + a_2^2 \int_{V} \varepsilon |E_2|^2 \, dv}{4} = \frac{a_1^2 H_{11} + a_2^2 H_{22}}{4} ,
\]

(6.3.15)

\[
P_{ld} \approx |a_1|^2 P_{ld}^D ,
\]

(6.3.16)

\[
P_{lc} \approx |b_2|^2 P_{lc}^C ,
\]

(6.3.17)

where \(P_{ld}^D\) and \(P_{lc}^C\) are the power losses for the dielectric insert and cavity respectively.

Normalizing the fields such that \(H_{11} = H_{22} = 1\), one can express the quality factor given by (6.3.7) for the coupled system as
\[ Q = \frac{\omega}{|a_1|^2 \omega_1 + |b_2|^2 \omega_2}. \quad (6.3.18) \]

Here

\[ Q_d = \frac{\omega_1}{2P_{ld}}, \quad (6.3.19) \]
\[ Q_c = \frac{\omega_2}{2P_{lc}}, \quad (6.3.20) \]

and the total loss is

\[ P_l = \frac{1}{2} \left( \frac{\omega_1 |a_1|^2}{Q_d} + \frac{\omega_2 |a_2|^2}{Q_d} \right). \quad (6.3.21) \]

For the synchronous case, \( \omega_1 = \omega_2 = \omega_0 \) and \( |a_1| = |a_2| = |b_1| = |b_2| = 1/\sqrt{2} \), the quality factors of the coupled modes are written as

\[ Q^{++} = 2\sqrt{1-|\kappa|} \frac{Q_d Q_c}{Q_d + Q_c}, \quad \text{and} \]
\[ Q^{+-} = 2\sqrt{1+|\kappa|} \frac{Q_d Q_c}{Q_d + Q_c}. \quad (6.3.23) \]

Where \( Q^{++} \) and \( Q^{+-} \) are the \( Q \) factors for the symmetric and anti-symmetric modes respectively. From the above equations it is clear that the two values are not equal. The difference between them is equal to

\[ Q^{+-} - Q^{++} \approx 2|\kappa| \frac{Q_d Q_c}{Q_d + Q_c}. \quad (6.3.24) \]
6.3.3 Filling factor

The filling factor $\eta$ is a measure of the compactness of the magnetic field. It is equal to

\[ \eta = \frac{\int_{V_{\text{sample}}} |H_\perp|^2 \, dv}{\int_{V_{\text{cavity}}} |\vec{H}|^2 \, dv}. \]  \hspace{1cm} (6.3.25)

Here $|H_\perp|$ is the magnetic field intensity perpendicular to the static magnetic field. Using similar arguments to those of the previous subsection, one can find out that when the fields are normalized ($H_{11} = H_{22}$), the filling factor for the coupled system is expressed in terms of the uncoupled ones as

\[ \eta = |a_1|^2 \eta_1 + |a_2|^2 \eta_2 + 2a_1 a_2 \int_{V_{\text{sample}}} \mu_0 \vec{H}_1 \cdot \vec{H}_2 \, dv \]

\[ \approx |a_1|^2 \eta_1 + |a_2|^2 \eta_2. \]  \hspace{1cm} (6.3.26)

For the synchronous case the filling factor is equal to the average of both filling factors,

\[ \eta = \frac{1}{2}(\eta_1 + \eta_2). \]  \hspace{1cm} (6.3.27)

This is a direct consequence of the fact that when the two uncoupled modes have equal frequencies, the resulting coupled modes have equal contributions from the uncoupled modes.

6.4 Results and Discussions

In this section the formulae derived in the previous section are applied to type A and type B resonators when inserted in a cylindrical cavity. The dielectric resonator is
operating in the $TE_{010}$ mode and the cavity is resonating in its $TE_{011}$ mode. As inferred from equation (6.3.4), the coupling coefficient is related to the relative permittivity and areas by

$$\kappa \propto \sqrt{\epsilon_r \frac{A_D}{A_C}}. \quad (6.4.1)$$

This suggests that $\left(\frac{\kappa_{\epsilon_r=30}}{\kappa_{\epsilon_r=261}}\right) \approx 4$ to $5$. In fact the actual ratio is even higher since in (6.4.1) all other parameters were assumed to be fixed which is not true.

It is interesting to compare the values of the coupling coefficient, $\kappa$, to those computed using the circuit model proposed in [6]. Analyzing the circuit model, the coupling coefficient, named hereafter $\kappa'$ to distinguish it from the one given by equation (6.3.4), is found to be

$$\kappa' = \omega_1 \omega_2 \sqrt{L_C C_{cc} L_D C_{cc}}, \quad (6.4.2)$$

where $L_C$, $L_D$ are the cavity and dielectric inductance respectively while $C_{cc}$ is the coupling capacitance. In deriving the above equation, reasonable approximations were assumed; $C_{cc} \ll C_C, C_D$, $L_C |_{C_{cc}} C_{cc} \ll \frac{1}{\omega_1^2}$, $C_{cc} \ll \frac{1}{\omega_2^2}$. The exact expressions for these lumped circuit parameters are defined in [6]. Noting that

$$\omega_1^2 = \frac{1}{L_D C_D}, \quad \omega_2^2 = \frac{1}{L_C C_C}, \quad (6.4.3)$$

equation (6.4.2) can be written as

$$\kappa' = \frac{C_{cc}}{\sqrt{C_D C_C}}. \quad (6.4.4)$$

By using the formulae defined for $C_{cc}$, $C_D$ and $C_C$ [6], one gets
\[ \kappa' = 2 \frac{1}{\sqrt{2\varepsilon_r \beta C}} \sqrt{2(\beta l'_D + \sin \beta l'_D)}. \]  

Equation (6.4.5) is different from the one derived using ECMT. The main difference is the absence of the explicit dependence on the area overlap \( A_D/A_C \) and provided all other parameters are fixed, \( \kappa' \) is inversely proportional to \( \sqrt{\varepsilon_r} \) rather than directly proportional as equation (6.4.1) suggests. Type B resonator is inserted in a cavity \( (d_C = l_C = 4.1598 \text{ cm}, f_{TE_{011}} = 9.5 \text{ GHz}) \) and the coupling coefficients \( \kappa \) and \( \kappa' \) are calculated using equations (6.3.4) and (6.4.5) respectively. The \( \beta \) parameter is the wave number along the z-axis inside the dielectric material and it can be determined by solving the transcendental equation \([11, 14]\)

\[ \tan \left( \frac{\beta l}{2} \right) = \frac{\alpha}{\beta}. \]  

(6.4.6)

Here \( \alpha \) is the attenuation in free space and it is equal to \( \alpha = \sqrt{\frac{2.405}{r_D}} - k_0^2 \). The coupling coefficients \( \kappa \) and \( \kappa' \) are plotted against the dimensions of the dielectric resonators which are changed over the interval \( (d_D = l_D = 1.3 - 2.1 \text{ mm}) \). The results are depicted in Figure 6-2.
Figure 6-2. Coupling coefficient using ECMT and the lumped circuit model. The cavity has a fixed dimension of \( d=l=4.1598 \) cm and the dielectric resonator has a high relative permittivity of 261 and its dimension was allowed to change.

It is clear from Figure 6-2 that the values of the coupling coefficients calculated using both methods are close in value around the synchronous condition \( (l_D \approx 1.7 – 1.9 \text{ mm}) \). However, the coupling coefficient calculated using ECMT spans a larger range. The symmetric and anti-symmetric frequencies were calculated for both methods (ECMT and Lumped Circuit Model) and the error, compared to ANSOFT simulations, are shown in Figure 6-3.
Figure 6-3. The error in the frequencies of the coupled modes for both ECMT and the lumped circuit model. The frequency values were compared to the full-wave finite elements simulations.

Energy Coupled Mode Theory gives slightly better results when compared to the lumped circuit model especially when the frequencies of the two uncoupled modes are not close to one another. Such observation can be correlated to the difference between the coupling coefficients depicted in Figure 6-2.

Previously, ECMT and the lumped circuit model were solved for type A resonator and the cavity’s diameter was allowed to change from 2.5 cm to 5.4 cm [5]. It was shown that ECMT gives slightly better error curves. In the current article, the coupling coefficients for this last scenario are calculated and plotted in Figure 6-4.
Figure 6-4 illustrates that the coupling coefficient for type A resonators is an order of magnitude higher than that shown in Figure 6-2. This is attributed to the increase in the overlap area. Again, the calculated coupling coefficients $\kappa$ and $\kappa'$ using both methods, are close in value when the resonators are near synchronization. Consequently, one can argue that the lumped circuit model can predict the system behavior efficiently especially when the two resonators are synchronized.

The high values for the coupling coefficients calculated in the current paper explain why the anti-mode in the case of a shield $(\omega_2 >> \omega_1)$ has a significant dielectric component for type A dielectrics [5]. Figure 6-5 illustrates how the ratio $\lambda = (a_2/a_1)^2$ behaves with respect to the square of the ratio of the two uncoupled frequencies $\gamma^2 = (\omega_1/\omega_2)^2$ for different coupling coefficient values.
Figure 6-5. The ratio $\lambda = \left( \frac{a_2}{a_1} \right)^2$ plotted versus the ratio $\gamma^2 = \left( \frac{\omega_1}{\omega_2} \right)^2$ for different $\kappa$ values.

Figure 6-5 clearly shows that when coupling increases the modes tend to stay coupled especially for large coupling coefficient values. This is best observed in the anti-symmetric mode $(\gamma^2 < 1)$.

The quality factor together with the coupling coefficient determines whether the coupled modes overlap or not. The quality factor was calculated in the previous section. To test the validity of the quality factor expression for the coupled system, given by equation (6.3.18), one can start by applying it to type B resonators inserted in a cavity $(d_C = l_C = 4.1598 \text{ cm}, f_{TE_{01}} = 9.5 \text{ GHz})$. The cavity is silver plate and hence its quality factor is approximately 32,000, while the dielectric material has a loss tangent of $7.5 \times 10^{-4}$ ($Q = 1333.3$) [6]. The obtained values are then compared to those obtained using HFSS finite elements simulator as shown in Figure 6-6.
Figure 6-6. Quality factor for type B resonators inserted in a silver-plated cavity

\[ d_C = l_C = 4.1598 \text{ cm}, f_{\text{TE}_{011}} = 9.5 \text{ GHz}, Q = 32,000. \]  

The resonators’ dimensions were allowed to change from \( D = 1.3 - 2.1 \text{ mm} \) and have a loss tangent of \( \tan \delta = 7.5 \times 10^{-4} \).

From Figure 6-6 one can notice that when the two modes are synchronous, the quality factor of the coupled structure decreases significantly compared to that of the empty cavity. Although the high dielectric constant increases the filling factor (fields compactness), this comes out at the expense of lowering the quality factor. Consequently by returning to equation (6.1.1) one can write the ratio of signal intensities of the coupled structure to that of an empty cavity as (provided that the power is kept constant)

\[
\frac{S_{\text{with insert}}}{S_{\text{empty}}} = \frac{\eta_{\text{with insert}}}{\eta_{\text{empty}}} \times \frac{Q_{\text{with insert}}}{Q_{\text{empty}}}. \tag{6.4.7}
\]

From equation (6.4.7) it is clear that if the dielectric material is highly lossy (low \( Q \)-value), the signal intensity may deteriorate rather than get enhanced after inserting the dielectric material. It is worth to notice that when there is a large difference between
\(Q_1\) and \(Q_2\) equations (6.3.22) and (6.3.23) predict that the quality factor at synchronous is approximately equal to \(2 \times \min(Q_1, Q_2)\). Indeed for the case in hand and from Figure 6-6, the synchronous condition occurs when \(l_D = 1.75\) mm where the calculated average \(Q\) for the two modes is found to be 2600 which is approximately equal to double the value of the minimum quality \((Q_{\text{min}} = Q_1 = 1333.3)\).

The above procedures are repeated but the dielectric loss tangent is decreased to \(\tan \delta = 10^{-6}\) which means that the dielectric quality factor is tremendously high \((Q \approx 10^6)\). The results are shown in Figure 6-7.

![Figure 6-7. Quality factor for type B resonators inserted in a silver-plated cavity](image)

\(d_C = l_C = 4.1598\) cm, \(f_{TE011} = 9.5\) GHz, \(Q \approx 32,000\). The resonators’ dimensions were allowed to change from \(l_D = 1.3 - 2.1\) mm and have a loss tangent of \(\tan \delta = 10^{-6}\).

Again, from Figure 6-7, the quality factor at the synchronous condition is approximately double the minimum uncoupled quality factor. In this case the minimum

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quality factor is that of the cavity alone. In this situation both ratio terms in the right hand side of equation (6.4.7) is going to increase, hence increasing the signal intensity over that of the empty cavity.

Applying formulae (6.3.22),(6.3.23) and (6.3.27) to (6.4.7), one can determine an expression for the signal enhancement in terms of the uncoupled parameters,

\[
\frac{S_{\text{with insert}}}{S_{\text{cavity}}} \approx \frac{\eta_1}{\eta_2} \times \frac{Q_1}{Q_1 + Q_2}.
\]  

(6.4.8)

From which it can be deduced that for a high loss dielectric material \( Q_1 << Q_2 \), the signal enhancement ratio is

\[
\frac{S_{\text{with insert}}}{S_{\text{cavity}}} \approx \frac{\eta_1}{\eta_2} \times \frac{Q_1}{Q_2}.
\]  

(6.4.9)

While for a low loss dielectric material \( Q_1 >> Q_2 \) the signal enhancement ratio is dictated by the dielectric alone

\[
\frac{S_{\text{with insert}}}{S_{\text{cavity}}} \approx \frac{\eta_1}{\eta_2}.
\]  

(6.4.10)

When the coupling coefficient \( \kappa \) is high as for type A resonators, the approximate equation (6.3.18) is only accurate around the synchronous condition. Therefore one need to apply the general expressions (6.3.12), (6.3.13) and (6.3.14). The reason behind this is that the overlap terms which were neglected in the derivation of expression (6.3.18) are no longer small. However using the general expressions, ECMT can still be used to give very accurate values for the quality factors. Indeed, for type A resonator, the cavity dimensions were allowed to change from 3.4 cm to 5.4 cm. This corresponds to a span
of $\pm2$ GHz around the synchronous condition ($f \approx 9.7$ GHz). The results were compared to those simulated using HFSS as shown in Figure 6-8.

As shown in Figure 6-8, the tendency of the coupled modes for type A resonator to decouple is lower than that of type B resonators. This can be attributed to the larger coupling coefficient. Figure 6-8 also illustrates that the tendency of the anti-mode to decouple is much lower than that of the symmetric one. Consequently this observation corroborates with the findings of [5] and Figure 6-5.

One might be interested in exciting only one of the coupled modes (either the symmetric or anti-symmetric). Therefore, it is vital to measure how well the two modes are separated. One such measure is to find the ratio of the difference between the two coupled frequencies versus the average bandwidth or
\[ \Phi = \frac{f_{\text{anti}} - f_{\text{sym}}}{0.5(BW_{\text{sym}} + BW_{\text{anti}})}. \]  

(6.4.11)

The minimum separation distance between the coupled modes occurs when the two modes are synchronous (at which both modes deviate the most from the uncoupled ones). Noting that \( BW = f / Q \), one can find that \( \Phi \) can be expressed as

\[ \Phi = 2\kappa \frac{Q_d Q_c}{Q_d + Q_c}. \]  

(6.4.12)

For type \( B \) ferroelectric resonators when the dielectric loss tangent is \( 7.5 \times 10^{-4} \), \( \Phi \) is found to be \( \approx 62 \). For type \( A \) resonators with the same loss tangent of \( 7.5 \times 10^{-4} \), \( \Phi \) is approximately 375. For practical ceramic type \( A \) resonators the loss tangent may be an order magnitude less and hence \( \Phi \) increases. For both types of resonators the two modes are well separated. However, as the permittivity increases, the coupling coefficient decreases according to equation (6.3.4)\(^1\). Hence if the quality factor is not large enough, the two modes may overlap.

### 6.5 Summary and Conclusions

Using ECMT, expressions for the coupling coefficient \( \kappa \), the quality factors \( Q \), and the filling factors \( \eta \) for a cavity with a dielectric insert were obtained. The coupling

\(^1\) This is because for very high dielectric constants, the dielectric resonator has to be smaller to have the same resonant frequency and hence its cross sectional area decreases.
The coupling coefficient was found to be proportional to the square root of the relative permittivity as well as to the overlap area. The coupling coefficients calculated using ECMT were compared to those derived using the circuit model proposed in [6]. It was found that both methods give close values when the uncoupled frequencies were close. However, the coupling coefficient calculated using ECMT spans a larger range of values. ECMT is shown to give slightly better results. The coupling coefficient of a cavity with a dielectric resonator having a moderately high relative permittivity \( \varepsilon_r \approx 30 \) was shown to be an order of magnitude higher than that of resonators having a very high relative permittivity \( \varepsilon_r \approx 261 \). Consequently, it was inferred that this is due to the increase in the overlap area. The high values of the coupling coefficient, especially when \( \varepsilon_r \) is relatively low and the cavity is small, explain why the anti-mode in the case of a shield \( (\omega_2 >> \omega_1) \) has a significant dielectric component.

A formula for the quality factor of the coupled system was derived. It was shown that the quality factor depends on the eigenvectors, uncoupled frequencies and the uncoupled quality factors. The formula was applied to a resonator with a high dielectric constant resonator with different loss tangents (\( \tan \delta = 7.5 \times 10^{-4} \) and \( 10^{-6} \)). Comparing the values found to those of HFSS, gives an excellent agreement. It was noticed that when the two uncoupled resonators have the same frequency (synchronous condition), the quality factors of the symmetric and anti-symmetric modes are slightly different. This observation was verified using HFSS and corroborates with the findings of [6]. It is observed that when the quality factor of the dielectric resonator is much smaller than that of the cavity, the coupled quality factors decrease significantly compared to that of the
empty cavity. It was shown that in general the quality factor at the synchronous condition is approximately equal to double the minimum of $Q_1$ and $Q_2$ provided there is a large difference between the two values.

A simple expression for the filling factor of the coupled system was derived. It was shown that the filling factor is the average of the two uncoupled modes when the resonators are synchronous.

An expression for the signal enhancement ratio (compared to the empty cavity signal intensity) was found. For low loss resonators the signal enhancement ratio is proportional to the ratio of the filling factors. However, when the dielectric insert is lossy, both the uncoupled quality and filling factors are needed to estimate the signal enhancement.

For relatively moderate dielectric inserts ($\varepsilon_r \approx 30$), the overlap integral must be taken into account when calculating the quality factors. It was argued that this is due to the high value of the coupling coefficient. However, ECMT is still capable of calculating the quality factors especially near the synchronous condition.

The separation between the modes compared to the average bandwidth was calculated for the two types of dielectric resonators. It was shown that the separation between the frequencies of the two coupled modes is significantly greater than five times the average bandwidth. Consequently, exciting one coupled mode will probably not excite the other one. However as the permittivity increases, the coupling coefficient decreases and if the quality factor of the dielectric insert is not large enough the two modes may overlap.
It is conjectured that the findings here can be directly applied to the case of a loop-gap inserted in a cavity. The results and conclusions of this article suggest that if an effective EPR probe is to be designed, one needs to evaluate the different parameters and how they relate. As was shown, a high filling factor dielectric insert with low $Q$ may negatively affect the signal enhancement. For extremely high loss dielectric loss tangents and/or for lossy samples, the coupled modes may overlap (the two modes are separated by less than their average bandwidth). Therefore, the current research suggests that optimization procedures may be needed for the design of an efficient probe. ECMT was capable of finding expressions for the signal enhancement ratio. Thus one can argue that ECMT can be used to find expressions for parameters which depend on the fields’ distribution. One such crucial parameter in the field of EPR spectroscopy is the resonator efficiency which depends on the filling and the quality factors [6]. In unsaturated EPR sample the ratio of signal intensities is proportional to square the ratio of the resonator efficiencies. Finding expressions for the resonator efficiency is crucial for better probe design whether it is the signal intensity of a cavity that needs to be improved using an insert, or a dielectric resonator that needs a suitable enclosing shield.

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References and Notes


7 Electron Paramagnetic resonance probe design based on the lambda efficiency parameter

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The candidate made the mathematical derivations and processed the computational and numerical calculations in this publication, worked in collaboration with Dr. Mattar to interpret the results and with Dr. Mattar and Dr. Tervo to publish the manuscript.

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Abstract

Expressions are obtained for the lambda efficiency of a system composed of a cavity with a dielectric insert in terms of those of the uncoupled ones. Two important design problems are studied. Given a certain cavity, it is shown that lambda will be close to that of the dielectric insert whenever the cavity acts as a shield. Working near synchronization (at which both modes have the same resonant frequency) where the coupled fields have contributions of those of the cavity and the insert is also discussed. Generally if the cavity is lossy, it is shown that the exact value of the dielectric quality factor is irrelevant as long as it is large compared to that of the cavity. Thus the insert which has the highest free space filling factor will lead to the best coupled lambda efficiency. However for low loss cavities, it is shown that one should pick the insert which has the highest free space lambda efficiency regardless of its filling factor. Given a certain dielectric resonator, it is proven that for high loss dielectric inserts the shield can boost the lambda efficiency over the free space value. This can be very helpful for relatively low efficiency dielectrics as well as lossy samples such as polarized liquids. It is argued that a system consisting of different open structures (loop-gap, dielectric and split-ring resonators) may be used in a way such that their $B_1$ values collaborate and hence increase the lambda efficiency of the combined structure.
7.1 Introduction

A loop-gap or a dielectric material inserted in a cavity is proven to provide a significant enhancement to the signal intensity for electron paramagnetic resonance (EPR) spectroscopy [1-4]. Usually the size of the insert is much smaller than that of the cavity. Consequently this implies that the filling factor of the coupled structure increases due to the concentration of the magnetic field in the insert [1]. The exchange between the insert and cavity modes is at a maximum when the frequency of the insert mode is close to that of the cavity mode [5]. This situation (hereafter called the synchronous condition) was proven to be very helpful if the signal intensity of a standard conventional cavity needs to be improved without modifying the coupling to the microwave bridge [1]. However if signal enhancement is of higher priority, the inserts should be housed in a small shield instead [2, 6]. In the latter case, unless the shield is very tight, coupling to the microwave bridge through an iris may be difficult due to the diminishing fields’ values at the shield surface [6]. Stacking two dielectric resonators inserted in a cavity gives the user the extra ability to tune the frequency of the cavity beside the signal intensity improvement [3, 7-8].

The signal intensity of an EPR probe is proportional to the resonator’s parameters [1, 9-10]

\[ S \propto \eta Q P^{1/2} \]  \hspace{1cm} (7.1.1)

Here \( S \) is the signal intensity, \( \eta \) is the resonator filling factor [10], \( Q \) is the resonator quality factor and \( P \) is the incident power. Although the insert leads to an increase in the filling factor, the quality factor of a lossy insert may be low in such a way that the signal intensity may not be significantly improved [1, 6]. For lossy inserts, an expression for
the signal intensity enhancement was derived [11]. Namely the signal enhancement with respect to the empty cavity was found to be

\[ \frac{S_{\text{with insert}}}{S_{\text{cavity}}} \approx \frac{\eta_1}{\eta_2} \times \frac{Q_1}{Q_2}. \]  

(7.1.2)

Here the subscripts “1” and “2” correspond to the insert and cavity modes respectively.

For low loss insert, the signal enhancement can be written as [11]

\[ \frac{S_{\text{with insert}}}{S_{\text{cavity}}} \approx \frac{\eta_1}{\eta_2}. \]  

(7.1.3)

In another words for a low loss insert, the signal enhancement is proportional to the ratio of the filling factors. Usually for a lossy insert it is better to express the signal enhancement in terms of the lambda efficiencies [6, 10]

\[ \frac{S_{\text{with insert}}}{S_{\text{cavity}}} \approx \Lambda_{\text{with insert}}^2 \Lambda_{\text{cavity}}^2. \]  

(7.1.4)

The lambda efficiency \( \Lambda \) is defined as [6]

\[ \Lambda = \frac{B_m}{2\sqrt{P}}, \]  

(7.1.5)

where \( B_m \) is the magnetic field density at the sample.

Generally, the lambda efficiency is crucial in understanding the properties of EPR resonators. The coupling between the \( TE_{01\delta} \) dielectric mode and the \( TE_{011} \) cavity mode was studied in [6] using a lumped circuit model where the lambda efficiency and other important parameters were calculated. It was inferred that the lambda efficiency of the coupled system is close in value to that of the insert (dielectric insert in this case). It was
also shown that when the two resonators are synchronous the lambda efficiency of the coupled system is approximately 98.5% of that of the dielectric resonator in free space.

The current authors used energy coupled mode theory formalism (ECMT) [12] to study how the two resonators (dielectric insert and enclosing cavity) interact [5]. In fact, ECMT was able to predict and calculate the frequencies and eigenvectors of the coupled modes [5]. Expressions for the coupling coefficient, quality and filling factors of the coupled system were determined [11]. As was shown, the quality and filling factors change tremendously depending on the frequency separation between the two uncoupled modes [6, 11]. Therefore, to design an effective probe, an optimum configuration, taking care of all constraints, is necessary.

The aim of the current paper is to derive expressions for the lambda efficiency of the coupled system in terms of those of the uncoupled ones. Two important design problems are considered. The first one deals with the selection of an appropriate insert for a given cavity, while the second problem deals with the design of an optimal shield to house a given insert.

Section 7.2 defines the system and the problem in a concise sense where properties such as the eigen-frequencies, eigenvectors and the electric fields are shown. Expressions for the coupling coefficient, quality and filling factors are presented. Section 7.3 constitutes the main core needed to study the system. In this section, expressions for the lambda efficiency of the coupled system are derived. Section 7.4 applies the results obtained to different scenarios. The results are verified using finite element simulation. Conclusions and discussions are provided in section 7.5.


7.2 Problem description

Although a loop-gap can be used, the discussion hereafter will be restricted to the case of a dielectric insert. However it is conjectured that the analysis is valid for other open structure resonators such as loop-gaps and split-rings. The system studied here is shown in Figure 7-1. It consists of a dielectric resonator inserted in the center of a cylindrical cavity. The holder, not shown in the figure, is of a material with low loss and low permittivity so its effect is negligible.

![Figure 7-1. System structure of a dielectric resonator inserted in a conducting cavity. The dielectric insert is held inside a hollow low loss/low permittivity holder (not shown).](image)

The two modes of interest are the dielectric $TE_{01\delta}$ mode and the cavity $TE_{011}$ mode.

Energy Coupled Mode theory is an eigenvalue equation which can be written as

\[ U \lambda = \omega^2 a, \]  

\[ U = (H^{-1}D^\dagger \Omega) \] is the polarization operator,
\[ \mathbf{V} = (\mathbf{G}^{-1} \boldsymbol{\Omega} \mathbf{D}) \] is the free-space operator, \hspace{1cm} (7.2.3)

where

\[ H_{ik} = \int_{V} \varepsilon E_i^* \cdot \overline{E}_k \, dv, \] \hspace{1cm} (7.2.4)

\[ G_{ik} = \int_{V} \mu H_i^* \cdot \overline{H}_k \, dv, \] \hspace{1cm} (7.2.5)

\[ D_{ik} = \int_{V} \varepsilon_j E_i^* \cdot \overline{E}_k \, dv, \] \hspace{1cm} (7.2.6)

and

\[ \boldsymbol{\Omega} \equiv \Omega_{mn} = [\omega_1 \omega_2 \ldots \omega_n] \mathbf{I} = \begin{pmatrix} \omega_1 & 0 & \cdots & 0 \\ 0 & \omega_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \omega_n \end{pmatrix}, \] \hspace{1cm} (7.2.7)

where \( \overline{H}_i \) and \( \overline{E}_i \) are the magnetic and the electric fields of the \( i^{th} \) resonator respectively.

The system of equations (7.2.1), (7.2.2) and (7.2.3) were solved for the case in hand where the coupling coefficient (\( \kappa \)), eigenvalues (\( \omega \)) and the eigenvectors (\( a_i^{++}, a_i^{+-} \)) were found to be [5]

\[ \kappa = \frac{Y_{12}}{\sqrt{H_{11} H_{22}}}, \] \hspace{1cm} (7.2.8)

\[ Y_{12} = \varepsilon_0 (\varepsilon_r - 1) \int_{DR} \overline{E}_1^* \cdot \overline{E}_2 \, dv, \]

\[ \omega^2 = \frac{\alpha_1^2 + \alpha_2^2}{2} \pm \sqrt{\left(\frac{\alpha_1^2 - \alpha_2^2}{2}\right)^2 + \alpha_1^2 \alpha_2^2 \kappa^2}, \] \hspace{1cm} (7.2.9)

\[ a_2^{++} = \left( \frac{1}{2\kappa} (\gamma^2 - 1) + \frac{1}{\sqrt{4\kappa^2 (\gamma^2 - 1)^2 + \gamma^2}} \right) a_1^{++}, \] \hspace{1cm} (7.2.10)
for the symmetric mode and

\[ a_2^{+-} = \left( \frac{1}{2\kappa} (\gamma^2 - 1) - \sqrt{\frac{1}{4\kappa^2} (\gamma^2 - 1)^2 + \gamma^2} \right) a_1^{+-} \]  \hspace{1cm} (7.2.11)

for the anti-symmetric case. Here \( \gamma^2 \) is equal to

\[ \gamma^2 = \left( \frac{\omega_1}{\omega_2} \right)^2. \]  \hspace{1cm} (7.2.12)

The quality factor was shown to be a function of the uncoupled quality factors as well as of the eigenvectors [11]. A closed form expression for the quality factor can be written down as

\[ Q = \frac{\omega}{\sqrt{a_1^2 \omega_1^2 + b_1^2 \omega_2^2}} Q_1 \]  \hspace{1cm} (7.2.13)

and the power loss for the coupled structure is found to be

\[ P_l = \frac{1}{2} \left( \frac{\omega_1 |a_1|^2}{Q_1} + \frac{\omega_2 |a_2|^2}{Q_2} \right). \]  \hspace{1cm} (7.2.14)

Similarly, the filling factor for the coupled system can be written as

\[ \eta = |a_1|^2 \eta_1 + |a_2|^2 \eta_2 \]  \hspace{1cm} (7.2.15)

### 7.3 Analysis

Equipped with the findings presented in the previous section, one can start by finding expressions for the lambda efficiency of the coupled system. Noting that

\[ B = b_1 B_1 + b_2 B_2, \]  \hspace{1cm} (7.3.1)
the lambda efficiency $\Lambda$ can be written as

$$\Lambda = \frac{|b_1 B_{1m} + b_2 B_{2m}|}{2\sqrt{P_i}}.$$  \hfill (7.3.2)

Here $P_i$ is given by equation (7.2.14)$^2$. The variables $B_{1m}$ and $B_{2m}$ are the maximum magnetic field density of the dielectric resonator and cavity respectively. Using algebraic manipulation, the lambda efficiency of the coupled system can be related to the lambda efficiency of the uncoupled system as

$$\Lambda = \frac{1}{\sqrt{1 + \zeta^2}} |\Lambda_1 + \zeta \Lambda_2|,$$  \hfill (7.3.3)

where $\Lambda_1$ and $\Lambda_2$ are the dielectric and cavity lambda efficiencies respectively while $\zeta$ is equal to

$$\zeta = \frac{a_2}{a_1} \left( \frac{Q_1}{Q_2} \times \frac{\alpha_2}{\alpha_1} \right)^{1/2}.$$  \hfill (7.3.4)

In deriving relation (7.3.3) it was assumed that $b_j \approx a_j$.

When the two resonators are synchronous, $a_i = \pm a_2$ and $P_i = 0.5 / (P_{i1} + P_{i2})$

therefore, equation (7.3.2) is reduced to

$$\Lambda = \frac{|B_{1m}|}{2\sqrt{P_{i1} + P_{i2}}} \pm \frac{|B_{2m}|}{2\sqrt{P_{i1} + P_{i2}}}.$$  \hfill (7.3.5)

---

$^2$ $P_i$ is equal to the supplied power $P$ in steady state.
7.4 Results and Discussions

In this section the formulae derived in the previous section will be applied to different schemes. First the lambda efficiency is calculated for the system previously studied in [5, 11]. Specifically, the dielectric resonator has the following properties: \( \varepsilon_r = 261, f_{TE_{01,\delta}} = 9.5 \text{ GHz} \), the aspect ratio (diameter to height) is one, the diameter and height are allowed to change from 1.3 to 2.1 mm and the dielectric loss tangent is \( 7.5 \times 10^{-4} \) \( (Q = 1333.33) \). The cavity is silver coated with the properties: diameter and height are equal to 4.1598 cm, \( f_{TE_{01}} = 9.5 \text{ GHz} \) and \( Q \approx 32,000 \). The calculated lambda efficiency versus dielectric insert diameter is depicted in Figure 7-2.

\[
\Lambda \left( \frac{G}{\sqrt{W}} \right)
\]

![Figure 7-2. \( \Lambda \) of both the symmetric and the anti-symmetric modes of the coupled system of a high dielectric resonator inserted in a silver plated cavity.](image)

\[
\begin{align*}
\Lambda \left( \frac{G}{\sqrt{W}} \right)
\end{align*}
\]
The values of the lambda efficiency calculated using ECMT and depicted in Figure 7-2 are consistent with those obtained previously [6]. Therefore, the formulae derived in the previous section, namely equations (7.3.2) and (7.3.3), can be used to study the behavior of \( \Lambda \) for different scenarios. It is interesting how a coupled-mode formalism, when applied to the case where resonators strongly couple is accurately capable of calculating expressions based on the field distributions. Two important scenarios are discussed in the next two subsections. The first is: given a cavity, one needs to pick a suitable dielectric resonator to enhance the signal intensity. In this case the parameters for the enclosing cavity are fixed. In the second scenario, the dielectric resonator is given and one needs to design the housing shield such that the lambda efficiency is maximized.

7.4.1 Improving the cavity \( \Lambda \) using an insert

In this subsection it is assumed that the cavity has a fixed lambda efficiency \( \Lambda_2 \).

One may be tempted to select a very small dielectric insert. In this case \( \omega_1 \gg \omega_2 \), so the cavity is considered as a large shield. Consequently \( (a_2^{++}/a_1^{++}) \rightarrow \infty \) and \( (a_2^{+-}/a_1^{+-}) \rightarrow 0 \), this leads to

\[
\Lambda^{++} \rightarrow \Lambda_2, \quad \text{(7.4.1)}
\]

and

\[
\Lambda^{+-} = \Lambda_1. \quad \text{(7.4.2)}
\]
A glance at equation (7.4.2) reveals that the anti-symmetric mode has a very high lambda efficiency value provided that a tiny dielectric insert was used. However it is difficult to excite this mode through the cavity iris due to the smallness of the fields near the cavity wall [6]. Therefore a large shield configuration is impractical in this case. Another problem which may arise is that the dielectric mode may couple with higher cavity modes as well. However as was previously discussed, this coupling usually has an insignificant effect [5].

Considering the other extreme condition, a large insert where \( \omega_1 \ll \omega_2 \). In this case, the cavity acts as a small shield where this situation \( \left( a_2^+ / a_1^+ \right) \to 0 \) and \( \left( a_2^- / a_1^- \right) \to \infty \) thus

\[
\Lambda^{++} \to \Lambda_1, \tag{7.4.3}
\]

and

\[
\Lambda^{+-} \to \Lambda_2. \tag{7.4.4}
\]

Equation (7.4.3) shows that the symmetric mode tends to the dielectric one. This was previously observed based on the coupled fields [5]. Depending on the insert size this mode may be easily coupled to the microwave bridge. However for a given material, as one increases the insert size, the lambda efficiency decreases. Figure 7-2 illustrates this behavior where it is shown that, when the dielectric dimensions increase, the lambda efficiency of the symmetric mode monotonically decreases after it reaches its maximum value. Therefore, one may need to work near synchronization \( \omega_1 \approx \omega_2 \) where the symmetric mode attains its maximum. Near synchronization, the fields are mixes of both
the cavity and insert fields. This means that coupling to the microwave bridge can be easily achieved through the cavity iris.

By noting that near synchronization $\gamma^2$ can be approximated by $1 + \frac{2(\omega_1 - \omega_2)}{\omega_2}$, the ratio $a_2/a_1$ is found to be

$$\frac{a_2}{a_1} = 1 \pm \left( \frac{1 \pm \kappa}{\kappa} \right) \frac{\omega_1 - \omega_2}{\omega_2}. \quad (7.4.5)$$

Here the plus sign corresponds to the symmetric mode and the negative sign is taken for the anti-symmetric one. For the symmetric mode and assuming that the coupling coefficient $\kappa$ is approximately constant, one can substitute (7.4.5) back in the lambda efficiency expression (7.3.3), to find an expression for $\Lambda$ as a function of $\gamma$ and $Q_1/Q_2$.

If the lambda efficiency of the insert is assumed to be constant and equal to its value at the synchronous condition (for instance, $40 \text{ G/} \sqrt{\text{W}}$ for the dielectric resonator shown in Figure 7.2), a three-dimensional plot of the ratio $\Lambda_1/\Lambda_2$ is obtained. Two resonators; one with a relatively high lambda efficiency ($\Lambda_1 \approx 23 \text{ G/} \sqrt{\text{W}}$) and the other with a low lambda efficiency ($\Lambda_1 \approx 4 \text{ G/} \sqrt{\text{W}}$) are inserted in a cavity which has a typical lambda efficiency value of $2 \text{ G/} \sqrt{\text{W}}$. Figure 7.3 depicts the change in the lambda efficiency around the synchronous condition as a function of the relative frequency $\gamma$ and the relative quality factor $Q_1/Q_2$. 

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Figure 7-3. The normalized lambda efficiency as a function of the relative frequency and the relative quality factor.

From Figure 7-3 it is noticed that as the ratio $Q_1/Q_2$ decreases, the lambda efficiency of the coupled system approaches the dielectric insert lambda efficiency. However, if the cavity quality factor is low ($Q_1 \gg Q_2$), the coupled efficiency is much smaller than that of the dielectric resonator. Accordingly, one can conclude that: given a specific cavity, a dielectric insert with a high lambda efficiency and relatively low quality factor will increase the lambda efficiency of the coupled system up to that of the insert in free space. The ferroelectric resonator used in [6] satisfies these requirements ($\Lambda_1 \approx 40 \frac{G}{\sqrt{W}}, Q \approx 1333$). Figure 7-4 illustrates how this resonator behaves near the synchronous condition.
Figure 7-4. The normalized lambda efficiency as a function of the relative frequency and the relative quality factor for a ferroelectric resonator.

As shown in Figure 7-4, whenever \( Q_1 << Q_2 \) the lambda efficiency of the coupled system is approximately equal to that of the dielectric resonator in free space \( (\Lambda_1) \).

Figure 7-4 also shows that for a lossy cavity \( (Q_1 >> Q_2) \), the dielectric insert will slightly improve the lambda efficiency compared to that of the dielectric resonator. In this case, knowing that \( \xi = \sqrt{Q_1/Q_2} \), which reduces equation (7.3.3) to

\[
\Lambda \approx \frac{\Lambda_1}{\xi} + \Lambda_2.
\]  

(7.4.6)

For a lossy cavity \( \Lambda_2 \) is very small, therefore
Equation (7.4.7) says that as long as $Q_1 >> Q_2$, the lambda efficiency can be controlled by the dielectric resonator compactness represented by $B_{lm}^3$. The maximum value $B_{lm}$ depends on the dielectric constant and the resonator’s dimensions (filling factor). Thus regardless of the exact insert quality factor (as long as $Q_1 >> Q_2$), the signal enhancement is a function of the insert filling factor alone. This result agrees with what was previously derived using the expressions of the filling and quality factors [11]. Therefore for lossy cavities, the main parameter affecting the signal enhancement is the dielectric resonator filling factor and the insert quality factor has an insignificant contribution. While for low loss cavities, the insert’s lambda efficiency has the dominant effect on the signal enhancement.

To verify the above findings, HFSS eigenmodes solver is used to calculate the lambda values for the above two scenarios and the results are depicted in table 1.

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3 This is because the fields are normalized ($W_{E}^{(1)} = W_{E}^{(2)}$). So the smaller the dielectric insert the higher is $B_{lm}$. 

215
Table 1 Lambda efficiency for the two scenarios $Q_1 \ll Q_2$ and $Q_2 \ll Q_1$.

<table>
<thead>
<tr>
<th>Cavity Insert</th>
<th>$Q_2 \gg Q_1$</th>
<th>$Q_1 \gg Q_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Q_2 = 30,000, \Lambda_2 = 2.5G/\sqrt{W}$</td>
<td>$Q_2 = 3000, \Lambda_2 = 0.776G/\sqrt{W}$</td>
<td></td>
</tr>
<tr>
<td>$\varepsilon_r$</td>
<td>261</td>
<td>29.2</td>
</tr>
<tr>
<td>$\Lambda_1 (G/\sqrt{W})$</td>
<td>12.65</td>
<td>23</td>
</tr>
<tr>
<td>$Q_1$</td>
<td>133</td>
<td>15,000</td>
</tr>
<tr>
<td>$\Lambda (G/\sqrt{W})$</td>
<td>12.44</td>
<td>20.96</td>
</tr>
</tbody>
</table>

From table 1, it can be seen that when the cavity is of low loss ($Q_2 \gg Q_1$) the resonator which has the highest free space lambda efficiency gives a better coupled lambda efficiency value (21 compared to 12.5) even though its filling factor is lower. On the other hand, for a lossy cavity ($Q_1 \gg Q_2$) the resonator that has the higher filling factor will lead to higher coupled lambda efficiency although it has the lowest free space lambda efficiency.

When the quality factors of the two uncoupled resonators are close in value, $\xi = 1$. Under this condition, equation (1.3.3) is written as

$$\Lambda = \frac{1}{\sqrt{2}} (\Lambda_1 + \Lambda_2).$$

(7.4.8)

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4 For example Murata DRD0600265R®.

5 For example Murata DRD0650288F®.
To verify relation (7.4.8), the HFSS eigenmodes solver is used to calculate the coupled lambda efficiency of the Murata DRD0600265R® resonators ($\Lambda \approx 23 \text{ G/}\sqrt{\text{W}}$) inserted in a 4.1598 cm $\times$ 4.1598 cm cylindrical cavity with $Q_2 = 15,000$. The calculations show that according to (7.4.8) the lambda efficiency is found to be $\approx 18 \text{ G/}\sqrt{\text{W}}$ which is very close to the HFSS result ($18.6 \text{ G/}\sqrt{\text{W}}$). Usually $\Lambda_2 << \Lambda_1$, therefore equation (7.4.8) can be simplified to

$$\Lambda = \frac{1}{\sqrt{2}} \Lambda_1. \quad (7.4.9)$$

From equations (7.4.9) and (7.1.4) it can be inferred that when the two resonators (cavity and dielectric) are synchronous and having the same quality factor, the signal enhancement is half that of the dielectric alone.

### 7.4.2 Designing an enclosing shield for a given dielectric resonator

Given a dielectric resonator with a fixed lambda and quality factor, one needs to design a suitable enclosing shield. The main requirement considered here is to maximize the lambda efficiency of the coupled system. Equation (7.3.3) is solved for different enclosing shield dimensions and the results are reported in Figures 7-5 and 7-6 for typical dielectric materials.
Figure 7-5. Lambda efficiency of a dielectric resonator with $\varepsilon_r = 261, \Lambda = 40$ enclosed in a silver plated shield.

Dielectric Properties

<table>
<thead>
<tr>
<th>Diameter</th>
<th>1.75 mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Height</td>
<td>1.75mm</td>
</tr>
<tr>
<td>$\varepsilon_r$</td>
<td>261</td>
</tr>
<tr>
<td>Q</td>
<td>1333.3</td>
</tr>
<tr>
<td>$\Lambda(\varepsilon/\sqrt{w})$</td>
<td>40</td>
</tr>
</tbody>
</table>

Shield: Silver plated $\sigma = 6.3 \times 10^7$ (S/m)
Radius 1.4-2.75 cm, Height 2.8-5.5 cm.

Figure 7-6. Lambda efficiency of a dielectric resonator with $\varepsilon_r = 29.2, \Lambda = 23$ enclosed in a silver plated shield.

Dielectric Properties

<table>
<thead>
<tr>
<th>Diameter</th>
<th>6.0 mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Height</td>
<td>2.65mm</td>
</tr>
<tr>
<td>$\varepsilon_r$</td>
<td>29.2</td>
</tr>
<tr>
<td>Q</td>
<td>15,000</td>
</tr>
<tr>
<td>$\Lambda(\varepsilon/\sqrt{w})$</td>
<td>23</td>
</tr>
</tbody>
</table>

Shield: Copper $\sigma = 5.8 \times 10^7$ (S/m)
Radius 1.4-2.75 cm, Height 2.8-5.5 cm.
Formulae reported in the literature for the shield’s quality factors, lambda efficiencies and eigen-frequencies were used to obtain the results depicted in Figures 7-5 and 7-6 [6, 13].

Using the previously reported results for high permittivity resonators [6] and Figures 7-2, 7-5 and 7-6, it is noticed that the lambda efficiency asymptotically approaches the dielectric free space value when the shield gets tighter. This is usually the case unless the dielectric is highly lossy or equivalently $Q_i << Q_2$. Indeed in this case the shield can be designed in a way so that it boosts the lambda efficiency. For the synchronous condition this can be explained by returning to equation (7.3.5). From the equation it can inferred that when $P_{11} >> P_{12}$ the lambda factor of the symmetric mode can be written as

$$\Lambda \approx \Lambda_1 + \frac{B_{2m}}{2\sqrt{P_{11}}} - \frac{1}{2} \frac{P_{12}}{P_{11}} \left( \Lambda_1 + \frac{B_{2m}}{2\sqrt{P_{11}}} \right).$$

(7.4.10)

When the net value of the second and third term at the right hand side of equation (7.4.10) is positive, then $\Lambda > \Phi_1$. Using simple algebra one can find the condition when lambda of the coupled system is greater than the dielectric resonator’s free space value to be

$$\frac{B_{2m}}{B_{1m}} > \frac{1}{2(1-\nu)}$$

(7.4.11)

where $\nu = P_{12}/P_{11} = Q_i/Q_2$. Therefore condition (1.4.11) can be approximated to

$$\frac{B_{2m}}{B_{1m}} > \frac{1}{2} \frac{Q_i}{Q_2}.$$
Compared to the dielectric resonator, the fields in the cavity (or shield) are spread over a larger area. Therefore, it is safe to assume that $B_{2m} \ll B_{lm}$. Consequently when $\nu$ is small, the condition (7.4.12) may be met especially if the shield is designed as a long tube. To verify that the cavity can indeed boost the lambda efficiency according to equation (7.4.10) and condition (7.4.12), a structure composed of a long tube shield housing a dielectric resonator with $\varepsilon_r = 20$, is simulated using ECMT and verified using HFSS eigenmodes solver. The lambda efficiency of the coupled system was calculated where the cavity conductivity is allowed to change over orders of magnitude. The system structure and the coupled lambda efficiency are shown in Figure 7-7.

![Figure 7-7. The lambda efficiency of a dielectric inserted in a long shield.](image)

As shown in Figure 7-7, the lambda efficiency of the coupled system is significantly boosted (12.5% more than the free space one). The shield was chosen such...
that the $TE_{011}$ mode has the same frequency of the dielectric $TE_{01\delta}$ mode (11.3 GHz). It is worth noting that this structure is impractical because the quality factors for both the cavity and dielectric are extremely high. However from condition (7.4.12) the ratio $\nu = Q_1/Q_2$ is what really matters.

For low epsilon, high loss resonators or for high lossy samples, optimizing $\Lambda$ can be very important. Such resonators have moderately low lambda efficiency so any boost from the shield is highly appreciated. In the following discussion, the same dielectric resonator utilized in Figure 7-7 is used but with a much lower quality factor ($Q_1 = 1000$). This resonator has a lambda efficiency of $4 G/\sqrt{W}$ (one order of magnitude less than the one shown above). Using HFSS, the lambda factor is calculated where the dielectric resonator was enclosed in a small shield ($Diameter = 2.8\, \text{cm}, Height = 3.5\, \text{cm}, f_{TE_{011}} \approx 13.9\, \text{GHz}$). The value of lambda is found to be $\approx 6.3 G/\sqrt{W}$ at $f^{++} \approx 11\, \text{GHz}$. This means that the shield boosted the efficiency by 58% which is translated into 250% signal enhancement. Using ECMT the lambda efficiency is calculated for different shield dimensions and the results are presented in Figure 7-8.

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6 This is because the signal ratio is proportional to the square of lambda for unsaturated samples.
Figure 7-8. Lambda efficiency for a coupled system consisting of a lossy dielectric resonator and a shield.

Figure 7-8 shows that certain shield dimensions give a boost to the lambda efficiency. One can pick up a point on the hump and calculate the value of lambda. One such point is when the dimensions of the shield are: height = 6 cm, radius = 1.95 cm.

Accordingly, using equation (7.3.3) the value of lambda is found to be $4.57 \, G/\sqrt{W}$. Applying the more accurate expression (7.3.2) one can find that lambda is equal to $5.47 \, G/\sqrt{W}$ at $f^{++} \approx 9.58$ GHz. Using HFSS, the lambda efficiency is found to be $5.35 \, G/\sqrt{W}$ which is very close to the value predicted by ECMT. Thus by careful design, an enhancement in the lambda efficiency can be achieved. In fact for the case in hand, $\Lambda$ has been improved by 35% resulting in 180% in signal intensity enhancement.
compared to the free space value. In this configuration the shield has a $TE_{011}$ frequency of $9.7 \text{ GHz}$. This means that the shield acts as a large shield (i.e., $\omega_1 > \omega_2$) contrary to what was expected. The eigenvector is calculated using ECMT to show that the mode is cavity-like. Indeed if the uncoupled fields are normalized, one can find that $a_2/a_1 \approx 3.7$. Thus, it can be inferred that the mode can be easily excited through an iris. Using HFSS the fields of the coupled structure are shown in Figure 7-9.

$$f \approx 9.58 \text{GHz, } \lambda \approx 5.4 \frac{\text{G}}{\sqrt{\text{W}}}$$

Figure 7-9. Fields for a coupled system consisting of a low lambda, high loss dielectric inserted in a large shield.

Figure 7-9 illustrates how the fields are localized inside the dielectric resonator. It is worth noting that ECMT was unable to accurately estimate the value of lambda for a tight shield. This may be attributed to the effect of the shield wall which was not taken into
account while deriving the ECMT eigenvalue equation. However, it is still capable of finding the coupled frequencies accurately.

### 7.5 Summary and Conclusions

Expressions for the lambda efficiency of a system composed of a cavity with a dielectric insert in terms of those of the uncoupled ones were obtained. Two important design problems are studied. The first one is concerned with the selection of an appropriate insert for a given cavity, while the second problem deals with the design of an optimal shield for a given insert. For the first type of problem it was shown that lambda will be close to that of the dielectric insert when the cavity acts as a shield. However, coupling to the microwave bridge is not guaranteed. Another alternative is by working near the synchronization condition where the fields are still a mix of both the cavity and the insert fields. Consequently, coupling to the microwave bridge can be easily achieved through the cavity iris. If the dielectric insert has a relatively high quality \((Q_1 >> Q_2)\), the insert filling factor plays the main role in the signal enhancement, while the exact value of the quality factor is irrelevant. Therefore for lossy cavities, the insert which has the highest filling factor will result in the highest coupled lambda efficiency. On the other hand, if the cavity has a high quality factor one should pick the resonator which has the highest lambda efficiency regardless of the value of the filling factor (provided that the inequality \(Q_1 << Q_2\) holds).
It was shown that when the two uncoupled systems (dielectric insert and cavity) have the same quality factor, the signal enhancement is half that of the dielectric insert alone.

For the second class of design problems, it was found that the lambda efficiency asymptotically approaches the dielectric free space value when the shield gets tighter. It was shown that for high loss dielectric inserts the shield can boost the lambda efficiency over its free space value. This can be very helpful for relatively low efficiency inserts. Using both ECMT and the HFSS finite element simulator, it was shown that a tight shield can indeed boost the efficiency by 58%. Even for a large shield a boost in efficiency was predicted by ECMT and verified by the HFSS eigenmodes solver. For the latter case, it was shown that the mode is cavity-like. Accordingly, one may infer that this mode can be easily coupled to the microwave bridge through an iris.

The current paper illustrated that a shield can indeed improve the lambda efficiency of the dielectric resonator. From the expressions found here for the lambda efficiency, it can be argued that a system consisting of different open structures (loop-gap, dielectric and split-ring resonators) may be used in a way such that their $\bar{B}_i$ values reinforce each other and hence increase the lambda efficiency of the combined structure.

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References and Notes


8 Coupled Mode Theory in the presence of conductors

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Abstract

The method of images in electromagnetics is used with energy coupled mode
theory to study cases where conducting planes are present. Using the proposed method,
the case where a dielectric resonator inserted in a cavity is brought close to the cavity
wall is analyzed. It is shown that the dielectric resonator couples with its image located
outside the cavity. This results in an anti-symmetric $TE_{01\delta}^{++}$ mode. If the capacitive gap of
a split-ring resonator is brought close to a conducting plane, coupling with the image will
be through the symmetric mode. The case of a dielectric resonator sandwiched between
two conducting planes is also studied. In this case the eigenvalue operator is
approximated by an infinite symmetric tri-diagonal matrix. In addition, the resulting
$TE_{01\delta}^{++}$ mode has an effective coupling coefficient which is double the one obtained
when only one conductor is present. This last observation explains one of the advantages
of putting conducting planes behind the resonant coils in wireless power transfer systems.
8.1 Introduction

Energy Coupled mode theory (ECMT) was proven to be successful in predicting the frequencies, fields, coupling coefficients and quality factors for coupled structures [1-4]. The theory proposes that coupling can be thought of as the interaction between different sources, such as currents and polarization vectors of a resonator with the fields of another resonator [5]. This interpretation of the coupling coefficient between coupled structures helps in constructing a unified framework capable of studying both dielectric and conducting resonators. The coupling between a dielectric resonator and an enclosing cavity was studied in detail [2-3], where the frequencies and fields, predicted by ECMT, agree with both the finite element simulations and other results reported in the literature [6].

The main limitations of ECMT are the restrictions imposed on the boundary conditions. It was shown that as long as the wavelengths of the modes are considerably longer than the resonators’ dimensions, the internal boundaries do not alter the total fields considerably. This is true for most open structure resonators such as dielectrics, loop-gaps, split-rings). For the external boundary (imposed by the enclosing cavity), the open structure resonators have to be far enough from the cavity walls in order that the boundary conditions on the walls are approximately satisfied [1]. These constraints do not play a vital role for the cases studied by the current authors [2-4].

In a previous work it was shown that a system consisting of two dielectrics and a $TE_{102}$ cavity behaves as a coupled system, where the coupling between the two dielectric $TE_{010}$ modes and the $TE_{102}$ cavity mode results in three coupled modes, namely the
$TE^{+++}$, $TE^{++-}$ and $TE^{+-+}$ modes [7]. Finite element simulations illustrated that the frequencies of the last two modes increase abruptly as the two dielectrics approach the cavity walls. In this case, it was also noticed that the fields get smaller inside the dielectric materials. This observation can be attributed to the fact that the dielectric resonator close to the wall is similar to a Hakki-Coleman resonator but with one conducting plane [8]. Thus the boundary of the dielectric resonators can be modeled as both a magnetic and an electric wall at the same time. In other words, the fields approximately vanish on the boundaries. Since the field divergences are finite, the fields values are small inside the dielectric material [7].

Conducting planes were shown to significantly improve the transfer efficiency for wireless power transfer systems [9]. Mid-range wireless power transfer schemes depend on resonant inductive coupling [10-11]. Thus it is important to modify the coupled mode theory so that cases where conducting planes are present can be described by the theory.

The method of images is usually applied to situations which involve conducting surfaces. It is used for charges and antennas [12-15]. The method of images was applied to the case of a rectangular split-ring resonator inside a waveguide [16]. The split-ring showed coupling with image resonators induced by the waveguide walls.

In the current paper an attempt is made to combine the image method with ECMT to study cases where resonators interact with conducting planes [12, 14]. This method is named ECMT-I. Section 8.2 describes how ECMT-I can be applied for different cases. Section 8.3 shows typical cases studied by ECMT-I and verified using finite element simulations. Section 8.4 layouts the main findings of the current research and points to areas that can be explored in the future.
8.2 Analysis

Using the image method, a conducting surface is removed and suitable images are substituted instead. The main requirement is that the images interact with the real resonator to yield a perfectly electric wall at the geometrical loci of the conductor. Figure 8-1 illustrates a typical structure where a dielectric resonator is placed close to a conducting plane (for example, one of the cavity walls).

![Image](image.png)

**Figure 8-1. A typical structure of a dielectric resonator interacting with a conducting plane. (a) shows the original system. (b) illustrates the equivalent structure where the plane is replaced by an equivalent image resonator.**

For the system depicted in Figure 8-1, since the electric field of the $TE_{015}$ mode has to vanish on the surface of the conductor, the two resonators (real + image) are interacting in the anti-symmetric mode. Accordingly one expects that the mode frequency of the system consisting of a dielectric resonator close to a conducting plane is
higher than that of a dielectric in free space. Using coupled mode theory, the frequency is found to be

\[ f^{++} = f_0 \sqrt{1 + \kappa(2s)} . \]  

(8.2.1)

Here \( f^{++} \) is the frequency of the anti-mode, \( f_0 \) is the frequency of the dielectric resonator in free space while \( \kappa(2s) \) is the coupling coefficient at double the distance between the resonator and the conducting plane.

However if a split ring resonator is brought close to a conducting plane as shown in Figure 8-2, the resonators are going to interact in the symmetric mode in order that the tangential component of the electric field vanishes. Thus, the resulting mode has a frequency \( f^{++} \) which is lower than that of the resonator in free space.

\[ f^{++} = f_0 \sqrt{1 - \kappa(2s)} . \]  

This interpretation, based on coupled mode theory, explains why the frequency decreases when the gap of the split-ring is brought close to the waveguide wall [16]. Zhang et al. attributed this to the increase of gap capacitance [16].

Figure 8-2. A split-ring resonator is coupled to its image in the symmetric mode.
When a resonator is inserted between two conducting planes, one gets an infinite number of image resonators [16]. For the case of a dielectric resonator sandwiched between two conducting planes as shown in Figure 8-3, the equivalent coupled mode structure is an array of infinite number of images. Accordingly, the eigenvalue problem of the coupled system can be written as [1].

$$\omega_0^2 \begin{pmatrix} 1 & -\kappa_{12} & -\kappa_{13} & \cdots & -\kappa_{1n} & \cdots \\ -\kappa_{21} & 1 & -\kappa_{23} & \cdots & -\kappa_{2n} & \cdots \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ -\kappa_{m1} & -\kappa_{m2} & \cdots & 1 & -\kappa_{mn} & \cdots \\ -\kappa_{n1} & -\kappa_{n2} & \cdots & -\kappa_{n,(n-1)} & 1 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_m \\ a_n \\ \vdots \end{pmatrix} = \omega^2 \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_m \\ a_n \\ \vdots \end{pmatrix} \quad \text{(8.2.2)}$$

Here $\omega_0$ is the angular frequency of the dielectric resonator in free space, $\kappa_{ij}$ is the coupling coefficient between the $i^{th}$ and $j^{th}$ resonators, $a_i$ is the coefficient multiplied by the electric field of the $i^{th}$ resonator and finally $\omega$ is the frequency of the coupled system.
Figure 8.3. One dielectric resonator between two conducting planes. (a) illustrates the original system while (b) shows the equivalent coupled system forming by the interaction of an infinite array of resonators.

Fortunately, the coupling coefficient decreases sharply as the distance between resonators increases. Therefore, the coupling coefficient between adjacent neighbors dominates and thus the system of equations (8.2.2) simplifies to

$$\omega_0^2 \begin{pmatrix}
1 & -\kappa & 0 & \cdots & 0 & \cdots \\
-\kappa & 1 & -\kappa & \cdots & 0 & \cdots \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & \cdots & -\kappa & 1 & -\kappa & \cdots \\
0 & 0 & \cdots & -\kappa & 1 & \cdots \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
\end{pmatrix} \begin{pmatrix}
a_1 \\
a_2 \\
\vdots \\
a_m \\
a_n \\
\vdots \\
\end{pmatrix} = \omega^2 \begin{pmatrix}
a_1 \\
a_2 \\
\vdots \\
a_m \\
a_n \\
\vdots \\
\end{pmatrix}. \quad (8.2.3)$$
In equation (8.2.3) the subscripts of $\kappa_{ij}$ were dropped since all the coupling coefficients are equal. The operator shown on the left hand side of the above equation is a symmetric tri-diagonal matrix. The eigenvalues of this matrix satisfy the inequality [17]

$$\omega_0^2 (1 - 2\kappa) < \omega^2 < \omega_0^2 (1 + 2\kappa).$$

(8.2.4)

To satisfy the boundary conditions in the conductors’ positions, the dielectric resonators are going to couple through their anti-symmetric mode. Thus the mode of interest will be the $+-+-+-...$ mode. This mode has a coupled frequency of $\omega_0 \sqrt{1 + 2\kappa}$.

8.3 Results and Discussions

The coupling between a dielectric resonator and a cavity was studied previously [2, 6]. It was assumed that the dielectric resonator is installed at the cavity center. In this case, the resonator is far away from the cavity walls and hence the interaction with its images is negligible. Therefore the coupling coefficient between the dielectric and the cavity was calculated using the fields of the dielectric $TE_{01\delta}$ and the cavity $TE_{011}$ modes only [2]. However, if the dielectric is brought close to one of the cavity walls, as shown in Figure 8-4, coupling with the image may be significant.
In this latter case the coupling is between the dielectric $TE_{01\delta}^{\pm}$ mode (anti-mode as a result of the coupling between the dielectric and its induced image) and the cavity $TE_{011}$ mode. A dielectric resonator ($\varepsilon_r=29.2$, Diameter = 6 mm, Height = 2.65 mm and $f_{TE_{01\delta}}=9.7$ GHz) inserted into a cylindrical cavity (Diameter = Height = 4.1 cm, $f_{TE_{011}}=9.7$ GHz) is allowed to move along their common axis. The frequencies of both the symmetric and the anti-symmetric modes were calculated using ECMT, ECMT + image method, and HFSS eigenmodes solver. Figure 8-5 shows how the frequencies of the symmetric and the antisymmetric modes change with respect to the distance $s$ between the dielectric and the upper cavity wall.
As illustrated in Figure 8-5, incorporating the method of images with ECMT (EMCT-I) gives more accurate results particularly for the anti-symmetric mode. As the dielectric moves further from the cavity center, the cavity electric field decreases

\[
|E| \propto \cos \left( \frac{\pi}{d} z \right)
\]

[14]. Accordingly, the coupling coefficient decreases and the modes tend to decouple. The symmetric mode then tends to the cavity mode [7], while the anti-mode tends to the dielectric \( TE^\pm_{01\delta} \) mode. Thus, for the anti-symmetric mode, the effect of the dielectric mode dominates, unlike the symmetric mode which is cavity-like. Accordingly, both methods (ECMT and ECMT-I) give comparable results for the symmetric mode, unlike the anti-symmetric mode where ECMT-I gives considerably better results.
The eigenvalue equation (8.2.3) represents the system consisting of a dielectric resonator sandwiched between two parallel planes as shown in Figure 8-3. Of interest is the $TE_{01\delta}$ mode since each resonator is coupled to the adjacent ones with a 180° phase shift. As already shown, the frequency of this mode is the upper limit of inequality (8.2.4) or

$$f_{TE_{01\delta}} = \sqrt{1 + 2\kappa(2s)} f_0.$$  \hspace{1cm} (8.3.1)

Equation (8.3.1) is solved for different distances, $s$. The results are then compared to the values obtained using HFSS eigenmodes solver as shown in Figure 8-6.

Figure 8-6. Frequency of the resonant mode for a dielectric resonator sandwiched between two conducting planes.

Figure 8-6 verifies formula (8.3.1). Comparing the frequency expression (8.3.1) to expression (8.2.1) one can see that the effective coupling coefficient when the two conductors are present is double that when only one conductor is present. This
conclusion explains the advantage of using two plane conductors behind the resonant coils used in wireless power transfer systems [9].

8.4 Summary and Conclusions

A developed method, ECMT-I, using the image method and ECMT is applied to study cases when coupled structures are in close proximity to conducting surfaces. The ECMT-I method shows that the increase in frequency when a dielectric resonator is brought close to a conducting plane is due to the induced anti-symmetric mode. Application of this method explains why the frequency decreases when the gap of a split-ring is brought close to a conductor wall. This is due to the fact that coupling with the induced image is done through the symmetric mode which is lower in frequency.

A dielectric resonator with a relative permittivity of 30 was brought close to a cavity top wall. ECMT-I gives better results compared to those of ECMT alone particularly for the anti-symmetric mode. When the dielectric is close to the cavity wall the resonant coupled modes tend to the uncoupled ones. Hence the symmetric mode tends to the cavity mode and the anti-symmetric mode tends to the dielectric one. Thus, for the symmetric mode, both methods (ECMT and ECMT-I) give comparable results. However, for the anti-symmetric mode, the two methods give considerably different results, where ECMT-I shows a better error curve. This is because unlike ECMT, ECMT-I takes into account the coupling of the dielectric with its image.

The case of a dielectric resonator sandwiched between two conducting planes was also studied. It is shown that this case is equivalent to an infinite array of coupled resonators. The resulting mode has an effective coupling coefficient that is double the
one resulting if only one plane is present. This last observation explains the advantage of putting conducting planes behind the resonant coils in wireless power transfer systems [9].

The new ECMT-I method opens the door for studying the coupling of two resonant coils in the presence of conducting planes. As already shown, one advantage of this scheme is the increase in the effective coupling coefficient. Another advantage is the reduction in radiation loss due to the presence of the conductors [9].

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References and Notes


9 General discussion and conclusions

The frequency, filling factors and field distributions of the DR/TE\textsubscript{102} probe, made up of two dielectric resonators in a rectangular cavity, are assessed by simulation using the finite integration technique. It was observed that the three uncoupled modes interact to give three coupled ones, namely $TE^{+++}$, $TE^{++-}$ and $TE^{+-+}$ modes. The cavity, which has long been treated as an enclosing shield, interacts with the two dielectric resonators in a way similar to that between resonators studied by lumped circuit models and coupled mode formalisms. Accordingly, with the aim of studying the effect of inserts on the cavity performance, one observed that coupled mode formalisms presented in the literature were unable to capture the essence of the coupling represented by the off-diagonal terms [1-2]. Therefore, a coupled-mode formalism was derived from first principles. The main aim of the formalism is to be general and respect the boundary conditions and internal interfaces. The formalism was written as an eigenvalue problem, where the eigenvalues represent the square of the frequencies and the eigenvectors are the fields’ coefficients.

It was proven that our formalism respects the law of conservation of energy and hence named Energy Coupled Mode Theory, ECMT for short. The effect of external and internal boundaries was also discussed. Energy coupled mode theory can be used for the analysis of different set of problems, for example EPR probes, magnetic resonance imaging (MRI), and wireless power transfer via resonant inductive coupling.

Using ECMT, a physical interpretation of the coupling coefficient was given. This interpretation together with the formulas derived is believed to be general enough to
encompass cases where dielectrics and conductors are present. We concluded that the coupling coefficient is always the difference between the magnetic and electric part and hence explaining Awai’s results [3].

Energy Coupled Mode Theory was then applied to the case of a dielectric resonator inserted in a cylindrical cavity. This situation is important in EPR spectroscopy as well as in dielectric constant measurements. It is also challenging since generally the modes are strongly coupled. The results obtained by ECMT agree to an excellent degree with those obtained using finite elements simulations. Because the dielectric is inserted in the cavity, coupling exists even when the two modes do not have the same frequency. This is true especially when the cavity is small. It was shown that ECMT can give accurate results for high coupling coefficient values. It is proposed that ECMT can be used to derive closed form expressions for the fields of the coupled system. It is also shown that perturbation methods cannot be applied when the two uncoupled systems have the same frequency, even if the dielectric is very small. Indeed, in this case, and because of coupling, the fields will be a blend of the two uncoupled modes.

The coupling coefficient was calculated for the case of one dielectric resonator in a cavity and it was shown that the coupling is stronger for low permittivity values. This is because the dimensions of low permittivity resonators are large and hence the ratio of the overlap areas increases.

Coupled mode formalisms are usually used to calculate eigenvalues (frequencies). In the current thesis, this step was pushed further to find the eigenvectors (the fields). Parameters such as the quality factor, filling factors, resonator efficiency were calculated. Energy coupled mode formalism was able to predict the behavior of these highly field-
dependent parameters. Consequently, the behavior of these parameters was used to study EPR probes. Two important classes were carefully examined. The first one is of a cavity that needs to be optimized by inserting a dielectric (or a loop-gap) to improve its performance. The second class discusses the design of a shield for a given dielectric resonator. The findings were verified using finite element simulations. Using ECMT, the probe designer needs to take into account several parameters, for example the uncoupled frequencies, filling, and quality factors. It is shown that a lossy dielectric resonator which has a very high dielectric constant may deteriorate the EPR signal rather than improving it. It is also proven that if properly designed, a shield can improve the EPR signal of a dielectric resonator.

Finally, ECMT was modified to deal with resonators close to conducting planes. The original theory assumed that conducting walls are far enough apart so that the fields of the open structure resonators (dielectrics, loop-gaps, split-rings, micro-strips, etc) are negligibly small near the boundaries. This is true for many classes. However, as was shown in the chapter 2, when the dielectrics get close to the cavity walls the frequency will change abruptly. Therefore, the well-known image method was used together with ECMT to study situations when the resonators are close to conducting planes. It is shown that the open structure resonator couples with its image in such a way which renders the location of the conducting plane a perfectly conducting wall. Therefore it can couple either symmetrically or anti-symmetrically. For the case of dielectrics, the resonator anti-symmetrically couples with its image and hence the resulting frequency increases. However when the gap of a split-ring is close to a conducting plane, the coupling is
symmetric. This last conclusion is important while one is studying the behavior of meta-
materials near conducting planes.

Main Contributions

To summarize, a list of the main contributions is provided:

1. It is shown that the interactions between two dielectric resonators and a cavity result in three coupled modes ($TE^{+++}$, $TE^{++-}$ and $TE^{--+}$).

2. A general coupled-mode theory (ECMT) is developed. The theory can deal with an arbitrary number of resonators and modes.

3. A unified formula for the coupling coefficient is derived and its physical origin is unveiled.

4. ECMT is applied to the important case of one dielectric resonator in a cavity, where expressions for the coupled frequencies and eigenvectors are derived.

5. Using ECMT, field dependent parameters such as the coupling coefficient, lambda efficiency, quality and filling factors are derived and calculated for different scenarios.

6. Design procedures for designing probes consisting of a high dielectric insert and a conducting cavity are proposed. The design procedures are applied to different scenarios and verified using finite element simulations.

7. It is shown that for a lossy dielectric resonator or/and lossy sample, the shield can improve the resonator efficiency.

8. The method of images is used together with ECMT to study cases when resonators are close to conducting surfaces.
9. ECMT can be used to find closed form expressions for the fields of coupled systems, provided that the fields of the uncoupled subsystems are known beforehand.

**Future work**

For two dielectrics inserted in a cavity, the $TE^{++}$ and $TE^{+-}$ modes are degenerate for some separation distance between the two dielectrics. This condition is not encountered if the dielectrics are left in free space. Therefore, it is concluded that this is due to coupling with the cavity mode. Equipped with ECMT, one can study this case and find expressions for coupled frequencies and how the fields interact. The behavior of the lowest mode, $TE^{+++}$, which is used in EPR spectroscopy, can be fully studied using the proposed theory.

Cases where loop-gaps are present can be investigated. A loop-gap has a high filling factor and a lower $Q$ value and hence can be used in Pulsed EPR spectroscopy where the ringing needs to be minimized. Designing probes which contain cavities, dielectrics, split-rings, and others is indeed an exciting and open area.

It was shown that when a resonator was inserted between two conducting planes, the effective coupling is double that of two resonators in free-space. Therefore, this observation can be used to study and analyze the coupling between two capacitively loaded coils in the presence of conducting walls [4].

Enhancing wireless power transfer using relay coils is a promising technique which can be used to steer power over from a source coil to a load [5]. Therefore, ECMT can be used to analyze and predict the behavior of such systems.
Metamaterials, materials with a negative relative permeability, were manufactured and used for the last decade [6-8]. Metamaterials can be fabricated using arrays of split-ring resonators. Therefore, the coupling between the split-rings can be thoroughly studied using ECMT. The behavior of the ensemble of the resonators needs to be investigated. This is true especially if the coupling coefficient is alternating between being predominately magnetic to being predominantly electric.

Recently, a coupled mode formalism which takes care of the radiating field components was applied to implantable devices [9]. Taking the radiating fields into account can be very helpful in minimizing radiation losses. For example, the field components of the anti-symmetric mode tend to destructively interfere with each other at the far field and hence decrease radiation. This is very similar to how antenna elements interact [10-11].

Energy coupled mode theory can be applied to millimeter waves where small sized relaying systems can be used for signal transmission. This is equivalent to wireless relaying power as was shown in [5, 12] and coupled resonators optical waveguides, CROW, in the optical range [13-15].

Finally, applying ECMT to micro and nano-scale systems is a challenging area. One may need to incorporate quantum effects. But having a general theory which can be applied to a wide range of the electromagnetic spectrum is worth the investigation and study.
References and Notes


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