Dielectric microwave resonators in TE_{011} cavities for electron paramagnetic resonance spectroscopy

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(Received 30 June 2008; accepted 25 July 2008; published online 5 September 2008)

The coupled system of the microwave cylindrical TE_{011} cavity and the $TE_{01\delta}$ dielectric modes has been analyzed in order to determine the maximum achievable resonator efficiency parameter of a dielectric inserted into a cavity, and whether this value can exceed that of a dedicated $TE_{01\delta}$ mode dielectric resonator. The frequency, Q value, and resonator efficiency parameter Λ for each mode of the coupled system were calculated as the size of the dielectric was varied. Other output parameters include the relative field magnitudes and phases. Two modes are found: one with fields in the dielectric parallel to the fields in the cavity center and the other with antiparallel fields. Results closely match those from a computer program that solves Maxwell's equations by finite element methods. Depending on the relative natural resonance frequencies of the cavity and dielectric, one mode has a higher Q value and correspondingly lower Λ than the other. The mode with the higher Q value is preferentially excited by a coupling iris or loop in or near the cavity wall. However, depending on the frequency separation between modes, either can be excited in this way. A relatively narrow optimum is found for the size of the insert that produces maximum signal for both modes simultaneously. It occurs when the self-resonance frequencies of the two resonators are nearly equal. The maximum signal is almost the same as that of the dedicated $TE_{01\delta}$ mode dielectric resonator alone, $\Lambda \cong 40 \text{ G/W}^{1/2}$ at X-band for a $KTaO_3$ crystal. The cavity is analogous to the second stage of a two-stage coupler. In general, there is no electron paramagnetic resonance (EPR) signal benefit by use of a second stage. However, there is a benefit of convenience. A properly designed sample-mounted resonator inserted into a cavity can give EPR signals as large as what one would expect from the dielectric resonator alone. © 2008 American Institute of Physics.

[DOI: 10.1063/1.2976033]

I. INTRODUCTION

Dielectric resonators made from $KTaO_3$ crystals¹ have been inserted into cavities to enhance electron paramagnetic resonance (EPR) signals²⁻⁴ although strategies have not been systematic. The maximum achievable signal has not been discussed. References 2 and 3 report EPR signal enhancement ratios, which are sensitive to sample size and type, instead of resonator properties. This approach makes it difficult to compare the performance of the inserts with other resonator types. Nesmelov *et al.*⁴ reported a resonator efficiency parameter [see Eq. (4)] of $\Lambda \cong 6 \text{ G/W}^{1/2}$ and indicated that further optimization is likely to improve the results. A different method was taken by Blank *et al.*,⁵ who placed the dielectric in a small conducting shield. In this apparatus, the resonator efficiency parameter was estimated to approach $40 \text{ G/W}^{1/2}$.⁶ In that study, they compare their results to those of Nesmelov *et al.* and others and attribute their higher Λ to a full excitation of the $TE_{01\delta}$ dielectric mode (Sec. II B). They also argue that full $TE_{01\delta}$ mode excitation was not achieved for the inserts. This raises the sci-

entific question of what the maximum achievable resonator efficiency parameter by a dielectric insert is and whether this value can exceed that of a dedicated $TE_{01\delta}$ mode dielectric resonator.

The present study answers this question and the results are consistent with those reported above. As we show, the maximum Λ of a $TE_{01\delta}$ mode $KTaO_3$ dielectric resonator is about $40 \text{ G/W}^{1/2}$ at room temperature and X-band, but can vary with temperature, crystal quality, sample size, and type. Analysis of the excitation of a $KTaO_3$ dielectric placed inside a resonant cavity shows that with iris-type coupling to the cavity wall, the maximum Λ is about 98.5% of the dedicated dielectric resonator. However, without careful design, much lower Λ values will be obtained because the optimum occurs under a narrow range of dielectric sizes and coupling must be made to the proper mode.

An analysis of the dielectric resonator inside a cavity is presented. We develop a lumped circuit model of the coupled system of the cylindrical TE_{011} cavity and the $TE_{01\delta}$ dielectric modes. This model permits the scanning of the size of the dielectric and the observation of the frequency, Q value, and resonator efficiency parameter for each mode of the coupled system. Other parameters include the relative field magnitudes and phases. Two modes are found: one with

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fields in the dielectric parallel to the fields in the cavity center and the other with antiparallel fields. For either mode, the magnetic fields are in both the cavity and the dielectric. In different limits, the fields can be primarily in either the cavity or the dielectric regions. Results closely match those from the finite element computer program Ansoft high frequency structure simulator (HFSS) (version 11.0, Ansoft Corporation, Pittsburgh, PA).

Depending on the relative natural resonance frequencies of the isolated cavity and dielectric resonators, one coupled mode will have a higher Q value and correspondingly lower Λ than the other. The mode with the higher Q value is preferentially excited by a coupling iris or loop placed in or near the cavity wall. The fields of this mode are higher at the walls. However, depending on the frequency separation between the modes, either mode can be driven. A relatively narrow optimum is found for the size of the insert that produces maximum signal for both modes simultaneously. This occurs when the self-resonance frequency of the cavity and dielectric resonators are nearly equal. The maximum signal is almost that of the insert resonator alone. A limiting case of our results is the placement of a dielectric resonator in a small conducting shield.⁵ In this limit, the resonator parameters correspond to those of the inserted resonator alone, although coupling to the other mode must be suppressed. For the correct mode, an insert in a larger shield has slightly higher Q value and therefore slightly higher EPR signal than in a small shield.

This work was inspired by observations of the fields using Ansoft HFSS driven mode solutions. The parallel mode was observed in some conditions and the antiparallel mode in others. The analytic lumped circuit model helped characterize and relate the two types of modes.

II. THEORY

We first give the natural resonance frequency, Q value, and resonator efficiency parameter for the isolated TE_{011} cavity mode and then the associated equivalent circuit and values of inductance, capacitance, and resistance. We then do the same for the isolated $TE_{01\delta}$ dielectric mode. Using these results, the coupled circuit is developed and modifications of the parameters are shown. Solution methods are discussed.

A. TE_{011} cavity mode and circuit model

The natural resonance frequency of a TE_{011} mode in a cylindrical cavity of radius r_c and axial length l_c is given by⁷

$$f_c = \frac{c}{2} \sqrt{\left(\frac{x'_{01}}{\pi r_c}\right)^2 + \frac{1}{l_c^2}}, \quad (1)$$

where c is the speed of light in vacuum and x'_{01} is the first nonzero root of the Bessel function $J'_0(x)=0$. Field solutions can be used to find the stored energy and the power dissipated in the cavity walls due to the surface currents, and these expressions can be used to determine the TE_{011} mode Q value,

$$Q_c = \frac{r_c}{\delta} \frac{1}{1 + \left(\frac{c}{2f_c l_c}\right)^2 \left(\frac{2r_c}{l_c} - 1\right)}. \quad (2)$$

In this equation, the skin depth is given by

$$\delta = \frac{1}{\sqrt{\pi f \mu_0 \sigma}}, \quad (3)$$

where μ_0 represents the magnetic permeability of free space and σ is the conductivity of the cavity walls. The EPR resonator efficiency parameter is given by⁸

$$\Lambda = \frac{B_1}{2\sqrt{P_l}}, \quad (4)$$

where B_1 is the peak magnetic field in the resonator and P_l represents the total power loss in the resonator. This expression has an additional factor of 2 in the denominator compared to Ref. 8, but is equivalent because of symbol definitions. The factor of 2 converts the linearly polarized B_1 of Eq. (4) into the circularly polarized component. Equation (4) can be evaluated from the field solutions,

$$\Lambda_c = \frac{\mu_0 10^4}{2\sqrt{P_{lc}}}, \quad (5)$$

where the TE_{011} mode power loss normalized to the peak rf magnetic field is given by

$$P_{lc} = \frac{\pi J_0^2(x'_{01}) r_c l_c}{2\sigma \delta} \left(1 + \frac{2\pi^2 r_c^3}{x_{01}^2 l_c^3}\right). \quad (6)$$

For the equivalent circuit of the cavity mode, we use the model of Smythe.⁹ The self-inductance and capacitance of cylindrical cavity modes are derived from the stored electric and magnetic energies and the cavity wall currents at resonance. For the TE_{011} cavity mode,

$$L_c = \frac{2\mu_0 c^2}{\omega_c^2 l_c}, \quad (7)$$

$$C_c = \frac{\epsilon_0 l_c}{2}, \quad (8)$$

where ϵ_0 represents the electric permittivity of free space and ω represents the radian frequency. The frequency in the inductance expression is evaluated at the natural resonance frequency of the cavity mode, Eq. (1), so that

$$f_c = \frac{1}{2\pi\sqrt{L_c C_c}}. \quad (9)$$

The series resistance is expressed in terms of the cavity mode Q value,

$$R_c = \frac{\omega_c L_c}{Q_c}. \quad (10)$$

The circuit is a series combination of the impedances $j\omega L_c$, $1/j\omega C_c$, and R_c , with the frequency in the impedance values a free parameter at the present stage in the analysis.

The resonator efficiency parameter, Eq. (4), may be evaluated from the lumped circuit values by substituting $B_1 = L_c i_c / A$ and $P_l = i_c^2 R_c$, where $L_c i_c$ represents the magnetic

flux, A is the effective area of the lumped circuit inductance, and i_c is the total lumped circuit cavity current,

$$\Lambda = \frac{L_c}{2A\sqrt{R_c}}. \quad (11)$$

By substituting Eqs. (7) and (10), using Eqs. (1) and (2), and setting the result equal to Eq. (5) with Eq. (6), an exact value for the effective area can be obtained,

$$A = \frac{|J_0(x'_{01})|}{x'_{01}} \left(\frac{\pi}{2} \right)^{1/2} r_c^2. \quad (12)$$

B. TE_{01δ} dielectric mode and circuit model

The electric fields of the TE_{01δ} mode in a cylindrical dielectric are purely azimuthal, like the cylindrical TE₀₁₁ mode. The natural resonance frequency can be derived assuming a magnetic boundary (axial magnetic field zero) at the radial edge of the dielectric $r=r_d$ and evanescent fields outside the dielectric for $|z|>l_d/2$ in a (φ, r, z) cylindrical coordinate system.^{10,11} These boundary conditions lead to a coupled system of equations that can be solved for the natural resonance frequency ω_d of the dielectric mode,

$$\zeta \tan\left(\frac{\zeta l_d}{2}\right) = \zeta_0, \quad (13)$$

$$\zeta = \sqrt{\epsilon_r \frac{\omega_d^2}{c^2} - \frac{x_{01}^2}{r_d^2}}, \quad (14)$$

$$\zeta_0 = \sqrt{\frac{x_{01}^2}{r_d^2} - \frac{\omega_d^2}{c^2}}, \quad (15)$$

where ϵ_r is the relative dielectric constant and x_{01} is the first root of the Bessel function $J_0(x)=0$. The third mode subscript in TE_{01δ} represents the (noninteger) number of half cycles of field variation along the axial length of the dielectric, $\delta \equiv l_d \zeta / \pi$.

It is well known that the resonance frequency predicted by Eqs. (13)–(15) is several percentage points low mainly because of the inaccuracy of the magnetic boundary condition.¹¹ The exact location of this boundary and the associated exact natural resonance frequency of the dielectric resonator depend on other nearby electromagnetic boundaries. Typical engineering applications take into account the presence of conducting walls in the design of the resonator.¹² However, to proceed with the present analysis, the natural resonance frequency of the *isolated* dielectric is needed. Ansoft HFSS simulations were made of the dielectric surrounded by a layer of free space, in turn, surrounded by absorbing boundary conditions. When the layer of free space is greater than about one-half wavelength in thickness, stable eigenmode frequencies and Q values are obtained. These eigenfrequencies can be assumed to be those of the isolated dielectric. For the dielectric constant and loss tangent of KTaO₃ at room temperature as described in Sec. III, the analytic frequencies predicted by Eqs. (13)–(15) over the range of dielectric sizes $1 \text{ mm} < l_d < 3 \text{ mm}$ for $2r_d/l_d=1$ are found to match the Ansoft eigenfrequencies when multiplied by the scale factor 1.0586. These frequencies also produce results

that agree well with the Ansoft HFSS simulations of the coupled dielectric-TE₀₁₁ cavity discussed in Sec. III.

Analytic field solutions were used to find expressions for the stored energy and the power dissipated in the dielectric, and these were used to determine the TE_{01δ} mode Q value,

$$Q_d = \frac{1}{\tan \delta}. \quad (16)$$

This equation neglects the electric field energy in vacuum and is therefore low by approximately one part in $1/\epsilon_r$. The Q value obtained from the Ansoft simulations of the isolated dielectric as described in the previous paragraph is found to be about one-third of that predicted by Eq. (16). About two-thirds of the losses of the dielectric resonator in free space are caused by radiation. The dielectric resonator is a magnetic dipole. This indicates that the dielectric mode cannot be truly isolated from its surroundings and that conducting boundaries must be used in any practical resonator design. However, it is accurate to use the real eigenfrequencies from Ansoft for those of the isolated dielectric because the natural resonance frequency depends on the Q value by only one part in $1/Q^2$.¹³

Ansoft HFSS was used to investigate the influence of different boundary conditions on the properties of the dielectric resonator surrounded by a layer of free space. When a resistive surface boundary condition of value equal to the characteristic impedance of free space was placed around the free-space layer, the Q value was stable at about one-third that predicted by Eq. (16) for a free-space thickness greater than about one-half free-space wavelength, $\lambda_{fs}/2$. As the free-space thickness was decreased, the Q value progressively decreased because of the absorption of the evanescent fields by the resistive layer. An alternative type of absorbing boundary in Ansoft is the perfect material layer (PML). With the PML, a perfectly absorbing boundary condition is obtained by forcing pure radiation fields within a layer of specified thickness. When the PML thickness is greater than about one-eighth free-space wavelength, stable solutions are obtained. With the free-space thickness greater than $\lambda_{fs}/2$, the same results were obtained with PML as with the resistive surface boundary. However, as the free-space thickness was decreased, the Q value increased to a value $(1+1/\epsilon_r)/\tan \delta$ [see Eq. (16) and discussion]. The Q value increases because the radiation fields are induced in the free-space region about one free-space wavelength around the dielectric.¹⁴ As the free-space thickness is reduced, the radiation fields are suppressed, leaving only dissipation in the dielectric. Surprisingly, the PML can be used to suppress the radiation. For a free-space thickness $\lambda_{fs}/8$, the real eigenfrequency is the same as for $\lambda_{fs}/2$ and the Q value is $(1+1/\epsilon_r)/\tan \delta$. As the free-space thickness is made smaller than $\lambda_{fs}/8$, the real eigenfrequency increases while the Q value remains nearly constant. The real eigenfrequency increases because the volume for the evanescent fields is reduced by the PML.

The resonator efficiency parameter, Eq. (4), can be evaluated from the field solutions,

$$\Lambda_d = \frac{\mu_0 10^4}{2\sqrt{P_{ld}}}, \quad (17)$$

where the $\text{TE}_{01\delta}$ mode power loss normalized to the peak rf magnetic field in the dielectric is given by

$$P_{ld} = \frac{\pi J_1^2(x_{01}) \epsilon_r \tan \delta \mu_0 \omega_d^3 r_d^4 \left(l_d + \frac{\sin \zeta l_d}{\zeta} \right)}{4x_{01}^2 c^2}. \quad (18)$$

The presence of the $\sin \zeta l_d / \zeta$ term in Eq. (18) indicates that the effective length of the dielectric is increased by an amount $\sin \zeta l_d / \zeta$ because the electric field is not zero at the axial edges of the dielectric $z = \pm l_d/2$.

The equivalent circuit values were determined by following the analysis of Sec. II A modifying the results for the dielectric constant and the increased effective length,

$$L_d = \frac{2\mu_0 c^2}{\epsilon_r \omega_d^2 \left(l_d + \frac{\sin \zeta l_d}{\zeta} \right)}, \quad (19)$$

$$C_d = \frac{1}{2} \epsilon_0 \epsilon_r \left(l_d + \frac{\sin \zeta l_d}{\zeta} \right). \quad (20)$$

The natural resonance frequency of the dielectric mode is

$$f_d = \frac{1}{2\pi\sqrt{L_d C_d}}. \quad (21)$$

The series resistance is again expressed in terms of the dielectric mode Q value

$$R_d = \frac{\omega_d L_d}{Q_d}, \quad (22)$$

and the circuit is a series combination of the impedances $j\omega L_d$, $1/j\omega C_d$, and R_d with the frequency in the impedance values a free parameter at the present stage in the analysis.

Following the analysis of Sec. II A, the resonator efficiency parameter, Eq. (4), may be evaluated from the lumped circuit values,

$$\Lambda = \frac{L_d}{2A\sqrt{R_d}}, \quad (23)$$

and by using Eqs. (19) and (22) and setting the result equal to Eq. (17), an exact value for the effective area of the dielectric mode can be obtained as

$$A = \frac{J_1(x_{01})}{x_{01}} \left(\frac{\pi}{2} \right)^{1/2} r_d^2. \quad (24)$$

C. Coupled TE_{011} and $\text{TE}_{01\delta}$ circuit model and solution method

The dielectric resonator inside the cylindrical cavity is illustrated in Fig. 1. Finite element simulation of the magnetic fields is also shown. The fields can be considered to be a superposition of the TE_{011} cavity mode fields and the $\text{TE}_{01\delta}$ dielectric mode fields. Because the axial TE_{011} field is nearly constant in the region where the $\text{TE}_{01\delta}$ magnetic field peaks ($r=0$) and goes through three-quarters of a cycle of oscillation ($0 < r \lesssim 3r_d$, Fig. 1), no significant TE_{011} magnetic flux

FIG. 1. (Color) Cylindrical KTaO_3 insert in cylindrical TE_{011} cavity with magnetic fields is shown. For this particular mode, the magnetic fields in the center of the dielectric are antiparallel to those that would be in the center of the cavity in the absence of the dielectric. (a) Entire cavity. (b) Expanded view near and inside the dielectric for the region boxed in part (a).

links the $\text{TE}_{01\delta}$ flux. Therefore, the magnetic coupling of the two modes is small. The two modes are magnetically nearly orthogonal because the volume integral of the dot product of the magnetic fields of the two modes is small. The same cannot be said of the electric fields. The electric fields are purely azimuthal for both $\text{TE}_{01\delta}$ and TE_{011} . Further, the electric fields of each of the modes are zero at the origin and go through only one-half cycle of variation in radius and axial length, although the scale lengths are different. Consequently, the dot product of the electric fields of the two modes is of a single sign and the volume integral is nonzero. The two modes are electrically nonorthogonal, and therefore, coupling of the two modes is primarily electric.

The circuit model that electrically links the TE_{011} and the $\text{TE}_{01\delta}$ LRC tank circuits is shown in Fig. 2. The coupling is done with a pi network, where the bridge coupling capacitance is C_{cc} . The parallel combination of C'_c and C_{cc} is the total TE_{011} capacitance C_c ,

$$C'_c = C_c - C_{cc}, \quad (25)$$

because in the absence of the dielectric, $\{C_d, L_d\} \rightarrow 0$, the cavity circuit should remain. Also, when the dielectric is nonresonant, its impedance is small and the cavity resonance frequency is preserved. The value of C_{cc} can be found by comparing Eqs. (8) and (20) and estimating the extent of axial overlap of the TE_{011} and $\text{TE}_{01\delta}$ electric fields

$$C_{cc} \cong \epsilon_0 \left(l_d + \frac{\sin \zeta l_d}{\zeta} \right). \quad (26)$$

With all the circuit values of self-inductance, resistance, and capacitance thus determined, the coupled circuit of Fig. 2 can be used to predict coupled resonance frequencies, Q

FIG. 2. Circuit model of coupled TE_{011} and $\text{TE}_{01\delta}$ modes.

FIG. 3. Real eigenfrequencies of coupled (solid) and isolated (dashed) TE₀₁₁ and TE_{01δ} modes. (a) Analytic lumped circuit model. (b) Ansoft HFSS eigenmode solutions.

values, and resonator efficiency parameters. Typically, the circuit is driven by an external coupling iris, and such a structure can be added to the circuit as described by Mett *et al.*¹⁵ However, we choose a simpler approach that neglects the effects of a coupling iris and that is directly comparable to Ansoft HFSS eigenmode results. In this approach, the circuit input impedance (shown in the Appendix) is set equal to zero and roots of the resulting equation are found. The roots are complex frequencies that represent the eigenvalues of the circuit. The imaginary part of the frequency quantifies how rapidly the mode decays in time, $e^{j\omega t} = e^{-\text{Im}(\omega)t} e^{j \text{Re}(\omega)t}$. The real parts of the frequencies are the natural resonance frequencies of the coupled system, and the Q values of the modes are given by¹³

$$Q_{cd} = \frac{\text{Re}(f)}{2 \text{Im}(f)}. \quad (27)$$

The resonator efficiency parameter can be found by Eq. (4) and the development of Eqs. (11) and (23). Since the sample is placed in the dielectric, $B_1 = L_d i_d / A$, $P_l = |i_{in}|^2 R_c + |i_d|^2 R_d$, and

$$\Lambda = \frac{L_d}{2A \sqrt{R_d + R_c |i_{in}/i_d|^2}}, \quad (28)$$

where A is given by Eq. (24). The current ratio can be obtained from the circuit of Fig. 2 by solving the coupled system of defined mesh currents and component voltage drops (shown in the Appendix) for the ratio i_{in}/i_d and evaluating Eq. (28) at the eigenfrequencies.

III. RESULTS

The coupled circuit equations were solved for a TE₀₁₁ mode in a fixed size X-band cylindrical cavity with a cylindrical dielectric insert of unity diameter to length ratio. The size of the insert was scanned and observations were made of the natural resonance frequencies, Q values, and resonator efficiency parameters of the coupled system. The computer program MATHEMATICA (version 6, Wolfram Research, Inc.,

Champaign, IL) was used. The corresponding system was modeled and analyzed with the finite element computer program Ansoft HFSS using the eigenmode solution method. A Dell Precision 690 workstation with dual dual-core 3.0 GHz processors and 16 GB of random access memory with WINDOWS XP 64 bits was used to run the programs. The TE₀₁₁ cavity was silver, of radius $r_c = l_c/2$, and length $l_c = 41.598$ mm, which corresponds to a natural resonance frequency of $f_c = 9.5$ GHz (X-band), unloaded Q value $Q_c = 31\,639$, and resonator efficiency parameter when matched of $\Lambda_c = 2.494$ G/W^{1/2}. The KTaO₃ insert was assumed to have a relative dielectric constant $\epsilon_r = 261$ and loss tangent $\tan \delta = 7.5 \times 10^{-4}$ at room temperature.^{3,16,17} The dielectric length was varied over the range $1 \text{ mm} < l_d < 3 \text{ mm}$, giving an isolated natural resonance frequency of 9.4947 GHz at 1.75 mm. At this diameter, the isolated dielectric resonator efficiency parameter $\Lambda_d = 41.01$ G/W^{1/2}. We first discuss the analytic results of the circuit model, then compare to Ansoft HFSS. Connection to a driven system is made.

A. Circuit model results

The real eigenfrequencies predicted by the circuit model are shown in Fig. 3(a). The eigenfrequencies of the coupled system are shown solid and the isolated eigenfrequencies of the cylindrical TE₀₁₁ cavity and TE_{01δ} dielectric are shown dashed. It is clear that for the coupled system there are always two modes—one near the isolated cavity frequency and one near the value for the isolated dielectric. The coupled system eigenfrequencies never cross. When the isolated eigenfrequencies are nearly equal, the coupled system frequencies exhibit maximum deviation from the isolated frequencies. The frequency separation is about an order of magnitude larger than f/Q , with Q corresponding to the dielectric. The modes are labeled parallel and antiparallel because when the current ratio i_d/i_{in} is evaluated using the circuit equations, Eq. (A2), Fig. 2, at the corresponding eigenmodes, the argument of the ratio is close to zero for the

FIG. 4. Q values of coupled (solid) and isolated (dashed) TE_{011} and $TE_{01\delta}$ modes. (a) Analytic lumped circuit model. (b) Ansoft HFSS eigenmode solutions.

parallel mode and close to π for the antiparallel. The phases of the electric and magnetic fields of the two modes from Ansoft HFSS show the same behavior. Magnetic fields of an antiparallel eigenmode are shown in Fig. 1.

The Q values predicted by the circuit model are shown in Fig. 4(a) with the coupled values solid and isolated values dashed. The parallel mode has a Q value near the cavity Q value when the isolated dielectric frequency is greater than 9.5 GHz ($l_d < 1.75$ mm) and the Q value decreases as the dielectric frequency approaches 9.5 GHz ($l_d \rightarrow 1.75$ mm). The Q value approaches the value of the isolated dielectric for $l_d > 1.75$ mm. The opposite is true for the antiparallel mode. The Q values of the two modes cross when the isolated resonance frequencies are nearly equal. The Q crossing is at about $l_d = 1.74$ mm, where $f_d = 9.549$ GHz, 0.5% above the cavity resonance $f_c = 9.5$ GHz. The Q value at the crossing is double the Q value of the isolated dielectric.

The corresponding resonator efficiency parameters are shown in Fig. 5(a). The Λ and Q values behave similarly, except that the mode with the highest Λ value always has the lowest Q value and visa versa. The Λ and Q values are

inversely related because the most localized fields give the highest Λ value. Since these fields are in the dielectric, the Q value is close to the inverse loss tangent, Eq. (16), and lower than that of the cavity. Conversely, the mode that has the more cavitylike fields has the highest Q value, the most diffused fields, and the lowest Λ . The Λ values of the two modes cross when the isolated resonance frequencies are nearly equal. The Λ crossing appears to occur at the same point as the Q crossing, $l_d \cong 1.74$ mm, where f_d is about 0.5% above the cavity resonance $f_c = 9.5$ GHz. The Λ value at the crossing is 98.5% of the Λ value of the isolated dielectric. The highest Λ for the coupled system is obtained from the mode that has fields closest to those of the isolated dielectric. The parallel mode fits this condition when $l_d > 1.75$ mm and the antiparallel mode when $l_d < 1.75$ mm.

The relative phase of the coupled system currents i_d and i_{in} obtained from the circuit model are shown in Fig. 6. Despite the variation of the phase of the currents of each mode as the isolated eigenfrequencies cross, the phase difference between the modes remains exactly π .

FIG. 5. Resonator efficiency parameter values of coupled (solid) and isolated (dashed) TE_{011} and $TE_{01\delta}$ modes. (a) Analytic lumped circuit model. (b) Ansoft HFSS eigenmode solutions.

FIG. 6. Relative phase of the coupled TE₀₁₁ and TE_{01δ} modes from the analytic lumped circuit model as obtained from the ratio of the dielectric current i_d to cavity current i_{in} . The value of $\arg(i_d/i_{in})$ evaluated for each eigenfrequency is plotted.

B. Comparison of analytic and finite element results

The coupled cavity-dielectric system was modeled using Ansoft HFSS and the dielectric size was varied. The eigenfrequencies and Q values obtained directly from the computer program are shown in Figs. 3(b) and 4(b). An excellent match to the circuit model, Figs. 3(a) and 4(a), is seen. The resonator efficiency parameter was evaluated from Eq. (4) using the Ansoft field solutions and shown in Fig. 5(b). These also compare well with those from the circuit model, Fig. 5(a). The finite element simulations of the Q and Λ values display a slightly stronger cavity-dielectric interaction than the circuit model for $l_d > 1.75$ mm and a slightly smaller interaction for $l_d < 1.75$ mm.

C. Connection to driven system

Eigenmode methods were used to obtain the solutions from both the circuit model and the finite element computer program. Individual eigenmodes are orthogonal. Orthogonality can mean that the fields are everywhere perpendicular, but this is not necessary. What is required for orthogonality is that the volume integral of the dot product of the fields is zero. Fields can be parallel if canceled by antiparallel fields.

A coupling iris can excite a superposition of orthogonal modes. Three conditions must be satisfied in order to excite a particular eigenmode: (1) the driving frequency should be within about $\pm 5(f/Q)$ of the natural resonance frequency of the mode;¹⁵ (2) the iris should have the same field symmetry as the mode near the iris; and (3) the mode fields should have significant strength at the location of the coupling iris. Unfortunately, the mode with the highest Λ has the weakest fields near the cavity walls and is therefore more difficult to excite using a conventional coupling iris. However, only 1.5% of the Λ is sacrificed at the mode crossing. Either mode can be coupled with a conventional iris at this condition. Far from the mode crossing, a special coupler placed close to the dielectric can be used to couple to the highest Λ mode. Al-

ternatively, the cavity can be made smaller, taking the form of a shield.⁵ This situation is captured on the right side of the mode charts of Figs. 3–5. As the cavity size decreases, the frequency of the cavity mode increases relative to the dielectric mode. In reality, there will be higher order dielectric modes between the lowest order dielectric and the cavity mode. For the lowest mode, a slight drop in Q value caused by the increase in wall currents will only slightly reduce Λ from the value obtained in the larger cavity.

With an iris, there is a splitting of all the modes shown in Figs. 3–5. Only one of the split modes can be coupled, depending on the sign of the iris reactance.¹⁵ The driven system with a conventional mutual-inductance-type coupler has been solved analytically. The results are consistent with the discussion of the preceding paragraph but also unnecessarily complicate the results presented in Figs. 3–5.

D. Other nonideal effects

The relative dielectric constant of KTaO₃ has a substantial inverse dependence on temperature. This implies that a dielectric insert would have a good match to a cavity only in a fairly narrow temperature range. Also, the dielectric loss tangent depends on the crystal quality and can be somewhat higher than the value used in our analysis. This increases the Λ value by $Q^{1/2}$. These effects are discussed in Ref. 5. Since our calculations were done for a solid cylindrical dielectric insert, they apply in the limit of a very small sample. A sample is normally placed in a hole in the dielectric, and this lowers the Λ value for two reasons. First, the magnetic fields are spread over a larger volume because the sample relative dielectric constant is lower than the dielectric. The effect of the placement of a sample hole in the dielectric is discussed in Ref. 3. Second, for a water sample, the loss tangent is larger than for the KTaO₃ and so the Q value is reduced. The influence of the sample can be found by finite element simulations.

IV. CONCLUSION

An analytic model of the excitation of a dielectric insert in a cavity has been developed. Results are in excellent agreement with finite element simulations. Results also resolve a conflict in the literature between a large resonator efficiency parameter observed for a dedicated TE_{01δ} mode dielectric resonator and a factor of five smaller for the case of a dielectric inserted into a cavity. We show that with careful design, a dielectric insert can perform almost as well as a dedicated dielectric resonator. We conclude that a conducting shield is necessary for a dielectric resonator to achieve maximum resonator efficiency. A small nonresonant shield gives maximum efficiency and a resonant cavity can also, but only under a narrow range of excitation of the proper mode. Extra design effort is needed to obtain the maximum signal benefit from the use of an insert.

With little modification, results of the present study can be applied to the insertion of a loop-gap resonator¹⁸ (LGR) into a cavity. LGRs have also been inserted into cavities to enhance EPR signals.^{19,20} By transformer action, it has been argued that an EPR signal level above cavity or LGR alone

might be expected. However, results of the present study indicate that signal levels only up to those of the LGR alone are achievable. The cavity is analogous to the second stage of a two-stage coupler, which does not provide any signal benefit. This conclusion is consistent with the previously reported results. Anderson *et al.*¹⁹ experimentally studied a LGR in a TE₁₀₂ cavity and observed a signal improvement over the cavity alone, but not above what was expected from the LGR alone. They also observed two relatively closely spaced modes that gave EPR signal, one above and one below the cavity resonance frequency. Britt and Klein²⁰ reported lower Q values and higher EPR signals than expected from the TE₁₀₂ cavity alone. Another conclusion of the present study is that the Q value at optimum Λ is nearly that of the inserted resonator. Since this Q value is much lower than the cavity, a different coupling iris is needed.

The analytical methods presented here can be used to determine the resonator efficiencies for other dielectric materials including SrTiO₃,¹⁰ quartz,²¹ sapphire, and rutile.²² Using the analytical expressions, the specific results are readily scalable to different dielectric constants and loss tangents.

ACKNOWLEDGMENTS

This work was supported by Grant Nos. EB001417 and EB001980 from the National Institutes of Health.

ABBREVIATIONS

- TE_{01δ} = dielectric resonator
- TE₀₁₁ = cavity
- EPR = electron paramagnetic resonance
- rf = radio frequency
- TE = transverse electric

APPENDIX: INPUT IMPEDANCE AND CIRCUIT EQUATIONS

The input impedance of the circuit of Fig. 2 is given by

$$Z_{\text{in}} = R_c + j\omega L_c + \frac{1}{j\omega(C_c - C_{cc}) + \frac{1}{\frac{1}{j\omega C_{cc}} + \frac{1}{j\omega C_d + \frac{1}{R_d + j\omega L_d}}}}. \quad (\text{A1})$$

A complete set of circuit equations for the circuit of Fig. 2 is derived from the defined mesh currents and component voltage drops and given by

$$\begin{aligned} v_{\text{in}} &= i_{\text{in}}(j\omega L_c + R_c) + v_{cc}, \\ v_{cc} &= \frac{i_{\text{in}} - i_{cc}}{j\omega(C_c - C_{cc})}, \\ v_{cc} &= \frac{i_{cc}}{j\omega C_{cc}} + v_d, \\ v_d &= \frac{i_{cc} - i_d}{j\omega C_d}, \\ v_d &= i_d(R_d + j\omega L_d). \end{aligned} \quad (\text{A2})$$

¹KTaO₃ is a cubic perovskite that has ferroelectric properties below 32.5 K and is sometimes referred to in literature as a ferroelectric or incipient ferroelectric material. Further details are given in footnote 18 of Ref. 5.

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