Theory of morphology-dependent resonances: shape resonances and width formulas

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Received March 17, 1992; accepted August 27, 1992; revised manuscript received August 28, 1992

The theory of morphology-dependent resonances of a spherical particle is developed in analogy with the theory of quantum-mechanical shape resonances. Exact analytic formulas for predicting the widths of the resonances for both real and complex indices of refraction are developed.

1. INTRODUCTION

The cross section for scattering electromagnetic energy by a dielectric sphere exhibits a series of sharp peaks as a function of the size parameter. These peaks are a manifestation of scattering resonances in which electromagnetic energy is temporally trapped inside the particle. A physical interpretation is that the electromagnetic wave is trapped by almost total internal reflection as it propagates around the inside surface of the sphere and that after circumnavigating the sphere the wave returns to its starting point in phase. These resonances are now generally referred to as morphology-dependent resonances (MDR's). A large body of literature has been written on the subject. A good review article, containing many references to the original literature, has recently been written by Hill and Benner.[1]

The present paper discusses two topics in the theory of MDR's. These are (i) an interpretation of MDR's as shape resonances and (ii) the derivation of exact analytic formulas for predicting the widths of these resonances. The theory of shape resonances is a familiar topic in atomic and molecular scattering theory. However, the fact that MDR's can be regarded as shape resonances[2,3] does not seem to be widely appreciated. This is evidenced by the general lack of any discussion or even mention of this interpretation in review articles and other published literature on MDR's. In this interpretation the electromagnetic energy is temporarily trapped near the surface of the sphere in a dielectric potential well. The energy enters and leaves the well by tunneling through the centrifugal barrier that forms the outer wall of the potential well.

Section 2 begins with a review of some of the basic equations for electromagnetic scattering from spherically symmetric particles. That section is presented mainly as matter of convenience. It helps to establish our conventions and notation and also gathers together equations that will be needed later in the paper. Section 3 discusses resonance theory and shows how MDR's can be interpreted as shape resonances. It is then shown how the boundary conditions that define a shape resonance state lead to the same mathematical conditions that define the location of an MDR. The section concludes with a discussion of some interesting problems that occur if the dielectric function of the particle (or a layer covering the particle) is permitted to be negative. Section 4 discusses several new exact analytic formulas for predicting the widths of resonances. Formulas are derived for both real and complex indices of refraction. Section 5 ends the paper with a summary and concluding remarks.

2. SCATTERING THEORY

This section briefly reviews the theory of electromagnetic scattering from a spherical particle. The basic equations needed in the remainder of the paper are presented, and some of the conventions and the notation to be used are established. The particle is assumed to be nonmagnetic. The radius of the particle is denoted by a, and the complex index of refraction, which may be a function of the radial coordinate r, is denoted by $m(r) = m_r(r) + im_i(r)$. In the region outside the sphere, $r > a$, the index of refraction is $m(r) = 1$ and the wave number is $k = 2\pi/\lambda$. The complex time dependence of the electric field is $\exp(-i\omega t)$. This time-dependence convention is the same as that used by Bohren and Huffman[4] but is opposite to that used by van de Hulst[5] and Kerker.[6] With this convention a positive imaginary part of index of refraction results in power absorption by the particle.

The electric field must satisfy the scattering boundary conditions and the following vector wave equation:

$$\nabla \times \nabla \times \mathbf{E} - k^2 m^2(r)\mathbf{E} = 0. \tag{1}$$

The solution to this equation is most easily computed by expanding the electric field in terms of the spherical vector wave functions

$$\mathbf{M}_{n,m}(r,\theta,\phi) = \frac{\exp(im\phi)}{kr} S_n(r)\mathbf{X}_{n,m}(\theta),$$

$$\mathbf{N}_{n,m}(r,\theta,\phi) = \frac{\exp(im\phi)}{k^2 m^2(r)}\left[\frac{1}{r}\frac{\partial T_n(r)}{\partial r}\mathbf{Y}_{n,m}(\theta) + \frac{1}{r^2}T_n(r)\mathbf{Z}_{n,m}(\theta)\right], \tag{2}$$

where the functions $\mathbf{M}_{n,m}(r,\theta,\phi)$ are the transverse electric (TE) modes and the functions $\mathbf{N}_{n,m}(r,\theta,\phi)$ are the

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transverse magnetic (TM) modes. The angular functions in these expressions are defined as

$$\mathbf{X}_{n,m}(\theta) = i\pi_{n,m}(\theta)\hat{\mathbf{e}}_\theta - \tau_{n,m}(\theta)\hat{\mathbf{e}}_\phi,$$
$$\mathbf{Y}_{n,m}(\theta) = \tau_{n,m}(\theta)\hat{\mathbf{e}}_\theta - i\pi_{n,m}(\theta)\hat{\mathbf{e}}_\phi,$$
$$\mathbf{Z}_{n,m}(\theta) = n(n+1)P_n^m(\cos\theta)\hat{\mathbf{e}}_r, \tag{3}$$

where

$$\pi_{n,m}(\theta) = \frac{m}{\sin\theta}P_n^m(\cos\theta),$$
$$\tau_{n,m}(\theta) = \frac{\partial}{\partial\theta}P_n^m(\cos\theta). \tag{4}$$

The function $P_n^m(\cos\theta)$ is the associated Legendre polynomial and $\hat{\mathbf{e}}_r$, $\hat{\mathbf{e}}_\theta$, $\hat{\mathbf{e}}_\phi$ are the unit orthogonal vectors associated with spherical coordinates. The functions $S_n(r)$ and $T_n(r)$ are the radial Debye potentials, which satisfy the following second-order differential equations[7,8]:

$$\frac{d^2S_n(r)}{dr^2} + \left[k^2m^2(r) - \frac{n(n+1)}{r^2}\right]S_n(r) = 0, \tag{5a}$$

$$\frac{d^2T_n(r)}{dr^2} - \frac{2}{m(r)}\frac{dm(r)}{dr}\frac{dT_n(r)}{dr} + \left[k^2m^2(r) - \frac{n(n+1)}{r^2}\right]T_n(r) = 0. \tag{5b}$$

The solutions to these equations must obey the initial conditions $S_n(0) = 0$ and $T_n(0) = 0$. These conditions are necessary to ensure that the electric field is finite at the origin.

In regions where the index of refraction has the constant value m, the two differential equations (5a) and (5b) have the same form, and the linearly independent solutions are Ricatti–Bessel functions,[9] which are defined as

$$\psi_n(mkr) = mkr\, j_n(mkr), \tag{6a}$$
$$\chi_n(mkr) = mkr\, n_n(mkr), \tag{6b}$$

where $j_n(mkr)$ and $n_n(mkr)$ are spherical Bessel functions. In the external region, $r \geq a$, where $m(r) = 1$, the general solutions are linear combinations of the Riccati–Bessel functions. For later use in the paper it will be convenient to define these external solutions as follows:

$$S_n(r) = B_n[\chi_n(kr) + \beta_n\psi_n(kr)], \tag{7a}$$
$$T_n(r) = A_n[\chi_n(kr) + \alpha_n\psi_n(kr)], \tag{7b}$$

where α_n, β_n, A_n, and B_n are constants. These functions must connect, in an appropriate manner at the surface of the sphere, with the solutions inside the sphere. The connection of the internal and external solutions is most easily carried out by using the log-derivative formalism.

The modified log-derivative functions of $S_n(r)$ and $T_n(r)$ are defined as

$$U_n(r) = \frac{1}{k}[S_n'(r)/S_n(r)], \tag{8a}$$

$$V_n(r) = \frac{1}{km^2(r)}[T_n'(r)/T_n(r)], \tag{8b}$$

where a prime denotes the derivative with respect to the argument of the function. Both of these functions are continuous at all points. This includes points where the index of refraction is discontinuous, such as at the surface of the sphere and, in the case of a layered sphere, at the boundaries between the layers. It will also be useful to define the log derivatives of the Riccati–Bessel functions by the relations

$$D_n(x) = \psi_n'(x)/\psi_n(x), \tag{9a}$$
$$G_n(x) = \chi_n'(x)/\chi_n(x). \tag{9b}$$

Substitute the external solutions defined by Eqs. (7a) and (7b) into the definitions of the modified logarithmic derivatives given by Eqs. (8a) and (8b) and evaluate at the surface of the sphere. Then use the continuity of the functions $U_n(r)$ and $V_n(r)$ across the boundary to obtain

$$U_n(a) = \frac{\chi_n'(ka) + \beta_n\psi_n'(ka)}{\chi_n(ka) + \beta_n\psi_n(ka)}, \tag{10a}$$

$$V_n(a) = \frac{\chi_n'(ka) + \alpha_n\psi_n'(ka)}{\chi_n(ka) + \alpha_n\psi_n(ka)}, \tag{10b}$$

where $U_n(a)$ and $V_n(a)$ are evaluated from the internal solution. These equations can be solved for α_n and β_n. The results are

$$\beta_n = -\frac{\chi_n(ka)}{\psi_n(ka)}\left[\frac{G_n(ka) - U_n(a)}{D_n(ka) - U_n(a)}\right], \tag{11a}$$

$$\alpha_n = -\frac{\chi_n(ka)}{\psi_n(ka)}\left[\frac{G_n(ka) - V_n(a)}{D_n(ka) - V_n(a)}\right]. \tag{11b}$$

For the special case of Mie scattering, in which the index of refraction has a constant value m, the solutions of the differential equations (5) in the region $0 \leq r \leq a$ are given by

$$S_n(r) = T_n(r) = \psi_n(mkr). \tag{12}$$

Substitute these functions into Eqs. (8a) and (8b) to obtain

$$U_n(r) = mD_n(mkr), \tag{13a}$$
$$V_n(r) = (1/m)D_n(mkr). \tag{13b}$$

Then substitute these expressions into Eqs. (11a) and (11b) to obtain

$$\beta_n = -\frac{\chi_n(x)}{\psi_n(x)}\left[\frac{G_n(x) - mD_n(mx)}{D_n(x) - mD_n(mx)}\right], \tag{14a}$$

$$\alpha_n = -\frac{\chi_n(x)}{\psi_n(x)}\left[\frac{mG_n(x) - D_n(mx)}{mD_n(x) - D_n(mx)}\right], \tag{14b}$$

where $x = ka$ is the size parameter.

It can be shown that α_n and β_n are related to the a_n and b_n coefficients of Mie theory by the formulas

$$b_n = \frac{1}{1 - i\beta_n}, \tag{15a}$$

$$a_n = \frac{1}{1 - i\alpha_n}. \tag{15b}$$

The a_n and b_n coefficients defined here are the same as the coefficients defined by Bohren and Huffman[4] and are

the complex conjugate of the coefficients defined by van de Hulst[5] and by Kerker.[6] All the usual formulas for cross sections and other quantities that are expressed in terms of the a_n and b_n coefficients are applicable.

3. RESONANCE THEORY

A. Quantum-Mechanical Analogy

The second-order differential equations (5a) and (5b) can be recast in a form similar to the radial Schrödinger equation. This well-known analogy is useful because with it one can formulate problems in such a way that familiar quantum-mechanical techniques can be used. To simplify the analogy, assume that the Schrödinger equation is expressed in units such that $\hbar^2/2\mu = 1$ (where $\hbar$ is Plank's constant and μ is the reduced mass). The radial Schrödinger equation then has the form

$$-\frac{d^2\psi(r)}{dr^2} + \left[V(r) + \frac{n(n+1)}{r^2}\right]\psi(r) = E\psi(r), \tag{16}$$

where $V(r)$ is the potential energy function and E is the total energy. Equation (5a) will be identical in form to the Schrödinger equation if we define the potential to be

$$V(r) = k^2[1 - m^2(r)] \tag{17}$$

and the energy to be

$$E = k^2. \tag{18}$$

[Equation (18) was obtained by comparing the equations for the case of free space, i.e., for $m(r) = 1$ and $V(r) = 0$.] We note immediately that one noteworthy difference between the quantum-mechanical and electromagnetic cases is that in the latter case the potential function is directly proportional to the energy (i.e., to k^2), whereas in the former case $V(r)$ is usually a fixed function, independent of the energy. This difference will lead to some interesting consequences that will be discussed in Subsection 3.C.

The total potential is the sum of the potential function $V(r)$ and the centrifugal potential. It is given by

$$V_n(r) = k^2[1 - m^2(r)] + \frac{n(n+1)}{r^2}. \tag{19}$$

The local wave number $p_n(r)$ is defined by the relation $p_n^2(r) = E - V_n(r)$. This can also be written in the form

$$p_n^2(r) = k^2m^2(r) - \frac{n(n+1)}{r^2}. \tag{20}$$

The quantity $p_n^2(r)$ is analogous to the kinetic energy in quantum mechanics. A region is classically allowed or classically forbidden depending on whether $p_n^2(r)$ is positive or negative, respectively.

Consider the special case of a spherical particle with a constant index of refraction m. The potential in this case is given by

$$V_n(r) = \begin{cases} k^2(1 - m^2) + n(n+1)/r^2 & r \le a \\ n(n+1)/r^2 & r > a \end{cases}. \tag{21}$$

Whether this potential is attractive or repulsive will depend on the values of both m^2 and k^2. The case of most interest in this paper is that of a dielectric particle with $m^2 > 1$ and with $k^2 > 1$. (Other cases will be considered in Subsection 3.C.) As a specific example consider the potential function $V_{40}(r)$ for a particle of radius a, index of refraction $m = 1.47$, and wave number $k = 33/a$. For convenience we choose the unit of length to be equal to the particle radius. Thus $a = 1.0$ and $k = 33$. The potential function $V_{40}(r)$ for this case is shown, drawn to scale, in Fig. 1. The most striking feature of this function is the presence of a potential well in the region $r_1 < r < a$. This is a classically allowed region in which $p_n^2(r) > 0$. The well is surrounded by the two classically forbidden regions $0 \le r < r_1$ and $a < r < r_2$ in which $p_n^2(r) < 0$. The points r_1 and r_2, defined by the relation $p_n^2(r) = 0$, are called the classical turning points.

In the equivalent quantum-mechanical problem a particle can tunnel through the classically forbidden region, $a < r < r_2$, into the classically allowed potential well. For certain values of the energy the particles will become temporally trapped in the well, oscillating back and forth many times before finally tunneling back through the classically forbidden region to the outside world again. These quasi-bound states are also known as resonances. The type of resonance described here is called a shape resonance. The name shape resonance means simply that the resonance behavior arises from the shape of the potential, i.e., the well and the barrier.[10] This particular type of shape resonance, in which the barrier is formed by the centrifugal potential, is also referred to as an orbiting resonance.[11] The latter name is particularly apt considering the usual interpretation of MDR's in terms of light rays propagating around the inside surface of the sphere.[1]

B. MDR's Interpreted as Shape Resonances

The electromagnetic scattering problem is similar to the quantum-mechanical problem. Electromagnetic energy can tunnel through the classically forbidden region and become temporarily trapped in resonance states. As I demonstrate, these are the familiar MDR's predicted by Mie theory. In the following discussion I assume that the index of refraction is a real quantity.

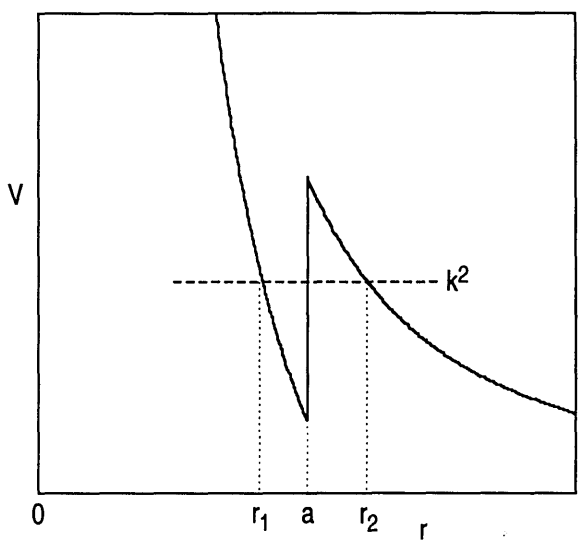

Fig. 1. Effective potential associated with a spherical dielectric particle.

In Fig. 1 the energy k^2 is approximately halfway between the top and bottom of the potential well. If the value of k^2 is changed, the shape of the potential well will also change. This is unlike the quantum-mechanical problem in which the potential is independent of the energy. As k is reduced in value, the bottom of the potential well will rise. For some value of k the energy k^2 will coincide with the bottom of the potential well. I refer to this energy as the bottom of the well and denote the value of k for which this occurs as k_B. The top of the well remains fixed in value as k^2 is varied. If k^2 is raised in value, it will eventually coincide with the top of the well. I refer to this as the top of the well and denote the value of k for which this occurs as k_T.

The classical turning points are defined by the condition $p_n^2(r) = 0$. Solving Eq. (20) for this condition gives the two turning points

$$r_1 = (n + 1/2)/km, \tag{22a}$$

$$r_2 = (n + 1/2)/k, \tag{22b}$$

where I have replaced $[n(n + 1)]^{1/2}$ with $n + 1/2$ and used the fact that $m(r_1) = m$ and $m(r_2) = 1$. These expressions for the turning points can be used to calculate the values of k_B and k_T. When $k = k_B$ the inner turning point must satisfy the relation $r_1 = a$, and when $k = k_T$ the outer turning point must satisfy the relation $r_2 = a$. Substituting these conditions into Eqs. (22) and solving for k gives $k_B = (n + 1/2)/ma$ and $k_T = (n + 1/2)/a$. It is more convenient to express these relations in terms of the dimensionless size parameter $x = ka$ rather than k. Thus the conditions for the bottom and the top of the potential well are given by

$$x_B = (n + 1/2)/m, \tag{23a}$$

$$x_T = n + 1/2. \tag{23b}$$

In quantum mechanics, only certain discrete energy levels are allowed in a one-dimensional potential well. The mathematical reason for this is that the boundary conditions can be satisfied only at these discrete energies. The problem of shape resonances is similar. The resonances occur only for energy values that satisfy the boundary conditions, which are quite similar to the boundary conditions for the bound-state problem.

The boundary conditions at $r = 0$ are given by $S_n(0) = T_n(0) = 0$. These conditions, which I stated above, must be met by all scattering solutions regardless of whether they are resonance states. The solutions that satisfy this condition are given by Eq. (12). The general form of the solutions in the region $r > a$ is given by Eq. (7). These functions are a linear combination of the Riccati–Bessel functions $\psi_n(kr)$ and $\chi_n(kr)$. In the classically forbidden region, $a < r < r_2$, these two functions have opposite behaviors. The function $\psi_n(kr)$ exhibits a rapid, exponentiallike growth in this region, while the function $\chi_n(kr)$ exhibits an exponentiallike decrease. At $r = r_2$ these functions cease their exponentiallike behavior and begin an oscillatory behavior in the region $r_2 < r < \infty$.

The condition that determines the discrete energy levels of a quasi-bound shape resonance is the requirement that the wave function exhibit an exponentiallike decay in the barrier region so that, if the barrier extended to $r \to \infty$, the wave function would decay to zero and the quasi-bound state would become a true bound state. This means that only the (exponentiallike) decreasing function $\chi_n(kr)$ is allowed in the barrier region. Translating this requirement back to the wave functions defined by Eq. (7) implies that the coefficient that multiplies the (exponentiallike) increasing function $\psi_n(kr)$ must be zero; i.e., $\beta_n = 0$ ($\alpha_n = 0$) at the location of a TE (TM) resonance, respectively. These conditions, which were obtained by satisfying the conditions for a shape resonance, are equivalent to the conditions commonly used to define the location of a MDR.[1] This is evident from Eqs. (15a) and (15b), which show that $\beta_n = 0$ ($\alpha_n = 0$) is equivalent to the condition that the imaginary part of the Mie coefficient b_n (a_n) is equal to zero.

Substituting $\beta_n = 0$ and $\alpha_n = 0$ into the formulas of Eqs. (14a) and (14b) gives the following equations that must be satisfied at the locations of TE and TM resonances, respectively:

$$G_n(x_0) = mD_n(mx_0), \tag{24a}$$

$$mG_n(x_0) = D_n(mx_0). \tag{24b}$$

These equations are satisfied by an infinite number of discrete values of the size parameter x_0. However, only the finite number of values of x_0 that lie in the range between the bottom and top of the potential well are considered to be resonant states. There are no solutions below the bottom of the well. The solutions above the top of the well are generally not considered to be resonances because they are too wide to have the properties associated with resonances, such as a sharp spike in the scattering cross section. (We note, however, that in some cases solutions that are only slightly above the top of the well are counted as resonances.) The bottom and the top of the potential well for the case $m = 1.47$ and $n = 40$ are $x_B = 27.5$ and $x_T = 40.5$. This potential supports three TE and three TM resonances between x_B and x_T. An accurate computer solution of the equations gives the following results: the TE resonances are located at 31.058854, 34.611195, and 37.653070 and the TM resonances are located at 31.519210, 34.996041, and 37.908035.

The wave functions for the three TE resonances are shown graphically in Fig. 2. These wave functions are the Debye potential functions $S_{40}(r)$, obtained by solving Eq. (5a). They are shown superimposed, at the proper level, upon the potential function $V_{40}(r)$. Within the region of the potential well, these wave functions resemble bound states. The lowest-level wave function has a single peak, the next level has two peaks (positive and negative), and the third level has three peaks. The number of peaks in the classically allowed region of the potential well, $r_1 \leq r \leq a$, is called the order number and is denoted by l. This number, along with the mode number n and the label TE or TM, uniquely identifies a resonance. Electromagnetic energy is temporarily trapped in the potential well. It can enter and leave by tunneling through the outer centrifugal barrier of the potential well. The width of the resonance is inversely proportional to the lifetime of the trapped energy, which in turn is determined by the rate of tunneling through the barrier. The levels near the bottom of the well must tunnel through a larger barrier than the upper levels. Therefore the lower levels have a longer

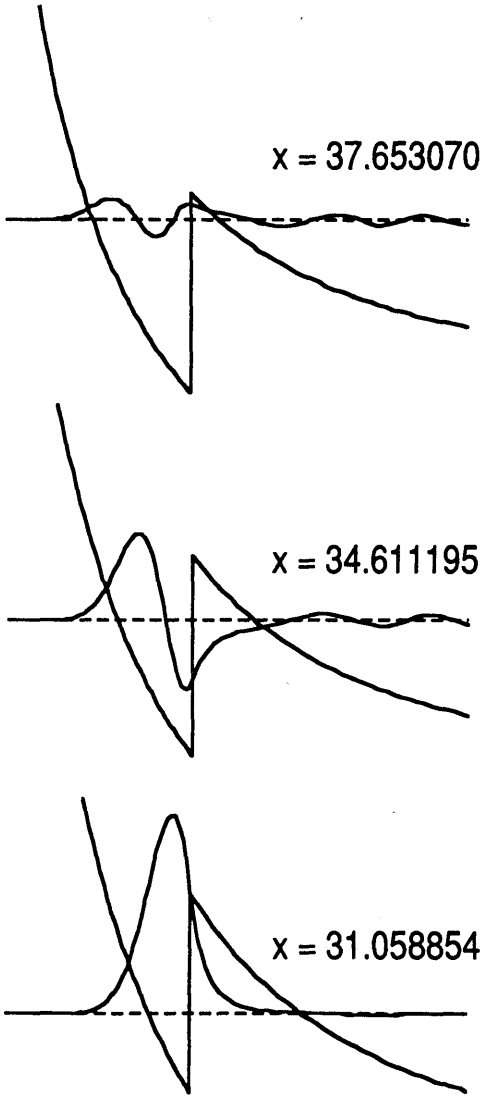

Fig. 2. Radial wave functions for the three TE, $n = 40$ resonances.

lifetime and hence a narrower width than the upper levels. The widths of the three TE resonances [which were calculated by using Eq. (32) of Section 4] are 0.00008782, 0.01023, and 0.1297.

Figure 3 shows the dramatic change that the wave function experiences as the system traverses the TE, $n = 40$, $l = 2$ resonance, located at $x_0 = 34.611195$. For graphical convenience the particle radius is $a = 1.0$. The top panel of Fig. 3 shows the wave function for the case $x = 34.911195$, which is above the resonance. The wave function $S_{40}(r)$ is shown superimposed, at the proper level, upon a plot of the potential function. The wave function shows an exponentiallike increase in the tunneling region. Because of this growth, the amplitude of the wave function the region $r > r_2$, outside the particle, is much greater than the amplitude inside the particle. The center panel shows the case $x = 34.611195$, which is on resonance. In this case the wave function decays in an exponentiallike manner in the tunneling region. This is the behavior that is opposite to that from the previous case. The amplitude of the wave function inside the particle is now much larger than the amplitude outside. The result is that, as one approaches the particle, the field strength increases rapidly in the region $a < r < r_2$, which is the layer just outside the surface, and then continues to rise to a maximum inside the particle near the surface. This increased field strength near the surface (both inside and outside the particle) is a characteristic resonance phenomenon. Finally, the bottom panel shows the case $x = 34.311195$, which is below the resonance. The behavior in this case is very similar to that in the top panel; i.e., the wave function increases in an exponentiallike fashion in the tunneling region, resulting in a small amplitude inside the particle relative to the amplitude outside. However, in this case the exponentiallike growth in the tunneling region is in the negative direction compared with that in the top panel. This results in a 180° phase shift of the outside wave function compared with its phase in the top panel. This 180° phase shift is also a characteristic feature of a shape resonance.

The amplitudes of the wave functions shown in Figs. 2 and 3 cannot be directly compared with one another

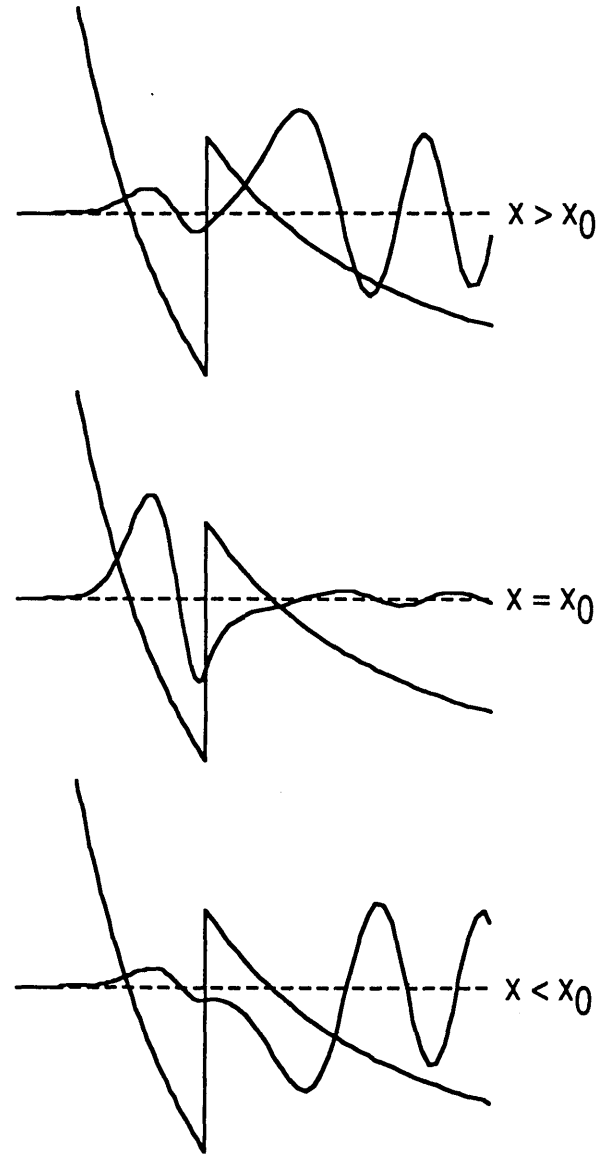

Fig. 3. Behavior of the TE wave function in the vicinity of a resonance: behavior for a size parameter value slightly above resonance (top); on resonance (middle); below resonance (bottom).

because each of these functions has been individually normalized to fit on the graph. To compare the peak amplitudes, it is necessary to normalize the wave functions so that they all have the same amplitude at $r \to \infty$. If we choose the wave amplitude at infinity to be 1, the following results are obtained: The peak amplitudes of the wave functions shown in Fig. 2 are (from top to bottom); 5.00, 18.67, and 225.25. The peak amplitudes (inside the particle) for the wave functions shown in Fig. 3 are (from top to bottom) 0.379, 18.67, and 0.274.

The picture that has been developed in this section, which portrays an MDR as a quasi-bound state, trapped in a potential well and connected to the outside world by tunneling, gives added intuition and insight into the nature of electromagnetic scattering resonances. This intuition is especially valuable for more-complicated problems in which the particle has a layered structure[12] or a continuously varying index of refraction.[13]

C. Particles With Negative Dielectric Functions

The dielectric function $\epsilon(\omega)$ of many materials is negative over a portion of the frequency spectrum. Examples are metals in the range $\omega < \omega_p$, where ω_p is the plasma frequency, and crystalline solids, such as NaCl, in the range $\omega_T < \omega < \omega_L$, where ω_T and ω_L are the transverse and longitudinal optical frequencies.[14] In this discussion let us assume that the real part of the dielectric function is negative and that the imaginary part is small and can be set equal to zero. The index of refraction is related to the dielectric function by $m^2 = \epsilon$. Thus at a frequency where $m^2 < 0$ the potential function given by Eq. (17) is a positive quantity.

As the first example case, consider a layered particle with a positive dielectric core covered by negative dielectric layer. The core has a radius $a_1 = 1.0$ and an index of refraction $m_1 = 1.47$. The outer layer has a thickness $\Delta a = 0.05$ and an index of refraction $m_2 = 0.8i$ (where i is the imaginary unit). The potential function $V_n(r)$ for the case $n = 40$ and $k = 45$ is shown, plotted to scale, in Fig. 4. The bottom of the potential well is $k_B = (n + 1/2)/m_1$. This is the same as in the previous example problem. However, there is no top to the potential well as defined previously. That is, there is no value k_T for which k^2 coincides with the top of the well. As the value of k^2 is increased, the top of the barrier also increases in such a manner that it always exceeds k^2. The wave function can tunnel through this barrier and become temporarily trapped in resonant states, just as in the previous analysis.

Consider next a sphere that is composed entirely of a negative dielectric material. This is an interesting system because it has both scattering-state and bound-state solutions. This occurs because the potential defined by Eq. (17) changes from a repulsive barrier when $k^2 > 0$ to an attractive potential well when $k^2 < 0$. To illustrate this, we consider a particle of radius $a = 1.0$ and an index of refraction $m = 0.8i$. Figure 5(a) shows the potential $V_n(r)$ and the energy level k^2 for the case $n = 40$ and $k = 45$. The potential forms a repulsive barrier that keeps the wave function from penetrating beyond a skin depth into the particle. The region inside the particle is classically forbidden, and the region outside is classically allowed. This situation is reversed if we let $k^2 < 0$. Then the classically allowed region is inside the particle and the classically forbidden region is outside. This is shown in Fig. 5(b), where the system is identical to that in Fig. 5(a) with the exception that we now let $k = 70i$. Because $k^2 < 0$, the potential is negative. Thus an attractive potential well is formed as shown. This situation is analogous to the quantum-mechanical bound-state problem. Only selected eigenvalues of k^2 are allowed because the wave function must satisfy boundary conditions similar to those for resonances. The difference, in this case, is that the wave function cannot tunnel through a barrier but must continue to decay exponentially to zero. Thus these are true bound states. There is no radiative energy loss. (However, the inevitable internal energy loss that occurs in any real system will cause these modes to decay. In order for these modes to exist there must be some mechanism to pump energy into them to replace the internal losses.) A part of the wave function penetrates into the forbidden region outside the sphere to form an evanescent wave near the surface of the sphere.

The allowed eigenvalues of k can be computed in a manner analogous to that used to calculate the locations of the resonances. The spectrum of eigenvalues, $k_{n,l}^2$, forms a sequence of negative values that begins at the upper (least negative) value and decreases in quantized steps for $l = 1, 2, 3, \ldots$. An upper bound to this sequence is obtained when k^2 coincides with the bottom of the potential well. This upper bound (which is a negative number) is given by

$$k_U^2 = [n(n + 1)]/m^2a^2. \tag{25}$$

For the example I am considering, $k_U^2 = -2562.5$ (i.e., $k_U = 50.62i$). The spectrum of eigenvalues $k_{n,l}^2$ begins at a value below this upper bound and forms a decreasing sequence of quantized levels that continues without end. In quantum mechanics the energy eigenvalues begin at a ground state near the bottom of the potential well and increase in quantized steps. At first sight the present system does not seem to behave in this way since the eigenvalues decrease in quantized steps. The reason for the apparent difference is that the bottom of the potential well is decreasing at an even faster rate than the eigenvalues $k_{n,l}^2$. Therefore the interval between the levels

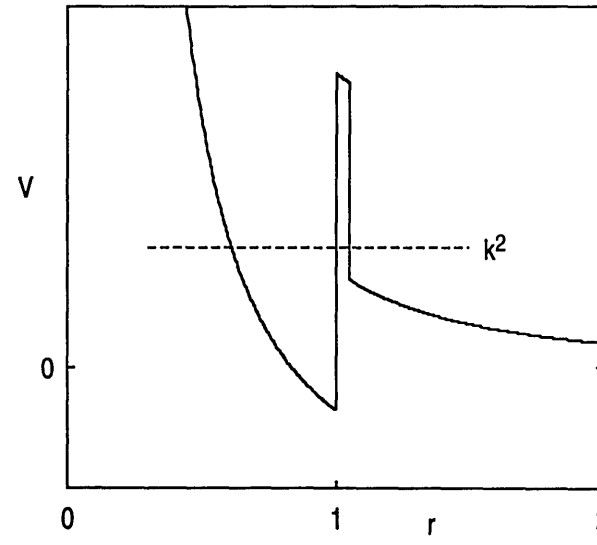

Fig. 4. Effective potential function for a layered sphere with a positive dielectric core covered by a negative dielectric layer.

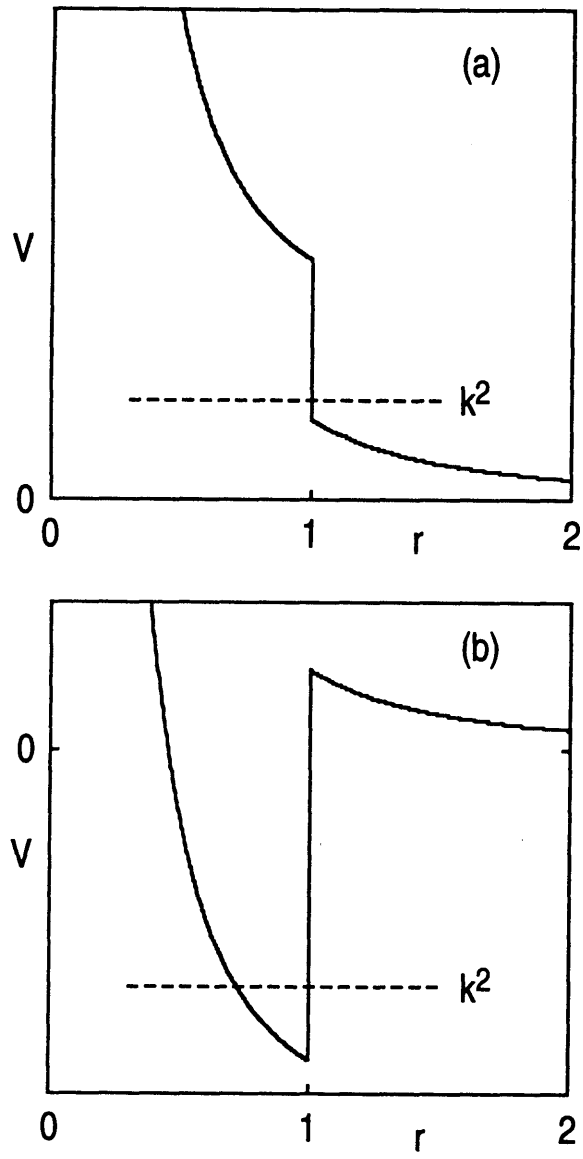

Fig. 5. Effective potential associated with a negative dielectric particle. (a) $k^2 > 0$, (b) $k^2 < 0$.

$k_{n,l}{}^2$ and the bottom of the well actually increases in quantized steps exactly as in the quantum-mechanical case.

4. RESONANCE WIDTHS

Useful exact analytic expressions for calculating resonance widths are derived in this section. These formulas cover the four cases involving TE and TM resonances for both real and complex indices of refraction.

A. TE Resonance, Real Index of Refraction

A TE resonance is characterized by a sharp peak in the real part of the $b_n(x)$ coefficient.[1] The resonance is located at a size parameter that satisfies the relation $\beta_n(x_0) = 0$. Since the index of refraction is real, it follows from Eq. (14a) that the function $\beta_n(x)$ is real. This fact, combined with Eq. (15a), gives the following expression for the real part of $b_n(x)$:

$$\mathrm{Re}[b_n(x)] = \frac{1}{1 + \beta_n{}^2(x)}. \tag{26}$$

At the center of the resonance this function has a maximum value $\mathrm{Re}[b_n(x_0)] = 1$, which drops off sharply on either side of x_0. The width of the resonance, $w_n(x_0)$, is defined to be the distance between the points $x_{\pm 1}$ on either side of x_0 where the amplitude has decreased to half its maximum value, i.e., to $\mathrm{Re}[b_n(x_{\pm 1})] = 1/2$. It follows from Eq. (26) that the half-amplitude points satisfy the relation $\beta_n{}^2(x_{\pm 1}) = 1$.

To a good approximation, the function $\beta_n(x)$ can be represented by the linear term of a Taylor series expansion around x_0:

$$\beta_n(x) = \beta_n'(x_0)\,(x - x_0), \tag{27}$$

where the prime denotes the derivative with respect to x. Within this linear approximation the half-amplitude points are $x_{\pm 1} = x_0 \pm \Delta x$, where $\beta_n'(x_0)\,\Delta x = 1$. Thus the width is given by

$$w_n(x_0) = \frac{2}{\beta_n'(x_0)}. \tag{28}$$

Differentiate expression (14a) with respect to x and evaluate the result at x_0. The result is

$$\beta_n'(x_0) = -\frac{\chi_n(x_0)}{\psi_n(x_0)}\left[\frac{m^2 D_n'(mx_0) - G_n'(x_0)}{mD_n(mx_0) - D_n(x_0)}\right]. \tag{29}$$

This expression can be simplified with the aid of the following formulas:

$$D_n'(x) = [n(n+1)]/x^2 - 1 - D_n{}^2(x), \tag{30a}$$

$$G_n'(x) = [n(n+1)]/x^2 - 1 - G_n{}^2(x), \tag{30b}$$

$$G_n(x) - D_n(x) = [\psi_n(x)\chi_n(x)]^{-1}. \tag{31}$$

The last-named formula was obtained by use of the Wronskian relation for Riccati–Bessel functions.

Substitute the derivatives given by Eq. (30) into Eq. (29). Then use Eq. (24a) to replace $mD(mx_0)$ by $G(x_0)$. Finally, use Eq. (31) to simplify the result. The result of all this manipulation is a simple expression for $\beta_n'(x_0)$, which can be substituted into Eq. (28) to give the following simple analytic formula for the width of a TE resonance:

$$w_n(x_0) = \frac{2}{(m^2 - 1)\chi_n{}^2(x_0)}. \tag{32}$$

B. TM Resonance, Real Index of Refraction

Using the same analysis as in the previous case, one obtains the following expression for the width of a TM resonance:

$$\overline{w}_n(x_0) = \frac{2}{\alpha_n'(x_0)}. \tag{33}$$

Differentiate expression (14b) to obtain

$$\alpha_n'(x_0) = -\frac{m\chi_n(x_0)}{\psi_n(x_0)}\left[\frac{G_n'(x_0) - D_n'(mx_0)}{mD_n(x_0) - D_n(mx_0)}\right]. \tag{34}$$

Equations (30), (31), and (24b) are then used to simplify this expression. Substitute the simplified result into Eq. (33) to obtain the following exact formula for the TM

resonance:

$$\overline{w}_n(x_0) = 2\Big/\left\{(m^2 - 1)\chi_n^{\,2}(x_0)\left[\frac{n(n+1)}{m^2 x_0^{\,2}} + G_n^{\,2}(x_0)\right]\right\}. \tag{35}$$

The analytic formulas (32) and (35) are exact; i.e., they give results identical to those obtained by precise numerical calculations of the resonance widths.

C. TE Resonance, Complex Index of Refraction

If the index of refraction is allowed to become complex, the function $\beta_n(x)$, which depends parametrically on $m = m_r + im_i$, will also be complex. To indicate this dependence explicitly, let us write $\beta_n(m; x)$. The Taylor series expansion of $\beta_n(m; x)$, which was carried out above with respect to the size parameter x, can be extended to also include an expansion with respect to the index of refraction m. The size parameter x will be expanded around the resonance point x_0, as in the previous analysis, and the index of refraction m will be expanded along the imaginary axis around the point $m = m_r$. The result is

$$\beta_n(m; x) = \beta_n'(m_r, x_0)(x - x_0) + i\gamma_n(m; x), \tag{36}$$

where the imaginary component $\gamma(m; x)$ is given by

$$\gamma_n(m; x) = m_i \times \left[\frac{\partial \beta_n(m; x)}{\partial m}\right]_{m=m_r}. \tag{37}$$

The subscript on the bracketed expression indicates that the derivative is to be evaluated at $m = m_r$.

Substitute linear approximation (36) into formula (15a) and calculate the real part of $b_n(x)$. The result is

$$\mathrm{Re}[b_n(x)] = [1 + \gamma_n]/\{[1 + \gamma_n]^2 + [\beta_n'(x - x_0)]^2\}. \tag{38}$$

This function exhibits a resonance peak centered at x_0. Thus the position of the resonance is not altered by the addition of a small imaginary component to the index of refraction. However, the maximum value of the resonance peak at x_0 is changed. Evaluating Eq. (38) at x_0 gives

$$\mathrm{Re}[b_n(x_0)] = 1/(1 + \gamma_n). \tag{39}$$

The width of the resonance is defined to be the distance between the points where the amplitude has decreased to half of its maximum value. Thus

$$\mathrm{Re}[b_n(x_0 \pm \Delta x)] = 1/2(1 + \gamma_n), \tag{40}$$

where Δx is half of the width. Using Eqs. (38) and (40), we obtain $\beta_n'\Delta x = 1 + \gamma_n$. This expression can be solved for Δx. Then use the relation $w_n(m_i; x_0) = 2\Delta x$ and Eq. (28) to obtain

$$w_n(m_i; x_0) = w_n(0; x_0)[1 + \gamma_n], \tag{41}$$

where $w_n(m_i; x_0)$ is the width of the resonance at x_0 for the case $m_i \neq 0$ and $w_n(0; x_0)$ is the width of the same resonance with $m_i = 0$.

The peak amplitude of the function $\mathrm{Re}[b_n(x)]$ at x_0 is called the resonance height[15] and is denoted by $H_n(m_i; x_0)$. Combine Eqs. (39) and (41) to obtain the following useful expression:

$$H_n(m_i; x_0) = \frac{w_n(0; x_0)}{w_n(m_i; x_0)}. \tag{42}$$

This formula shows that the product of the height and the width of the resonance is a constant, equal to the undamped width $w_n(0; x_0)$. The resonance height is a useful quantity because it is a measure of how much a resonance is suppressed by the internal energy absorption. If no energy is absorbed, the height has a maximum value of 1. If the height is much less than 1, then the resonance is, for all practical purposes, suppressed out of effective existence.

Differentiate Eq. (14a) with respect to m to get

$$\frac{\partial \beta_n}{\partial m} = -\frac{\chi_n(x_0)}{\psi_n(x_0)}\left[\frac{D_n(mx_0) + mx_0 D_n'(mx_0)}{mD_n(mx_0) - D_n(x_0)}\right]. \tag{43}$$

Use Eqs. (30), (31), and (24a) to simplify this expression. The result is

$$\frac{\partial \beta_n}{\partial m} = \frac{x_0 \chi_0^{\,2}(x_0)}{m}\{[m^2 - 1] - [G_n'(x_0) + G_n(x_0)/x_0]\}. \tag{44}$$

Substitute this into Eq. (37) to get

$$\gamma_n(m; x_0) = \chi_n^{\,2}(x_0)(m_r^{\,2} - 1)\frac{m_i}{m_r}[1 - \epsilon_n]x_0, \tag{45}$$

where ϵ_n is given by

$$\epsilon_n = \frac{1}{(m_r^{\,2} - 1)}[G_n'(x_0) + G_n(x_0)/x_0]. \tag{46}$$

Combine the results contained in expressions (32), (41), and (45) to obtain the following formula for the width of a TE resonance:

$$w_n(m_i; x_0) = w_n(0; x_0) + 2x_0\frac{m_i}{m_r}(1 - \epsilon_n). \tag{47}$$

The quantity ϵ_n can be evaluated by an approximate semiclassical WKB analysis. The result shows that $|\epsilon_n| \approx O[1]/n$, where $O[1]$ is a number of order unity. Therefore, for most resonances, $|\epsilon_n| \ll 1$, and, to a good approximation, it can be neglected in Eq. (47). Thus the final simplified result for the width of a TE resonance is

$$w_n(m_i; x_0) = \frac{2}{(m_r^{\,2} - 1)\chi_n^{\,2}(x_0)} + 2x_0\frac{m_i}{m_r}. \tag{48}$$

The first term in this expression is proportional to the radiative energy loss from the particle, and the second term is proportional to the internal energy absorption in the particle.[1] The second term was derived previously by Arnold, who used a physical argument based on a consideration of the absorptive energy losses in a cavity.[16] This term prevents the extremely narrow resonances that are

sometimes predicted by theory when m_i is neglected. Formulas (47) and (48) show that the width is a linear function of m_i, as was previously reported.[15,17] Recent experimental results are consistent with this formula.[18]

This result can be used in Eq. (42) to calculate the height of the resonance. It is apparent that, in cases in which the undamped resonance width $w_n(0; x_0)$ is extremely small, a small value of m_i can lead, for all practical purposes, to the complete suppression of the resonance.

D. TM Resonance, Complex Index of Refraction

The analysis of this case is identical to that of the previous case, with α_n and a_n replacing β_n and b_n. Formula (14b) for $\alpha_n(m; x)$ must be differentiated with respect to m. The result, after simplifying with the aid of Eq. (24b), is

$$\frac{\partial \alpha_n}{\partial m} = -\frac{\chi_n(x_0)}{\psi_n(x_0)}\left[\frac{x_0 D_n'(mx_0) - G(x_0)}{G(x_0) - D(x_0)}\right]. \tag{49}$$

This result can be further simplified with the use of Eqs. (31), (30a), and (24b). The result is

$$\frac{\partial \alpha_n}{\partial m} = \frac{\chi_n^2(x_0)}{m}\left[x_0 + m^2 x_0 G_n^2(x_0) - \frac{n(n+1)}{m^2 x_0}\right]. \tag{50}$$

Then, with the aid of expressions (35) and (41), I obtain the following formula for the width of the TM resonance:

$$\overline{w}_n(m_i; x_0) = \overline{w}_n(0; x_0) + 2x_0\frac{m_i}{m_r}(1 - \bar{\epsilon}_n), \tag{51}$$

where

$$\bar{\epsilon}_n = \frac{G_n'(x_0) - G_n(x_0)/x_0}{(m^2 - 1)\left[G_n^2(x_0) + \dfrac{n(n+1)}{m^2 x_0^2}\right]}. \tag{52}$$

Similar remarks apply to the quantity $\bar{\epsilon}_n$ as applied to the quantity ϵ_n defined by Eq. (46). For most resonances, $|\bar{\epsilon}_n| \ll 1$ and can be neglected. Therefore the final simplified result for the width of a TM resonance is

$$\overline{w}_n(m_i; x_0) = \frac{2}{(m_r^2 - 1)\chi_n^2(x_0)\left[\dfrac{n(n+1)}{m_r^2 x_0^2} + G_n^2(x_0)\right]} + 2x_0\frac{m_i}{m_r}. \tag{53}$$

5. SUMMARY AND CONCLUDING REMARKS

The analogy between the radial Schrödinger equation and the differential equations for the radial Debye potentials has been exploited for the purpose of analyzing electromagnetic scattering resonances. These resonances are shown to be analogous to quantum-mechanical shape resonances. The picture developed in this paper views these resonances as a quasi-bound states, temporarily trapped in a potential well of the type illustrated in Fig. 1. This viewpoint provides some immediate intuitive insights into the nature of these resonances. For example, the top and the bottom of the potential well determine effective upper and lower bounds for the resonance levels. The resonance widths, which are inversely proportional to the decay time of the quasi-bound state, are determined by the rate at which energy can tunnel through the outer barrier of the potential well. Since the lower levels must tunnel through a larger barrier, the lower levels have a longer lifetime and thus have narrower widths than the upper levels.

The condition that defines a shape resonance is similar to the condition that defines a bound state in a potential well. This condition states that the wave function must decrease exponentially in the classically forbidden regions outside the well. The application of this boundary condition leads directly to Eqs. (24a) and (24b). These are the same equations that have been derived in the theory of MDR's.[1] Figures 2 and 3 show the dramatic change that occurs in the wave function at resonance. These figures show how the exponential behavior of the wave function in the classically forbidden region is responsible for the large electric field amplitudes near the surface of a particle at resonance.

The interpretation of resonances as the quasi-bound states of a potential well can be applied to more complicated systems than a simple dielectric sphere. I briefly described one such system, a layered sphere with a negative dielectric outer layer. (The potential function for this case is illustrated in Fig. 4.) It is obvious that one can use similar analysis to consider more-complicated problems in which the particle has a multilayered structure[12] or a continuously varying index of refraction.[13] This approach offers intuitive insights into these more complicated resonance problems than is available in the traditional picture, which views a resonance as a wave propagating around the sphere, confined by internal reflections.[1]

We have also used this analysis to describe briefly the interesting case of a negative dielectric sphere. This problem is interesting because the system has two distinct types of solution. We refer to these as the positive-energy ($k^2 > 0$) and negative-energy ($k^2 < 0$) solutions. For the positive-energy solution the potential in the interior of the particle is a repulsive barrier [illustrated in Fig. 5(a)], which keeps the wave function outside. This is a traditional scattering problem that can be calculated by Mie theory. For the negative-energy solution the potential inside the particle is a deep well [illustrated in Fig. 5(b)]. This case is not a resonance problem, but it is similar and can be analyzed by the same methods. In this case the energy cannot tunnel out of the well; therefore the electromagnetic modes are true bound states. If it were not for the inevitable internal losses, these states would have an infinite lifetime. These modes exist inside the particle, with only a surface evanescent wave penetrating outside the particle.

Exact analytic formulas for resonance widths were developed in Section 4. The final useful and simplified results are contained in the two formulas (48) and (53). These formulas predict the widths of TE and TM resonances, respectively, for both complex ($m_i \neq 0$) and real ($m_i = 0$) indices of refraction.

Note added in proof: I have become aware of a recent work in which formulas for resonance widths are derived by asymptotic analysis.[19]

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