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The static electric polarizability of a particle bound by a finite potential well

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We derive an expression for the static electric polarizability of a charged particle bound by a finite potential well by employing the elegant Dalgarno-Lewis perturbative technique. The derivation does not make explicit use of the continuum states, is much simpler than the usual perturbation derivation, and allows us to separate the contributions to the polarizability from the classically forbidden and classically allowed regions of the finite potential well. © *2011 American Association of Physics Teachers.*

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I. INTRODUCTION

The finite potential well provides an example of a spectrum of wave functions which includes bound and continuum (unbound) states. The bound states give the probability of a particle to be in the classically forbidden region where the total energy of the system is less than its potential energy.

In this paper, we discuss an example of the effectiveness and simplicity of the method of Dalgarno and Lewis[1] to determine the shift of the energy eigenvalues to second order in perturbation theory due to the interaction of an applied static electric field and a charged particle which is bound by a finite potential well. The energy shift due to this interaction is used to calculate the electric polarizability. The conventional method used to calculate the energy shift to second order involves an infinite sum or an integral that contains all possible states connected to the ground state by the interaction.[2] Some of these states, for example, scattering (unbound) states, can be very difficult or impossible to obtain in a large number of problems. With the use of the Dalgarno-Lewis method, knowledge of the scattering states is unnecessary.[2,3] It also allows us to highlight the contribution of the wave function in the classically forbidden region to the electric polarizability.

The method of Dalgarno and Lewis is not limited to simple models and has been used to determine the electric polarizability of the hydrogen atom[4,5] and the deuteron.[6]

The use of perturbation theory is suspect because a series in powers of the applied electric field strength does not converge due to the fact that an unbound solution with lower energy always exists.[7,8] Because the potential due to the electric field varies linearly with the displacement of the charged particle from the origin of the potential, a solution will always exist that corresponds to ionization of the charged particle. However, for laboratory-sized fields, second-order perturbation gives useful and physically correct results because the tunneling probability is extremely small, and the charged particle remains bound, with a small shift in energy.

II. THE DALGARNO-LEWIS METHOD

The method of Dalgarno and Lewis replaces the conventional way of calculating the energy shift in second-order perturbation theory with the solution of an inhomogeneous differential equation. We summarize here the basic results of the method. More details can be found in Refs. 1, 4, 5, 9, and 10.

The shift ΔE_0 of the ground state energy to second order in the applied electric field is given by

$$\Delta E_0 = \sum_{n=1}^{\infty} \frac{\langle \psi_0 | H' | \psi_n \rangle \langle \psi_n | H' | \psi_0 \rangle}{E_0 - E_n}. \tag{1}$$

Here ψ_0 is the ground state of the unperturbed system with ground state energy E_0. The functions ψ_n represent the excited states of the unperturbed system and H' is the perturbation Hamiltonian.

The first-order correction ϕ to the unperturbed state can be written as[4]

$$|\phi\rangle = \sum_{n=1}^{\infty} \frac{|\psi_n\rangle \langle \psi_n | H' | \psi_0 \rangle}{E_0 - E_n}. \tag{2}$$

The ket $|\phi\rangle$ satisfies the inhomogeneous differential equation,

$$(E_0 - H_0)|\phi\rangle = H'|\psi_0\rangle - \langle \psi_0 | H' | \psi_0 \rangle |\psi_0\rangle, \tag{3}$$

where H_0 is the unperturbed Hamiltonian. If we operate with H' on Eq. (2) and then take the inner product with ψ_0, we obtain the expression in Eq. (1), so that ΔE_0 can be written in terms of only ϕ, ψ_0, and H',

$$\Delta E_0 = \langle \psi_0 | H' | \phi \rangle. \tag{4}$$

To obtain ΔE_0 using the Dalgarno-Lewis method, we first solve Eq. (3) for ϕ. The final step is to use ϕ in Eq. (4) to obtain ΔE_0. The only stationary state we need is ψ_0, and we completely avoid the infinite sum in Eq. (1).

We next consider what we gain by avoiding the infinite sum and how we take advantage of the Dalgarno-Lewis method in obtaining the electric polarizability for the proposed model. Consider a charged particle bound by a finite potential well. The potential energy $V(x)$ is given by

$$V(x) = \begin{cases} -V_0 & \text{for } (-a < x < a) \\ 0 & \text{otherwise}, \end{cases} \tag{5}$$

where $2a$ is the width of the well. The one-dimensional Schrödinger equation for $V(x)$ in Eq. (5) produces a spectrum of bound states with even and odd parities, in addition to a continuum of unbound states.[11–13] The latter states $(E > 0)$

are given by oscillatory functions which extend to $x \to \pm\infty$.[12,13] Such states require careful attention in the sums, which present considerable mathematical difficulty. To our knowledge, an exact result for ΔE_0 for the finite potential has not been obtained using the infinite sum in Eq. (1).

The Dalgarno-Lewis method uses only the unperturbed ground state, ψ_0, to calculate the exact value of ΔE_0. The ground state ψ_0 has even parity and is given by[11]

$$\psi_0(x) = \begin{cases} N \cos K_0 a e^{k_0(x+a)} & (x < -a) \\ N \cos K_0 x & (-a < x < a) \\ N \cos K_0 a e^{-k_0(x-a)} & (x > a), \end{cases} \tag{6}$$

where E_0 is the eigenenergy of the state ψ_0 and is negative, $K_0^2 = (2m/\hbar^2)(V_0 - |E_0|)$, $k_0^2 = 2m|E_0|/\hbar^2$, and $K_0 a < \pi/2$. The normalization constant N is given by

$$N = \frac{1}{\sqrt{a}} \frac{1}{[1 + \sin K_0 a \cos K_0 a / K_0 a + \cos^2 K_0 a / k_0 a]^{1/2}} \tag{7a}$$

$$= \frac{1}{\sqrt{a}} \frac{1}{[1 + \sin \gamma_0 \cos \gamma_0 / \gamma_0 + \cos^2 \gamma_0 / \beta_0]^{1/2}}, \tag{7b}$$

where $\gamma_0 = K_0 a$ and $\beta_0 = k_0 a$. The electric dipole perturbation H' can be written as[2,3]

$$H' = -q\epsilon x. \tag{8}$$

The electric field ϵ is applied in the positive x direction and is assumed to exist both inside and outside the potential well. The electric polarizability α is then obtained from the definition $\Delta E_0 = -\alpha\epsilon^2/2$.

III. DERIVATION OF THE POLARIZABILITY

We rewrite Eq. (3) in the coordinate representation as

$$\left[E_0 + \frac{\hbar^2}{2m}\left(\frac{d^2}{dx^2}\right) - V(x)\right]\phi(x) = -q\epsilon x \psi_0(x). \tag{9}$$

The second term on the right-hand side of Eq. (3) vanishes because H' has odd parity and ψ_0 has even parity. Similarly, the energy shift to first order is equal to zero. We need to calculate $\phi(x)$ for $x < -a$, $|x| < a$, and $x > a$ separately. The function $\phi(x)$ and its derivative satisfy continuity conditions at the boundaries just like the unperturbed states [see Eq. (2)]. In addition, $\phi(x)$ has odd parity because in standard nondegenerate perturbation theory, the corrections to the unperturbed bound state are orthogonal to it. Consequently, Eq. (9) must be solved separately in just two regions.

The solution of an inhomogeneous second-order differential equation requires a linear combination of the solutions to the homogeneous equation along with a particular solution determined by integrals involving the Wronskian and the homogeneous solutions. In this case the solutions to the homogenous equation are well known, either decaying exponentials or oscillatory functions, depending on the region. To obtain the particular solution we follow the procedure in Ref. 14, which involves products of linear and quadratic functions in x with sinusoidal and exponential functions. The result is

$$\phi(x) = \begin{cases} \eta \dfrac{\cos \gamma_0}{\beta_0^3} e^{k_0(x+a)}[-(k_0 x)^2 + k_0 x - c_1] & (x < -a) \\ \dfrac{\eta}{\gamma_0^3}[c_2 \sin(K_0 x) - (K_0 x)\cos(K_0 x) - (K_0 x)^2 \sin(K_0 x)] & (-a < x < a) \\ \eta \dfrac{\cos \gamma_0}{\beta_0^3} e^{-k_0(x-a)}[+(k_0 x)^2 + k_0 x + c_1] & (x > a). \end{cases} \tag{10}$$

Here, $\eta \equiv mq\epsilon a^3 N/(2\hbar^2)$ and c_1 and c_2 are constants. We have already used the fact that $\phi(x)$ decays as $x \to \pm\infty$ and must be odd. In addition, the solutions must match at $x = \pm a$, which yields two conditions for the constants c_1 and c_2 leading to

$$c_1 = \tan^3 \gamma_0 \{\gamma_0 + (1 - \gamma_0^2)\cot \gamma_0 - \gamma_0 \cot^2 \gamma_0\} \tag{11}$$

and

$$c_2 = (\gamma_0 + \cot \gamma_0)^2. \tag{12}$$

Equation (4) gives the change in energy. If we use

$$\Delta E_0 = -\tfrac{1}{2}\alpha\epsilon^2 = -\tfrac{1}{2}(\alpha_{\text{in}} + \alpha_{\text{out}})\epsilon^2, \tag{13}$$

we can express the solution in terms of the polarizability, α.

Note that the Dalgarno-Lewis method allows us to separate the total polarizability into α_{in} and α_{out}, which represent the classically allowed contributions from the wave function in the well region ($-a < x < a$) and the classically forbidden contributions from outside the well region ($|x| > a$), respectively. Such a separation is useful for understanding the role of the wave function in the "forbidden" region, which is impossible with standard perturbation theory. For $|x| < a$, we obtain, after eliminating β_0 in favor of γ_0 and switching integration variables to $u \equiv K_0 x$,

$$\alpha_{\text{in}} = \frac{mq^2a^4}{\hbar^2} \frac{1}{\gamma_0^4} \frac{1}{\gamma_0 + \cot \gamma_0} \int_0^{\gamma_0} du[c_2 u \sin 2u - u^3 \sin 2u - u^2 \cos 2u - u^2]. \tag{14}$$

The integrals are straightforward, and the final result is

$$\alpha_{\rm in} = \frac{mq^2a^4}{\hbar^2}\frac{1}{\gamma_0^4}\frac{1}{\gamma_0+\cot\ \gamma_0}\left[\frac{1}{2}\cot\ \gamma_0\left(1+\frac{3}{2}\sin^2\ \gamma_0\right)+\frac{5}{4}\gamma_0\left[1-\frac{2}{5}(\cot^2\ \gamma_0+\cos^2\ \gamma_0)\right]-\gamma_0^2\cot\ \gamma_0-\frac{1}{3}\gamma_0^3\right]. \tag{15}$$

For the infinite square well $\gamma_0 \to \pi/2$, and

$$\alpha_{\rm in} \to \frac{mq^2a^4}{\hbar^2}\frac{20}{\pi^4}\left(1-\frac{\pi^2}{15}\right) \approx 0.07022\frac{mq^2a^4}{\hbar^2} \quad (V_0 \to \infty), \tag{16}$$

which is the known result.[10] For the δ-function potential we take the limit $2a \to 0$ with $V_0 \to \infty$, while the product aV_0 remains constant, and we obtain

$$\alpha_{\rm in} \to \frac{mq^2a^3}{6\hbar^2K_0^2} \to 0 \quad (V_0 \to \infty \ \text{as} \ a \to 0). \tag{17}$$

For $|x|>a$ we change integration variables to $u \equiv k_0x$ and obtain

$$\alpha_{\rm out} = \frac{mq^2a^4}{\hbar^2}\frac{2}{\beta_0^4}\frac{\cos^3\ \gamma_0}{\gamma_0\sin\ \gamma_0+\cos\ \gamma_0}\int_{\beta_0}^{\infty} du(u^3+u^2+c_1u)e^{-2(u-\beta_0)}, \tag{18}$$

and integration gives

$$\alpha_{\rm out} = \frac{mq^2a^4}{\hbar^2}\frac{1}{2\beta_0^4}\frac{\cos^3\ \gamma_0}{\gamma_0\sin\ \gamma_0+\cos\ \gamma_0}\times\left[\frac{5}{2}+5\beta_0+5\beta_0^2+2\beta_0^3+c_1(1+2\beta_0)\right]. \tag{19}$$

We have expressed Eq. (19) in terms of β_0 and c_1 because rewriting them in terms of γ_0 alone would complicate the expression with no apparent simplification. The limit for the infinite well potential can be taken, with $\gamma_0 \to \pi/2$, which leads to $\beta_0 \to (\pi/2)/\cos\ \gamma_0 \to \infty$ and $c_1 \to (\pi/2)/\cos^3\ \gamma_0 \to \infty$. Hence,

$$\alpha_{\rm out} \to \frac{mq^2a^4}{\hbar^2}\frac{4}{\pi^3}\cos^3\ \gamma_0 \to 0 \quad (V_0 \to \infty). \tag{20}$$

For the δ-function potential, both β_0 and c_1 approach zero because the well width $2a \to 0$, so that Eq. (19) yields

$$\alpha_{\rm out} \to \frac{5}{4}\frac{mq^2}{\hbar^2k_0^4} \quad (V_0 \to \infty \ \text{as} \ a \to 0), \tag{21}$$

which is the correct result.[2]

The limit for a very shallow well ($V_0 \to 0$ as $2a$ remains fixed) follows a similar procedure as for the δ-function potential. We obtain

$$\alpha_{\rm in} \to \frac{mq^2a^4}{\hbar^2}\frac{8}{3\pi^2}\frac{E_G}{V_0} = \frac{mq^2a^4}{\hbar^2}\frac{2}{3}\frac{1}{R^2} \quad (V_0 \to 0) \tag{22}$$

and

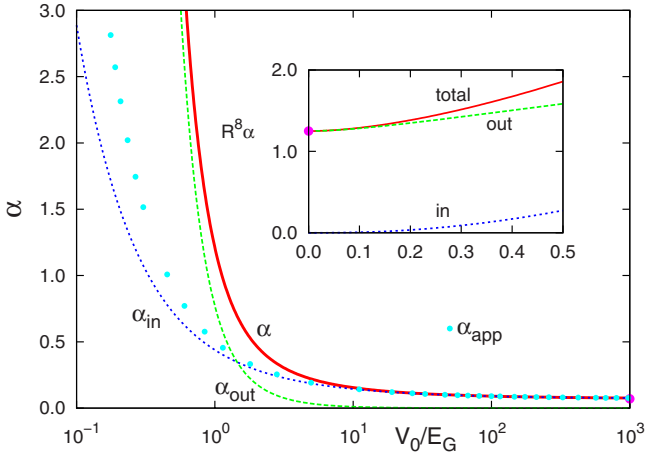

Fig. 1. Change in the polarizability α (plotted in units of $mq^2a^4/\hbar^2$) as a function of well depth (logarithmic scale). The solid curve gives the total contribution, the dotted curve gives the contribution from $x<|a|$, and the dashed curve gives the contribution from $x>|a|$. The filled circle at the far right indicates the limit, $\alpha=0.070225mq^2a^4/\hbar^2$, derived analytically in Eq. (16) for an infinite square well. There is a crossover from where the entire contribution comes from inside the well (large V_0) to where the polarizability is dominated from contributions from outside the square well (small V_0). The small filled circles are obtained by a straightforward approximation based on the infinite square well [see Eq. (26)]. This approximation is accurate for $R \gtrsim 4$, the same domain of accuracy for the ground state energy (Ref. 15). In the inset α is multiplied by R^8 to highlight the divergence of the polarizability as the potential well strength decreases, where most of the contribution comes from outside the well. The point at (0, 5/4) is the analytical limit, as discussed in the text. Note that the abscissa in the inset is the same as for the main figure, but in the inset V_0/E_G uses a linear scale starting from zero.

$$\alpha_{\rm out} \to \frac{mq^2a^4}{\hbar^2}\frac{320}{\pi^8}\left(\frac{E_G}{V_0}\right)^4 = \frac{mq^2a^4}{\hbar^2}\frac{5}{4}\frac{1}{R^8} \quad (V_0 \to 0), \tag{23}$$

where

$$R^2 \equiv \frac{2ma^2V_0}{\hbar^2} \tag{24}$$

is a dimensionless measure of the potential strength and

$$E_G \equiv \frac{\pi^2\hbar^2}{2m(2a)^2} \tag{25}$$

is the ground state energy for an infinite potential well with width $2a$. (Note that $R^2=\pi^2V_0/4E_G$.) Both inside and outside contributions diverge as the energy of the ground state approaches the lower bound of an infinite number of continuum excited states. However, the outer contribution dominates because the wave function becomes increasingly extended as the well becomes shallower.

IV. DISCUSSION

Figure 1 illustrates how the polarizability changes with increasing potential well depth (on a logarithmic scale). The solid curve is the total polarizability from the sum of Eqs. (15) and (19); also indicated are the separate contributions from the regions inside [Eq. (15)] and outside [Eq. (19)] the well. For deep potential wells the contribution from inside the well region is dominant [dotted curve given by Eq. (15)] and for shallow wells the contribution from outside the well

dominates [dashed curve given by Eq. (19)]; the source of the different contributions is also apparent from the asymptotic expressions—for large V_0 α_{in} in Eq. (16) dominates α_{out} in Eq. (20) and for small V_0 α_{out} in Eq. (23) dominates α_{in} in Eq. (22). These asymptotic results are expected because the amplitude of the ground state wave function becomes very small outside the well as the depth increases. From the more traditional perspective, the low-lying excited states have minimal amplitude outside the well, so contributions from the low-lying states (which are the only ones required in the traditional treatment of the infinite square well[10]) become negligible.

As the well depth decreases, the polarizability diverges according to the power law derived in Sec. III, given by Eq. (23). To examine this divergence more closely we show $R^8\alpha_i$ (i=in, out, and total) as a function of V_0/E_G in the inset of Fig. 1 for small values of V_0. For small values of R, perturbation theory in the applied field becomes suspect, and as the well becomes increasingly shallow, the size of the applied electric field for which second-order perturbation theory remains valid decreases. The analytical limit for vanishing small potential well strength is achieved in the inset of Fig. 1 [filled circle at (0, 5/4)], and the analytical limit for infinitely large potential strength is indicated by a filled circle at the far right in the main plot.

The calculations presented in this paper are straightforward, but lengthy, and it is interesting to examine a possibility motivated by the work in Ref. 15, where it was shown that a finite potential well of width $2a$ and depth V_0 can be approximated by a wider infinite potential well of width $2b$ with $b=(1+1/R)a$. This approximation produces small errors in the eigenvalues and the eigenfunctions belonging to the lowest energy states for $R \gtrsim 4$.[15] For example, in comparing the approximate and the exact energy eigenvalue for the lowest two energy states at $R=4$, the errors are 0.7% for the lowest energy even parity state and 3% for the lowest energy odd parity state. The approximation also produces a small error for the probability densities of the two states as a function of x (see Fig. 3 of Ref. 15). These results are significant for a comparison with our results because the lowest energy state is the only state which we use in our calculation of the polarizability, and the transition $n=1$ to $n=2$ produces almost all the contribution to the polarizability in the infinite potential well.

The simplest approach would be to determine an approximation, α_{app}, by replacing the width a in Eq. (26) by b, so that α_{app} is given by

$$\alpha_{app} = 0.070225 \frac{mq^2a^4}{\hbar^2}\left(1+\frac{1}{R}\right)^4. \tag{26}$$

We include in Fig. 1 small dots to indicate this approximation. This approximation works well for $V_0/E_G=(2R/\pi)^2 > 10$, which is a similar range to that found for the ground state energy. For shallower wells, this approximation fails because $\alpha \propto 1/R^8$ in this regime.

V. CONCLUSION

We have derived an expression for the static electric polarizability α of a charged particle bound by a finite potential well. The only stationary state of the system which we have used in our calculation is the unperturbed ground state of the particle. The continuum is not required for the calculation of the polarizability.[2,3]

Perhaps most importantly, we have been able to separate out contributions from the classically allowed region within the well and from the classically forbidden region outside the well. To our knowledge this separation is only possible with the Dalgarno-Lewis method. In addition, we have recovered well known limits, for which it is clear that only the classically forbidden region (given by α_{out}) produces the entire result for the δ-function potential and only the classically allowed region (given by α_{in}) produces the entire result for the infinite potential well.

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