The dynamic electric polarizability of a particle bound by a double delta potential

M A Maize and J J Smetanka

Department of Physics, Saint Vincent College, 300 Fraser Purchase Road, Latrobe, PA 15650, USA

E-mail: anis.maize@email.stvincent.edu and john.smetanka@email.stvincent.edu

Received 13 January 2008, in final form 14 February 2008
Published 25 March 2008
Online at stacks.iop.org/EJP/29/497

Abstract
In this paper we derive an expression for the dynamic electric polarizability of a particle bound by a double delta potential for frequencies below and above the absolute value of the particle’s ground state energy. The derived expression will be used to study some of the fundamental features of the system and its representation of real systems. In addition we derive a general expression of the dynamic electric polarizability for a potential of multi-delta functions.

1. Introduction

The study of the electric polarizability, \( \alpha \), has been significant in many areas of physics. Calculation of \( \alpha \) has played an important role in educating us about the electromagnetic properties of atoms [1], the internal structure of nucleons [2, 3] and the basic properties of a solid [4], to name a few examples. Certainly, the study of the static electric polarizability, \( \alpha(0) \), has received more attention than the study of the dynamic polarizability, \( \alpha(\omega) \), at least at the level of a fundamental treatment [5]. From an educational point of view, determination of \( \alpha(\omega) \) gives an excellent example of the application of perturbation theory to the interaction of systems with time-dependent external sources. Second, \( \alpha(\omega) \) provides us with great knowledge of the dispersive electromagnetic properties of atoms based on the study of the linear response of the atomic charge to an external oscillating electric field of various frequencies, \( \omega \) [1, 6]. Third, we can obtain the static electric polarizability \( \alpha(0) \), by taking the static limit of \( \alpha(\omega) \). These are but a small fraction of the reasons we believe that the study of \( \alpha(\omega) \) is valuable to the basic learning of quantum mechanics and through its application enhancing our knowledge in many fields of physics and related disciplines.

Based on our fundamental knowledge of electromagnetism, application of an external electric field to a charge system can lead to charge displacement. The linear response of the
charge displacement (distortion) is expressed in terms of what we define as the induced electric dipole. The induced electric dipole is proportional to the applied field and the proportionality is given by the electric polarizability. To obtain the quantum $\alpha(\omega)$, we find the average of the electric dipole operator and divide it by the external time-dependent electric field, $\varepsilon(t)$ [5]. For the rest of the paper, the electric polarizability will always be in reference to the quantum mechanical problem.

The conventional perturbation method used to calculate either the static or dynamic electric polarizability involves an infinite sum or integral that contains all possible states allowed by the electric dipole transition [7]. Some of these states, for example, the scattering states, can be very difficult or impossible to obtain in a large number of cases [7]. In this work, the only states we are going to use in our calculation are the ground state of the unperturbed system and the complete set of the free particle states $|k\rangle (|k\rangle = \frac{1}{\sqrt{2\pi}} e^{ikx})$. With this choice we avoid unnecessary approximations and mathematical difficulties. Contrary to specialized papers, this work is beneficial to both advanced undergraduate and first-year graduate students.

The double delta potential has been used extensively for a variety of purposes [8–10]. Most notably, this potential has been employed to demonstrate the quantum features of a system that resembles the motion of an electron in the field of two nuclei [8]. A calculation of the eigenstates and eigenfunctions of the bound system of the double delta potential with comparison to the results for actual molecules had been reported by Lapidus [9]. Most recently, Bonfim and Griffiths considered the example of the double delta potential in presenting their approach to obtain closed form expressions for the bound-state energies in the one-dimensional problem [10].

In calculating $\alpha(\omega)$, we study the perturbative interaction between a charged particle, which is initially in the ground state of the system, and an applied time-dependent electric field [5]. As reported in [8–10], the double delta potential allows for one or two bound (negative energy) states. We will do our calculations for both cases while staying within the ‘non-degenerate’ conditions [10]. In section 2 we provide theoretical insight into how we calculate $\alpha(\omega)$ in the case of the double-delta potential. In addition we establish a general expression for $\alpha(\omega)$ in the case of the multi-delta potential. In section 3, we present our numerical results with analysis. Finally, we give concluding remarks.

### 2. Determination of $\alpha(\omega)$

The unperturbed Hamiltonian $H_0$ is given by

$$H_0 = -\hbar^2 \frac{\partial^2}{\partial x^2} - g[\delta(x + a) + \delta(x - a)],$$  

(1)

where $g$ is the strength of the potential and $m$ is the mass of the particle occupying the ground state. Now let $p = \frac{2mga}{\hbar}$. For $p < 1$, the solution of the wave equation $H_0\psi = E\psi$ will produce one bound (negative energy) state and a continuum of unbound states. The bound state, we will call $\psi_0$, is given by [8–10]

$$\psi_0(|x| > a) = N(k_0a) \cosh(k_0x) e^{-k_0(|x| - a)}$$  

(2a)

and

$$\psi_0(|x| < a) = N(k_0a) \cosh(k_0x),$$  

(2b)

where $N(k_0a) = \sqrt{\frac{2k_0}{e^{2k_0a} - 1}}$, $k_0$ is related to the bound state energy, $E_0$, by

$$E_0 = -\frac{\hbar^2 k_0^2}{2m},$$  

(3)
with $k_0$ and $g$ related by the equation

$$\frac{2mg}{\hbar^2} = k_0[1 + \tanh(k_0a)]. \quad (4)$$

For $p \geq 1$, a second bound (negative energy) state will satisfy (1) in addition to $\Psi_0$ and a continuum of unbound states. Let us call the second bound state $\Psi_1$ and its eigenenergy $E_1$, where $E_1 = -\frac{\hbar^2k_1^2}{2m}$. $\Psi_1$ is obtained by replacing $k_0$ by $k_1$ and the cosh function by the sinh function in (2a) and (2b). Also, $\Psi_1$ has an overall negative sign in the region $x < -a$. Here $k_1$ and $g$ are related by

$$\frac{2mg}{\hbar^2} = k_1[1 + \coth(k_1a)]. \quad (5)$$

As long as $p$ is not close to or greater than 5, $\Psi_0$ is the lowest energy state of the system. For $p$ close to or larger than 5, $E_0$ will be very close to $E_1$ and we will be in the region of double degeneracy [10]. For our calculation in this paper, we consider only the non-degenerate case, $p < 5$.

To determine $\alpha(\omega)$, we study the interaction between a particle of charge $q$ that is initially in the ground state of the system and an external time-dependent electric field of variable frequency $\omega$ [5]. Taking the electric field to be parallel to the $x$-axis, the basic expression of $\alpha(\omega)$ is [5]

$$\alpha(\omega) = -q^2 \left[ \int \langle \Psi_0 | x | k' \rangle \langle k' | G(\pm \omega) | k \rangle \langle k | \Psi_0 \rangle \, dk \, dk' \right. \right.$$

$$+ \left. \int \langle \Psi_0 | x | k' \rangle \langle k' | G(-\omega) | k \rangle \langle k | \Psi_0 \rangle \, dk \, dk' \right], \quad (6)$$

where the completeness of the free particle states $|k\rangle$ and $|k'\rangle$ has been employed. $q\hat{x}$ is the dipole operator with $G(\pm \omega)$ defined by

$$G(\pm \omega) = G(\pm \omega) + G(\pm \omega)V(x)G(\pm \omega), \quad (7)$$

with $V(x)$ being the binding potential. $G(\pm \omega)$ and $G_0(\pm \omega)$ are given in terms of $\hat{T}$, $H_0$, $\hbar\omega$ and $E_0$ by

$$G(\pm \omega) = \frac{1}{E_0 \pm \hbar\omega - H_0} \quad (8)$$

$$G_0(\pm \omega) = \frac{1}{E_0 \pm \hbar\omega - \hat{T}} \quad (9)$$

where $\hat{T} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2}$. To calculate $\alpha(\omega)$ (from (6)), we need to calculate the matrix elements $\langle \Psi_0 | x | k' \rangle$, $\langle k' | G(\pm \omega) | k \rangle$, and $\langle k | x | \Psi_0 \rangle$. Calculations of the matrix elements $\langle \Psi_0 | x | k' \rangle$ and $\langle k | x | \Psi_0 \rangle$ for either the double or the single delta can be done with a simple one-dimensional integration. To calculate $\langle k' | G(\pm \omega) | k \rangle$ for the multi-delta function potential, we first start with the simpler, general double-delta potential $V(x) = -[g_1\delta(x + a) + g_{-1}\delta(x - a)]$. Then we add delta functions at $+2a$ with strength $g_2$ and at $-2a$ with strength $g_{-2}$ and so on. With the aid of the detailed derivations of [11], $\langle k' | G(\pm \omega) | k \rangle$ for the multi-delta function potential can then be written as

$$\langle k' | G(\pm \omega) | k \rangle = G_{0k}(\pm \omega)\delta(k - k') - \frac{G_{kk}(\pm \omega)}{2\pi} \sum_{n=1} \left[ g_n A_n(\pm \omega, k) e^{i nk} + g_{-n} A_{-n}(\pm \omega, k) e^{-i nk} \right], \quad (10)$$
where \( G_{sk}(\pm \omega) \) and \( A_{sk}(\pm \omega, k) \) are given by

\[
G_{sk}(\pm \omega) = \frac{1}{E_0 \pm \hbar \omega - \frac{k^2 z^2}{2m}} \tag{11}
\]

\[
A_{sk}(\pm \omega, k) = \int e^{i k_2 n a} \langle k_2 | G(\pm \omega) | k \rangle \, dk_2. \tag{12}
\]

\( G_{sk}(\pm \omega) \) is obtained by replacing \( k \) by \( k' \) in (11). With the expression given by (10) and the knowledge of the ground state of the system \( \Psi_0 \), we can obtain \( \alpha(\omega) \) for any multi-delta potential. The first term on the right-hand side of (10) is the only contribution of \( \langle k' | G(\pm \omega) | k \rangle \) to \( \alpha(\omega) \) in the case of a single delta localized at \( x = 0 \) [5, 7]. The same term is common to the double delta and higher count of deltas. Since the single delta can only support one bound state, the significant contribution of the multi-bound state system to the details of \( \alpha(\omega) \) then comes from the second term on the right-hand side of (10). In terms of photon scattering the term \( e^{i k n a} \) with the corresponding coefficient can be considered as a scattering of photons with momentum \( p' \), \((p' = \hbar k')\) by a system localized at \( x = n a \). Accordingly, the model given here for a multi-delta potential represents a simple periodic system.

In our paper, the contribution to \( \alpha(\omega) \) will come from the first term on the right-hand side of (10) and the terms associated with \( A_1 \) and \( A_{-1} \). We set \( g_1 = g_{-1} = g \). The determination of \( A_1 \) and \( A_{-1} \) is given in [11].

### 3. Numerical results and analysis

In all of our graphs, the vertical axis represents \( \alpha(\omega) \) multiplied by \( \frac{1}{\pi \epsilon_0} \left( 9.0 \times 10^9 \text{Nm}^2 \text{C}^{-2} \right) \) so that the final unit is in \( \text{m}^3 \). We do so because the polarizability is usually given in units of length cubed as introduced in undergraduate textbooks [12]. In figures 1(a) and (b), the dynamic electric polarizability displays the same characteristics as the case of the single delta [5]. Such similarity is not surprising since for \( p < 1 \) there is one bound (negative energy) state and a continuum of unbound states which is the same structure as in the case of the single delta. It is also important to observe that the threshold of the photoelectric effect takes place at \( h \omega = E_B \) (figures 1(b) and 2(b)) where \( E_B = -E_0 \). We know from our studies of the photoelectric effect that when \( h \omega \geq E_B \) \((E_B \text{ here represents the work function})\) the total absorption of a photon of energy \( h \omega \) can take place. Such absorption leads to the existence of the imaginary part.

In figure 2(a) we can see that the polarizability blows up when \( \omega \) is close to \( 0.75 \omega_B \) (numerical calculations give a more precise value of 0.7529\( \omega_B \)). This behaviour has been reported before in the study of the atomic dynamic electric polarizability and examples can be found in [1, 13, 14]. But why does \( \alpha(\omega) \) for \( \omega < \omega_B \) \((\alpha(\omega < \omega_B))\) blow up in the case of \( p = 1.5 \) and not in the case of \( p = 0.5 \)? For \( p \geq 1 \), the unperturbed system contains two bound states [8–10]. The blow up in \( \alpha(\omega < \omega_B) \) takes place at an \( \omega \) where \( h \omega \) is equal to the energy difference between the two bound states. Since the only bound state we used in our calculation is \( \Psi_0 \), our expression for the dynamic polarizability is then responsible for detecting the existence of a second bound state for the case of \( p = 1.5 \). Let us define \( \hbar \omega_1 \) to be the absolute value of the eigenenergy of the second bound state. Now the resonant frequency at \( \omega = 0.7529 \omega_B \) should be given by \( h \omega = E_B - \hbar \omega_1 \) resulting in \( \omega_1 = 0.2471 \omega_B \). Using the detailed expression derived for the bound states ((4) and (5)), we get the same value for \( \omega_1 \). From a pedagogical point of view, this gives a clear illustration of how the study of polarizability can be used to study the structure of a bound system.
The dynamic electric polarizability of a particle bound by a double delta potential

Figure 1. (a) Plot of \( \frac{\alpha(\omega < \omega_B)}{4\pi \varepsilon_0} \) in m\(^3\) versus \( \frac{\omega}{\omega_B} \) where \( \omega_B = \frac{E_B}{\hbar} \), \( a = 0.5 \) Å and \( p = 0.5 \). (b) Plot of \( \text{Re}\left[\frac{\alpha(\omega > \omega_B)}{4\pi \varepsilon_0}\right] \) (solid line) and \( \text{Im}\left[\frac{\alpha(\omega > \omega_B)}{4\pi \varepsilon_0}\right] \) (dashed line) in m\(^3\) versus \( \frac{\omega}{\omega_B} \) for \( a = 0.5 \) Å and \( p = 0.5 \). 

In comparing figures 1(b) and 2(b), we can see that the increase of \( p \) leads to a higher threshold frequency for the photoelectric effect (\( \omega_B \) is higher for \( p = 1.5 \)). This is because increasing \( p \) for the same \( a \) leads to stronger attraction.
To continue with learning the fundamental features of $\alpha(\omega)$ in our model, we test our results with extreme conditions and examine how these cases compare with the cases we have already presented. In figure 3 we plot $\alpha(\omega)$ for ($\omega < \omega_B$) for the case, $a = 10^9$ Å, $p = 0.5$ and...
The dynamic electric polarizability of a particle bound by a double delta potential

Figure 3. Plot of $\frac{4\pi \epsilon_0}{\omega_B} \alpha(\omega, a)$ in m$^3$ versus $\omega/\omega_B$ where $a = 10^9$ Å, and $p = 0.5$.

This case has an extremely large separation of the two deltas and an extremely weak binding. In comparing the results shown in figure 3 (for $\omega < \omega_B$) with the results shown in figure 1(a) ($p = 0.5$ and $a = 0.5$ Å), we find that for the same $\frac{2mga}{\hbar^2}$, $\alpha(\omega)$ is multiplied by a factor close to $10^{37}$ going from the smaller to the much larger separation. As $a$ becomes very large (figure 3), the binding becomes very small, i.e. $\omega_B$ is approaching zero, and the numerical results of $\alpha(\omega)$ demonstrate that the given system is approaching the state of a free particle. The same scaling is found for $\omega > \omega_B$ as well.

To complete the study of the extreme conditions, we consider the case of the very small $a$ and very large binding (very large $g$). In figure 4, we present $\alpha(\omega)$ versus $\omega/\omega_B$ for $p = 0.5$ and $a = 10^{-6}$ Å. This case demonstrates the effect of the very small separation in the case of the system of one bound state. The case of the two bound states for $a = 10^{-9}$ Å and $p = 1.5$ is given in figure 5. In comparing $\alpha(\omega)$ in the case of $p = 1.5$ (figures 2(a) and 5) we find that the resonance (the blowup of $\alpha(\omega)$) takes place at the same $\frac{2mga}{\hbar^2}$. The same result can be reached by glancing at (4) and (5). This is another example showing how the study of $\alpha(\omega)$ offers meaningful insight into the structure of the system.

At this point we have an abundance of examples (figures 1(a)–5) to aid our discussion of how $\alpha(\omega)$ behaves as $p$ and $a$ are changed. In comparing figure 1(a) to figure 4, we find that for the same $\frac{2mga}{\hbar^2}$, $\alpha(\omega)$ is multiplied by a factor of $10^{-23}$ going from the larger to the much smaller separation. Considering much smaller separation between the two deltas with much larger $g$ ($p = \frac{2mga}{\hbar^2}$) will increase the binding of the particle. This in turn will push the energy of the particle in its initial state $\Psi_0$ further below the higher energy state leading to lower magnitude of the polarizability.

Now, we pay attention to $\alpha(\omega)$ at various values for $a$ and the same $p$. The solution of (4) for $p = 0.5$ and $a = 0.5$ Å will produce $k_0 = 0.7388$ Å$^{-1}$ while the solution of (4) for the same $p$ and $a = 10^{-6}$ Å will produce $k_0 = 3.696 \times 10^5$ Å$^{-1}$. The ratio of these two particular values of $k_0$ raised to the fourth power is $1.6 \times 10^{-23}$, the exact factor by which $\alpha(\omega)$ for
\[ \frac{\alpha(\omega < \omega_B)}{4\pi\epsilon_0} \text{ in m}^3 \text{ versus } \frac{\omega}{\omega_B} \text{ where } a = 10^{-6} \text{ Å and } p = 0.5. \]

\[ \frac{\alpha(\omega < \omega_B)}{4\pi\epsilon_0} \text{ in m}^3 \text{ versus } \frac{\omega}{\omega_B} \text{ where } a = 10^{-9} \text{ Å and } p = 1.5. \]

\( a = 0.5 \text{ Å (shown in figure 1(a)) differs from } \alpha(\omega) \text{ for } a = 10^{-6} \text{ Å (shown in figure 4). The same scaling exists for cases with two bound states. For } p = 1.5 \text{ and } a = 0.5 \text{ Å, (4) will produce } k_0 = 1.758 \text{ Å}^{-1} \text{ while for the same } p \text{ and } a = 10^{-9} \text{ Å will produce } k_0 = 8.792 \times 10^8 \text{ Å}^{-1}. \) The ratio of these two \( k_0 \) to the fourth power is \( 1.6 \times 10^{-35}. \) Again \( \alpha(\omega) \) for \( p = 1.5 \) and
The dynamic electric polarizability of a particle bound by a double delta potential

Figure 6. Plot of $\frac{\alpha(\omega)}{\epsilon_0} \text{m}^3$ versus $p$ for systems with $a = 0.5$ Å.

The static polarizability $\alpha(0)$ can be obtained by setting $\omega = 0$ in our expression for $\alpha(\omega)$ (6) and performing a set of simple integration or by taking $\omega \rightarrow 0$ in the final expression of $\alpha(\omega)$ [11]. When we set $q = e, m = m_e, 2a = 0.74$ Å and $p = 1.22$ in our expression for $\alpha(0)$, we obtain $4.68 \times 10^{-31} \text{m}^3$. The acceptable value for the static polarizability of the H$_2$ ion is $4.69 \times 10^{-31} \text{m}^3$ [15]. This agreement demonstrates that simple models can be used within reason to study realistic systems. To study the relation between the static polarizability and the structure of the system, we use the basic expression for $\alpha(0)$ [5], which is given by:

$$\alpha(0) = 2q^2 \sum_n \frac{|\langle \Psi_n | x | \Psi_0 \rangle|^2}{E_n - E_0},$$  \hspace{0.5cm} (13)

where the summation over $n$ does not include the state $\Psi_0$. Referring to figure 6, $\alpha(0)$ at $p = 1$ is approximately 1/5 its value at $p = 0.5$. For $p < 1$, the states $\Psi_n$’s belong to the continuum. Increasing $p$ does increase $g$ and this will lead to the increase in the energy gap $E_n - E_0$. The increase in the energy gap is then instrumental in $\alpha(0)$ decreasing while $p$ increases. $\alpha(0)$ at $p = 1.5$ is approximately 1/2 its value at $p = 1.0$. From $p = 1.5$ to $p = 2.5$, $\alpha(0)$ is about constant and then there is a modest increase in its value from $p = 2.5$ to close to the end of the ‘non-degenerate’ region. The behaviour of $\alpha(0)$ beyond $p = 1.0$ does not then continue the precipitous drop which occurs for $p < 1.0$. As we discussed earlier, for $p \geq 1$, the system of states in our problem will contain two bound (negative energy) states in addition to the continuum. Due to this the polarization of the system will come from the transitions $\Psi_0$ to second bound state and $\Psi_0$ to continuum states. So we can conclude that the transitions $\Psi_0$ to the second bound state is what stopped the rapid decrease in $\alpha(0)$. In addition, there is then a
decrease in the energy gap between the two bound states which leads to the modest increase of $\alpha(0)$ shown in figure 6 for $p > 2.5$.

4. Conclusions

In this paper we demonstrate the effectiveness of relying on $\Psi_0$ and the complete set of free particle states $|k\rangle$, to derive the final expression for $\alpha(\omega)$ in the case of a particle bound by a double-delta potential and establish a general expression for $\alpha(\omega)$ in the case of the multi-delta potential. We believe that the work we present here is a modest addition to our learning of applications in the area of perturbing charged systems with time-dependent fields of variable frequency. Second, we demonstrate the relationship between the electromagnetic properties of a system and its structure. Finally, this problem can aid in preparing physics students towards doing more advanced work in many areas of theoretical physics.

References

[1] Glover R M and Weinhold F 1976 J. Chem. Phys. 65 4913–25
[2] Koester L, Waschkowski W, Mitsyna L V, Samosvat G S, Prokofjevs P and Tambergs J 1995 Phys. Rev. C 51 3363–71
[3] MacGibbon B E, Garino G, Lucas M A, Nathan A M, Feldman G and Dolbilkin B 1995 Phys. Rev. C 52 2097–109
[4] Kittle C 1996 Introduction to Solid State Physics 7th edn (New York: Wiley)
[5] Maize M A and Williams M 2004 Am. J. Phys. 72 691–4
[6] Chung K T 1971 Phys. Rev. A 4 7–11
[7] Maize M A and Burkholder C A 1995 Am. J. Phys. 63 244–7
[8] Frost A A 1956 J. Chem. Phys. 25 1150–4
[9] Lapidus I R 1970 Am. J. Phys. 38 905–8
[10] de Alcantara Bonfim O F and Griffiths D J 2006 Am. J. Phys. 74 43–48
[11] Maize M A and Smetanka J J 2008 Preprint 0801.1499v1
[12] Griffiths D J 1989 Introduction to Electrodynamics 2nd edn (Englewood Cliffs, NJ: Prentice-Hall)
[13] Saslow W M and Mills D L 1969 Phys. Rev. 187 1025–34
[14] Gavrila M 1967 Phys. Rev. 163 147–55
[15] Taylor J M, Dalgarno A and Babb J F 1999 Phys. Rev. A 60 R2630–32