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Interaction of a charge and an electric dipole in one dimension

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The quantum-mechanical interaction of an electric charge and an electric dipole in one dimension is investigated using the delta-function potential to represent the interaction between charges. It is found that there is a single bound state. The problem of scattering of a charge from an electric dipole is solved exactly and in Born approximation. Because the potential is not symmetric, a phase shift analysis does not yield the correct cross section.

I. INTRODUCTION

The one-dimensional delta-function potential has proved to be a useful model for developing insights into more complex three-dimensional problems. In recent years a number of authors have published papers in this Journal in which the model is applied to a number of problems.

Lapidus has discussed models for a diatomic ion[1] and molecular orbitals.[2] Two-electron systems have been studied by Lapidus,[3,4] Srivastava and Bhaduri[5] and Urumov.[6] Similar results have been obtained by Nielson.[7] The Hartree approximation has been discussed by Nogami, Vallieres, and van Dijk[8,9] and by Foldy.[10,11] Scattering from one-dimensional delta-function potentials has been discussed by Lapidus.[12,13]

More recently, Turner[14] has examined the quantum-mechanical interaction of an electron and an electric dipole. The electron-dipole problem is also soluble in one dimension using delta-function potentials for the interaction.

In this paper the interaction of a charge interacting with an electric dipole in one dimension is studied. It is found that a single bound state exists. The scattering problem is solved exactly and by using the Born approximation. Finally, a partial wave analysis following the formalism of Eberly[15] is carried out. Formanek[16] has shown that the phase shift analysis should yield the cross section only if the potential is symmetric. In this case the potential is antisymmetric and one does not obtain the correct cross section.

II. BOUND STATES

Consider the motion of a particle of mass m in a one-dimensional potential given by

$$V(x) = -Ze^2\delta(x+a) + Ze^2\delta(x-a). \quad (1)$$

The time-independent Schrödinger equation is

$$(-\hbar^2/2m)\psi''(x) + V(x)\psi(x) = E\psi(x), \quad (2)$$

which has bound state solutions

$$\psi_1 = A\exp(\kappa x), \text{ for } x \leq -a, \quad (3a)$$

$$\psi_2 = B\exp(\kappa x) + C\exp(-\kappa x), \text{ for } |x| \leq a, \quad (3b)$$

$$\psi_3 = D\exp(-\kappa x), \text{ for } x \geq a, \quad (3c)$$

where $E = -\hbar^2\kappa^2/2m$.

The solution $\psi(x)$ is continuous at $x = \pm a$, while $\psi'(x)$ has a discontinuity given by

$$\psi'(\pm a + \epsilon) - \psi'(\pm a - \epsilon) = \pm(2Z/a_0)\psi(\pm a), \quad (4)$$

where $a_0 = \hbar^2/me^2$.

Solutions of Eqs. (3) can be found only for energy eigenvalues which satisfy the condition

$$(\kappa a_0/Z)^2 = 1 - \exp(-4\kappa a). \quad (5)$$

For large values of a, Eq. (5) yields

$$E = -E_0, \quad (6)$$

where $E_0 = Z^2e^2/2a_0$, which is the bound state energy of one attractive delta-function potential well.

For small values of a, Eq. (5) yields

$$E = -E_0 4\lambda^2/(1+2\lambda^2)^2, \quad (7)$$

where $\lambda = p/ea_0$ and $p = (Ze)(2a)$ is the dipole moment of the system. There is only one bound state. $|E|$ has a maximum value of $E_0/2$ when $p = ea_p/\sqrt{2}$.

III. SCATTERING

In this section the scattering of a charge by an electric dipole is discussed. Exact expressions for the reflection and transmission coefficients are obtained. Scattering is also discussed using the Born approximation. Finally, the applicability of the method of partial waves is considered.

A. Reflection and transmission

The solutions of Eq. (2) for an incident wave of unit amplitude may be written as

$$\psi_I(x) = \exp(ikx) + r\exp(-ikx), \text{ for } x \leq -a, \quad (8a)$$

$$\psi_{II}(x) = b\exp(ikx) + c\exp(-ikx), \text{ for } |x| \leq a, \quad (8b)$$

$$\psi_{III}(x) = t\exp(ikx), \text{ for } x \geq a, \quad (8c)$$

where r, b, c, t are constants and $E = \hbar^2k^2/2m$.

Making use of the continuity condition and Eq. (4), one obtains

$$\exp(-ika) + r\exp(ika) = b\exp(-ika) + c\exp(ika), \quad (9)$$

$$ik[b\exp(ika) - c\exp(ika)] - ik[\exp(-ika) - r\exp(ika)] = -(2Z/a_0)/[\exp(-ika) + r\exp(ika)], \quad (10)$$

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$$t\exp(ika) = b\exp(ika) + c\exp(-ika), \quad (11)$$

$$ikt\exp(ika) - ik[b\exp(ika) - c\exp(-ika)] = (2Z/a_0)t\exp(ika). \quad (12)$$

Equations (9)–(12) may be solved for r and t. One obtains

$$r = \lambda\gamma(1-\gamma^2)(\gamma - i\beta)/[(\lambda^2+\beta^2)\gamma^2 - \lambda^2], \quad (13)$$

$$t = \beta^2\gamma^2/[(\lambda^2+\beta^2)\gamma^2 - \lambda^2], \quad (14)$$

where $\beta = 2ka$, $\gamma = \exp(-i\beta)$, and $\lambda = 2Za/a_0$.

For small values of a, one obtains the reflection and transmission coefficients

$$R = |r|^2 = \frac{4\lambda^2(1 + 4E_0/E - \lambda^2/3)}{1 + 4\lambda^2(1 + 4E_0/E - \lambda^2/3)}, \quad (15)$$

$$T = |t|^2 = \frac{1}{1 + 4\lambda^2(1 + 4E_0/E - \lambda^2/3)}. \quad (16)$$

Of course, $R + T = 1$.

B. Born scattering

Born scattering by a one-dimensional delta-function potential has been discussed by Lapidus.[13] We review the method here.

The solutions of Eq. (2) satisfy an integral equation

$$\psi(x) = \exp(ikx) - \int_{-\infty}^{\infty} G(x,x')U(x')\psi(x')dx', \quad (17)$$

where $U(x) = 2mV(x)/\hbar^2$ and $k^2 = 2mE/\hbar^2$. The Green's function for the "outgoing" wave solution is

$$G(x,x') = \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{\exp[ik'(x-x')]}{(k'^2 - k^2)dk'} = \frac{i}{2k}\exp(ik|x-x'|). \quad (18)$$

The Born series is obtained by expanding $\psi(x)$ in a power series with an expansion parameter of order U/k^2, *i.e.*,

$$\psi(x) = \sum_n \psi^{(n)}(x). \quad (19)$$

Then from Eq. (17),

$$\psi^{(n+1)}(x) = -\int_{-\infty}^{\infty} G(x,x')U(x')\psi^{(n)}(x')dx'. \quad (20)$$

For the potential energy given in Eq. (1),

$$\psi^{(n+1)}(x) = (2Z/a_0)G(x,-a)\psi^{(n)}(-a) - (2Z/a_0)G(x,a)\psi^{(n)}(a), \quad (21)$$

where

$$G(x, \pm a) = (i/2k)\exp(ik|x \mp a|). \quad (22)$$

Thus, to lowest order the scattered wave is

$$\psi^{(1)}(x) = (iZ/\alpha)\{\exp[ik(|x+a| - a)] - \exp[ik(|x-a| + a)]\}, \quad (23)$$

where $\alpha = ka_o$.

For $x > a$, $\psi^{(1)}(x) = 0$. Hence in lowest order, the scattering amplitude in the forward direction vanishes, i.e., $f_+^{(1)} = 0$.

For $x < -a$,

$$\psi^{(1)}(x) = (2Z/\alpha)\sin(2ka)\exp(-ikx). \quad (24)$$

Hence, in lowest order, the scattering amplitude in the backward direction is

$$f_-^{(1)} = (2Z/\alpha)\sin(2ka). \quad (25)$$

The total scattering cross section in first Born approximation is then

$$\sigma_{\text{tot}}^{(1)} = |f_+^{(1)}|^2 + |f_-^{(1)}|^2 = (4Z^2/\alpha^2)\sin^2(2ka). \quad (26)$$

For small values of a,

$$\sigma_{\text{tot}}^{(1)} = 4\lambda^2. \quad (27)$$

To second order the scattered wave is

$$\psi^{(2)}(x) = 2(Z/\alpha)^2\sin(2ka)\exp[ik(|x+a| + a)]. \quad (28)$$

For $x > a$,

$$\psi^{(2)}(x) = 2(Z/\alpha)^2\sin(2ka)\exp[ik(x+2a)], \quad (29)$$

which yields a forward scattering amplitude

$$f_+^{(2)} = 2(Z/\alpha)^2\sin(2ka)\exp(2ika). \quad (30)$$

For $x < -a$,

$$\psi^{(2)}(x) = 2(Z/\alpha)^2\sin(2ka)\exp(-ikx), \quad (31)$$

which yields a backward scattering amplitude

$$f_-^{(2)} = 2(Z/\alpha)^2\sin(2ka). \quad (32)$$

Thus,

$$\sigma_{\text{tot}}^{(2)} = 8(Z/\alpha)^4\sin^2(2ka). \quad (33)$$

For small values of a,

$$\sigma_{\text{tot}}^{(2)} = 8\lambda^2(E_0/E - \lambda^2/3). \quad (34)$$

The complete Born series may be obtained by continued iteration. The exact solution for small values of a is given by

$$\sigma_{\text{tot}} = |r|^2 + |1-t|^2 = \frac{4\lambda^2(1 + 8E_0/E - 2\lambda^2/3)}{1 + 4\lambda^2(1 + 4E_0/E - \lambda^2/3)}. \quad (35)$$

C. Phase shift analysis

In 1965, Eberly[15] developed a formalism for scattering in one dimension using a phase shift analysis. Lapidus[12] applied this method to the scattering from a single delta-function potential.

However, more recently Formanek[16] noted that the derivation of the partial wave formalism is correct only for "centrally symmetric" potentials, i.e., symmetric potentials for which $V(-x) = V(x)$. The potential given in Eq. (1) does not satisfy this condition. In fact $V(-x) = -V(x)$, i.e., $V(x)$ is antisymmetric.

In order to examine the validity of the critique by Formanek, we carry through the derivation of the phase shift analysis for electron-dipole scattering. We find that in this case the partial wave formalism does not yield the correct scattering cross section.

For $|x| \geq a$ we may write the solution of Eq. (2) as

$$\psi(x) = \exp(ikx) + f\exp(ik\epsilon x), \quad (36)$$

where f is the scattering amplitude and $\epsilon = \pm 1$ to the right and left of the dipole.

Expanding f in "partial waves"

$$f_\epsilon = i \sum_{l=0}^{1} \epsilon^l \exp(i\delta_l) \sin\delta_l. \quad (37)$$

The solutions to the right and left of the dipole are

$$\psi_+(x) = \exp(ikx) + f_+ \exp(ikx), \quad (38a)$$

$$\psi_-(x) = \exp(ikx) + f_- \exp(-ikx). \quad (38b)$$

The scattering amplitudes f_+ and f_- are given by $f_+ = t - 1$ and $f_- = r$, or

$$f_+ = \lambda^2(1 - \gamma^2)/[(\lambda^2 + \beta^2)\gamma^2 - \lambda^2], \quad (39)$$

$$f_- = \lambda\gamma(1 - \gamma^2)(\lambda - i\beta)/[(\lambda^2 + \beta^2)\gamma^2 - \lambda^2]. \quad (40)$$

In order to examine the validity of Eq. (37) it is necessary to obtain the "phase shifts", δ_l, from the boundary conditions given by Eq. (14). This calculation yields, for small values of a,

$$\tan \delta_0 = (\lambda/ka)/[(\lambda/ka) \tan ka - \tan^2 ka - 1] \rightarrow [\lambda/(\lambda - 1)]/ka, \quad (41)$$

$$\tan \delta_1 = -(\lambda/ka) \tan^2 ka/[(\lambda/ka) \tan ka + \tan^2 ka + 1]. \rightarrow -[\lambda/(\lambda + 1)]\, ka. \quad (42)$$

The total cross section for scattering obtained from the relation

$$\sigma_{\text{tot}} = 2 \sum_{l=0}^{1} \sin^2\delta_l, \quad (43)$$

yields

$$\sigma_{\text{tot}} = 2\{1 + [(2\lambda^2 - 1)/(\lambda + 1)^2](E/4E_0)\} \quad (44)$$

which does not agree with Eq. (35).

Formanek[16] has discussed the criteria necessary for carrying out a phase shift analysis of one-dimensional scattering. A necessary condition for the analysis is that $V(-x) = V(x)$, which corresponds to a centrally symmetric potential in three dimensions. In the latter case the scattering solutions must be eigenstates of the total angular momentum. In one dimension the requirement of symmetry corresponds to the condition that the scattering states must be eigenstates of the parity operator.

IV. SUMMARY

The quantum-mechanical interaction of a charge and an electric dipole in one dimension has been studied using the delta-function potential. It is found that there is one bound state of a charge and a dipole.

The exact solution to the scattering problem of a charge from an electric dipole has been obtained and the Born expansion has also been developed. Finally, it was shown that a partial wave analysis does not give the correct scattering cross section.

The delta-function potential provides a useful model for the study of quantum-mechanical systems because the system is simple and it is possible to evaluate all integrals in the calculations easily. Thus, this model provides a useful pedagogical tool as well as helping to develop insights into more complex problems.

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