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The quantum probability equation: II. Scattering state perturbation theory

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Abstract

The time-independent bound-state perturbation theory derived for the quantum probability equation (Milward G C and Wilkin C 2000 *J. Phys. A: Math. Gen.* **33** 7353) is extended to treat the scattering domain. Formulae for the changes in the partial wave phase shifts are derived to third order in the perturbing potential. The results are compared with those obtained for analytically soluble problems.

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1. Introduction

When the wavefunction $u(r)$ in a particular angular momentum state satisfies real boundary conditions, it is possible to recast the single-particle time-independent partial wave Schrödinger equation into one for the density distribution $P(r) = [u(r)]^2$. This leads, in the s -wave case, to the non-linear second-order equation

$$P(r) P''(r) = \frac{1}{2}[P'(r)]^2 + 2[U(r) - E] P(r)^2 \quad (1.1)$$

where both the particle energy E and the spherically symmetric potential $U(r)$ are measured in units of $\hbar^2/2m$. The equation is also valid for higher partial waves provided that a centrifugal barrier term $\ell(\ell + 1)/r^2$ is included in an effective potential.

In a previous paper [1], hereinafter referred to as I, we developed time-independent perturbation theory in the bound state domain for this and an equivalent third-order linear equation. In this approach, one cannot exploit orthogonality of different wavefunctions. Standard perturbation theory, involving the coupling to the excited states, is therefore not applicable. We derived instead a variant of the results of Bender [2], where the energy shift depends only upon the unperturbed probability density and the change in the potential. Explicit knowledge of neither the unperturbed potential nor the corresponding spectrum is required. It is the purpose of this paper to show that similar techniques can be used in the continuum.

Perturbation formulae for s -waves are derived in section 2 where, for simplicity, we assume that the potential vanishes beyond a finite radius R . As shown in section 3, the formulae are

still valid in the limit of $R \rightarrow \infty$, provided the perturbation vanishes faster than $1/r$ at large distances. Alternative forms for the second-order phase shift change are applied in section 4 to simple soluble cases. The relationship to some other perturbation approaches is discussed in section 5. Although most of our work deals specifically with the s-wave case, the formulae can be generalised to higher partial waves and the major changes required to accomplish this are outlined in section 6. The connection between bound- and scattering-state perturbation theory is discussed in section 7. Although the first-order bound-state formula may be obtained by simple extrapolation from positive energies, this is not straightforward for the second order. Some general conclusions are drawn in section 8.

2. S-wave scattering state perturbation theory

We here confine ourselves to s-wave scattering from a potential which vanishes identically for $r \geq R$, where R is some finite radius. The associated probability distribution behaves at large r as

$$\tilde{P}(r) = \frac{1}{k^2} \sin^2(kr + \delta) \quad \text{for } r \geq R \quad (2.1)$$

where δ is the s-wave phase shift. The symbol \tilde{P} distinguishes the scattering from the bound state density used in I, which satisfies rather an integral boundary condition. The probability density furthermore vanishes at the origin:

$$\tilde{P}(0) = 0. \quad (2.2)$$

We now suppose that the probability equation (1.1) may be solved for some potential $U_0(r)$ to give a density distribution $\tilde{P}_0(r)$ and a phase shift δ_0 . Consider then the perturbation expansion

$$U(r) = U_0(r) + \lambda W(r) \quad (2.3)$$

$$\tilde{P}(r) = \tilde{P}_0(r) + \lambda \tilde{P}_1(r) + \lambda^2 \tilde{P}_2(r) + \lambda^3 \tilde{P}_3(r) + \dots \quad (2.4)$$

$$\delta = \delta_0 + \lambda \delta_1 + \lambda^2 \delta_2 + \lambda^3 \delta_3 + \dots \quad (2.5)$$

where λ is some small parameter. It is our aim to derive expressions for the $\tilde{P}_n(r)$ and δ_n in terms of $\tilde{P}_0(r)$ and $W(r)$.

2.1. First-order phase shift correction

The boundary condition of equation (2.2) requires that $\tilde{P}_n(0) = 0$ for all n . Inserting equations (2.4), (2.5) into (2.1) and expanding to first order in λ gives the large- r limit:

$$\tilde{P}_1(r) = \delta_1 \frac{1}{k^2} \sin(2kr + 2\delta_0) \quad \text{for } r \geq R. \quad (2.6)$$

As in I, introduce the perturbation expansion of equation (2.4) into the probability equation (1.1) and expand to first order in λ . After eliminating the combination $[U_0(r) - E]$ by use of the unperturbed equation, the result may be integrated to give

$$\tilde{P}_1'(r) - \frac{\tilde{P}_1(r)\tilde{P}_0'(r)}{\tilde{P}_0(r)} = 2 \int_0^r W(r') \tilde{P}_0(r') dr'. \quad (2.7)$$

For $r \geq R$, we can use the asymptotic forms of equations (2.1), (2.6) to evaluate the left-hand side and this leads to the first-order change in the phase shift:

$$\delta_1 = -k \int_0^\infty W(r) \tilde{P}_0(r) dr. \quad (2.8)$$

2.2. First-order probability density correction

The first-order change in the probability density is obtained by dividing equation (2.7) by $\tilde{P}_0(r)$ to leave an exact derivative which can be integrated as

$$\tilde{P}_1(r) = 2\tilde{P}_0(r) \int_R^r \frac{1}{\tilde{P}_0(r')} dr' \int_0^{r'} W(r'') \tilde{P}_0(r'') dr'' + C(R) \tilde{P}_0(r) \quad (2.9)$$

where $C(R)$ is an integration constant whose value depends upon R .

The integration over r'' is now split into two intervals, $R \rightarrow r'$ and $0 \rightarrow R$. The latter integral is determined by the first-order phase shift change of equation (2.8). Furthermore, for $r \geq R$, the asymptotic behaviours of equations (2.1), (2.6) may be employed on the left- and right-hand sides and the value of $C(R)$ deduced. Hence

$$\tilde{P}_1(r) = 2\tilde{P}_0(r) \int_R^r \frac{1}{\tilde{P}_0(r')} dr' \left\{ \int_R^{r'} W(r'') \tilde{P}_0(r'') dr'' - \frac{\delta_1}{k} \right\} + 2\delta_1 \cot(kR + \delta_0) \tilde{P}_0(r). \quad (2.10)$$

2.3. Second-order corrections

The λ^2 terms which result from the insertion of equations (2.3)–(2.5) into (2.1) lead, after the elimination of the potential, to

$$\tilde{P}_2'(r) - \frac{\tilde{P}_2(r)\tilde{P}_0'(r)}{\tilde{P}_0(r)} + \frac{\tilde{P}_1(r)^2\tilde{P}_0'(r)}{2\tilde{P}_0(r)^2} - \frac{\tilde{P}_1(r)\tilde{P}_1'(r)}{2\tilde{P}_0(r)} = \int_0^r \tilde{P}_1(r') W(r') dr'. \quad (2.11)$$

The asymptotic boundary condition on $\tilde{P}_2(r)$ can be established by introducing the phase shift expansion of equation (2.5) into (2.1);

$$\tilde{P}_2(r) = \frac{\delta_2}{k^2} \sin(2kr + 2\delta_0) + \frac{\delta_1^2}{k^2} \cos(2kr + 2\delta_0) \quad \text{for } r \geq R. \quad (2.12)$$

When this is employed in equation (2.11), we find that

$$\begin{aligned} \delta_2 &= -\frac{k}{2} \int_0^\infty W(r) \tilde{P}_1(r) dr \\ &= -k \int_0^\infty W(r) \tilde{P}_0(r) dr \int_R^r \frac{1}{\tilde{P}_0(r')} dr' \left\{ \int_R^{r'} W(r'') \tilde{P}_0(r'') dr'' - \frac{\delta_1}{k} \right\} \\ &\quad + \delta_1^2 \cot(kR + \delta_0). \end{aligned} \quad (2.13)$$

Turning now to the probability correction, equation (2.11) is a linear first-order differential equation for $\tilde{P}_2(r)$. The solution with the correct boundary conditions is

$$\begin{aligned} \tilde{P}_2(r) &= \frac{\tilde{P}_1(r)^2}{4\tilde{P}_0(r)} + \tilde{P}_0(r) \int_R^r \frac{1}{\tilde{P}_0(r')} \left\{ \int_R^{r'} W(r'') \tilde{P}_1(r'') dr'' - \frac{2\delta_2}{k} \right\} dr' \\ &\quad + 2\delta_2 \tilde{P}_0(r) \cot(kR + \delta_0) - \delta_1^2 \tilde{P}_0(r). \end{aligned} \quad (2.14)$$

Higher-order terms are harder to evaluate and here we merely quote the formal result for the third order change in the phase shift:

$$\delta_3 = -\frac{k}{3} \int_0^\infty W(r) \tilde{P}_2(r) dr \quad (2.15)$$

which can be evaluated using equation (2.14).

3. The long-range limit

It is not possible to take the $R \rightarrow \infty$ limit directly in equation (2.13) because of the explicit $\cot(kR + \delta_0)$ term. This problem can be circumvented by defining the kernel

$$\tilde{K}(r', r) = \int_r^{r'} \frac{1}{\tilde{P}_0(r'')} dr'' \quad (3.1)$$

which differs from the analogous K used in I for the bound state case through the absence of multiplicative unperturbed probability factors. For the free unperturbed probability density,

$$\tilde{P}_0^{\text{free}}(r) = \frac{1}{k^2} \sin^2[kr + \delta_0] \quad (3.2)$$

the corresponding kernel can be evaluated explicitly

$$\tilde{K}^{\text{free}}(r', r) = \int_r^{r'} \frac{1}{\tilde{P}_0^{\text{free}}(r'')} dr'' = k \cot(kr + \delta_0) - k \cot(kr' + \delta_0). \quad (3.3)$$

The difference between the free and interacting kernel,

$$\Delta K(r', r) = \tilde{K}(r', r) - \tilde{K}^{\text{free}}(r', r) \quad (3.4)$$

remains finite when r or $r' \rightarrow \infty$.

After grouping terms and integrating by parts, the expression for $\tilde{P}_1(r)$ can be reduced to

$$\tilde{P}_1(r) = 4 \tilde{P}_0(r) [k \cot(kr + \delta_0) + \Delta K(\infty, r)] \int_0^r W(r') \tilde{P}_0(r') dr'. \quad (3.5)$$

and that for the phase shift to

$$\begin{aligned} \delta_2 = 2k^2 \int_0^\infty W(r) \tilde{P}_0(r) \cot(kr + \delta_0) dr \int_0^r W(r') \tilde{P}_0(r') dr' \\ + 2k \int_0^\infty W(r) \tilde{P}_0(r) \Delta K(\infty, r) dr \int_0^r W(r') \tilde{P}_0(r') dr'. \end{aligned} \quad (3.6)$$

It is crucial to note that the integrals converge at large r and, in fact, the limit $R \rightarrow \infty$ has been taken here.

An alternative form for δ_2 can be found by defining the auxiliary function

$$\delta_1(r) = -k \int_0^r W(r') \tilde{P}_0(r') dr' \quad (3.7)$$

for which $\delta_1(r) \rightarrow \delta_1$ as $r \rightarrow \infty$. Then

$$\delta_2 = \delta_1^2 \cot \delta_0 + \frac{1}{k} \int_0^\infty \left\{ \frac{\delta_1(r)^2}{\tilde{P}_0(r)} - \frac{\delta_1^2}{\tilde{P}_0^{\text{free}}(r)} \right\} dr. \quad (3.8)$$

This is probably the most important result of this paper. Just as for the energy shift for bound states investigated in I, the expression only involves two quadratures. The first term in equation (3.8) arises because the phase shift has been expanded in a perturbation series and it would not be present in an expansion for $\cot \delta$.

Although the integrands in equations (3.6) and (3.8) are well behaved at large r , there may be singularities in the integrands due to the vanishing of $\tilde{P}_0(r)$ at finite r . These are similar in nature to those occurring for excited states in the discrete spectrum studied in I. We adopt the same strategy of considering first the problem where k has a small positive imaginary part, $k \rightarrow k(1 + i\epsilon)$, taking the limit $\epsilon \rightarrow 0$ at the end of the calculation. Though this causes no problem in the analytic examples considered in the next section, it is more tedious to implement in numerical evaluations.

Formulae for higher-order phase changes can also be established in the $R \rightarrow \infty$ limit. For example, starting from equation (2.15),

$$\delta_3 = -\delta_1^3 + \frac{2}{3}\delta_1 \delta_2 \cot(\delta_0) - \frac{k}{3} \int_0^\infty \frac{\tilde{P}_1(r)^2 W(r)}{4\tilde{P}_0(r)} dr + \frac{2}{3k} \int_0^\infty \left(\frac{\delta_2(r) \delta_1(r)}{\tilde{P}_0(r)} - \frac{\delta_2 \delta_1}{\tilde{P}_0^{\text{free}}(r)} \right) dr. \tag{3.9}$$

4. Examples

4.1. Scattering length problems

The scattering length $a = -\lim_{k \rightarrow 0} \{\delta/k\}$ may be expanded in a perturbation series similar to that of equation (2.5) for the phase shift;

$$a = a_0 + \lambda a_1 + \lambda^2 a_2 + \lambda^3 a_3 + \dots \tag{4.1}$$

Outside the range of the potential, the unperturbed probability density behaves as

$$\tilde{P}_0(r) \rightarrow (r - a_0)^2. \tag{4.2}$$

In terms of the function

$$a_1(r) = \int_0^r W(r') P_0(r') dr' \tag{4.3}$$

the first correction to the scattering length is $a_1 = \lim_{r \rightarrow \infty} \{a_1(r)\}$. The zero-energy limit of equation (3.8) is

$$a_2 = \frac{a_1^2}{a_0} - \int_0^\infty \left\{ \frac{a_1(r)^2}{\tilde{P}_0(r)} - \frac{a_1^2}{\tilde{P}_0^{\text{free}}(r)} \right\} dr \tag{4.4}$$

where $\tilde{P}_0^{\text{free}}(r)$ is given by equation (4.2) for all values of r .

Consider first an attractive finite square well, $U_0(r) = -q^2 \theta(R - r)$, whose depth is perturbed by $W(r) = -\theta(R - r)$. Elementary manipulation of the explicit solution shows that the perturbations in the scattering length are

$$a_0 = R - \tan(qR)/q \tag{4.5}$$

$$a_1 = -\frac{1}{2q^3} \tan qR + \frac{R}{2q^2} \sec^2 qR \tag{4.6}$$

$$a_2 = \frac{3}{8q^5} \tan qR - \frac{3R}{8q^4} \sec^2 qR + \frac{R^2}{4q^3} \sec^2 qR \tan qR. \tag{4.7}$$

The auxiliary function of equation (4.3) becomes

$$a_1(r) = -\frac{1}{4q^3} \sin 2qr \sec^2 qR + \frac{r}{2q^2} \sec^2 qR \tag{4.8}$$

for $r \leq R$. Taking $r = R$, this yields the result of equation (4.6), and using this form in equation (4.4), leads directly to the desired result of equation (4.7).

For any specific potential, it is possible to evaluate the corrections due to a perturbation in other ways. These alternatives are not as simple if one is given instead the unperturbed probability density. As an example, suppose that at zero energy

$$\tilde{P}_0(r) = \frac{r^2(r + b)^2}{(r + a + b)^2} \tag{4.9}$$

for which the unperturbed scattering length $a_0 = a$. The perturbation $W(r) = \delta(r - R)$ leads to

$$\begin{aligned} a_1 &= \frac{R^2(R+b)^2}{(R+a+b)^2} \\ a_2 &= a_1^2 \left\{ \frac{2a(a+b)}{b^3} \ln\left(\frac{b+R}{R}\right) - \frac{(a+b)^2}{b^2 R} - \frac{a^2}{b^2(b+R)} \right\}. \end{aligned} \quad (4.10)$$

4.2. The centrifugal barrier potential

In the case of the angular momentum barrier potential

$$U_0(r) = \frac{\ell(\ell+1)}{r^2} \quad (4.11)$$

the probability density is given by

$$\tilde{P}_0(r) = [r j_\ell(kr)]^2 \quad (4.12)$$

with a phase shift $\delta_0 = -\frac{1}{2}\ell\pi$. For the perturbation

$$\lambda W(r) = \frac{\lambda}{r^2} \quad (4.13)$$

the probability density is similar to that of equation (4.12) but with an effective angular momentum of

$$\ell' = \sqrt{\left(\ell + \frac{1}{2}\right)^2 + \lambda} - \frac{1}{2} \approx \ell + \frac{\lambda}{2(\ell+1)} - \frac{\lambda^2}{(2\ell+1)^3} + \mathcal{O}(\lambda^3). \quad (4.14)$$

The phase shift perturbations are therefore

$$\delta_1 = -\frac{\pi}{2(2\ell+1)} \quad (4.15)$$

$$\delta_2 = \frac{\pi}{2(2\ell+1)^3}. \quad (4.16)$$

From equation (2.8) the first-order perturbation is

$$\delta_1 = -k \int_0^\infty \frac{1}{r^2} [r j_\ell(kr)]^2 dr = -\frac{\pi}{2(2\ell+1)} \quad (4.17)$$

which agrees with equation (4.15).

Turning to the second-order perturbation, the kernel of equation (3.1) becomes

$$\tilde{K}(r', r) = \int_r^{r'} \frac{dr''}{r''^2 j_\ell(kr'')^2} = k \left[\frac{n_\ell(kr')}{j_\ell(kr')} - \frac{n_\ell(kr)}{j_\ell(kr)} \right] \quad (4.18)$$

which means that

$$\delta_2 = -2 \int_0^\infty j_\ell(x) n_\ell(x) dx \int_0^x [j_\ell(y)]^2 dy. \quad (4.19)$$

The latter integration can be performed using hypergeometric functions and leads to the expected result of equation (4.16).

Our perturbation method can therefore handle potentials which behave asymptotically like $1/r^2$, and this relevant to the discussion of higher partial waves carried out in section 6.

5. Comparison with other approaches

5.1. Born approximations

In the limiting case where the unperturbed potential vanishes, the unperturbed s-wave density is that of a plane wave $\tilde{P}_0(r) = \sin^2(kr)/k^2$, and the first-order change in the phase shift of equation (2.8) becomes

$$\delta_1 = -\frac{1}{k} \int_0^\infty W(r) \sin^2(kr) dr \quad (5.1)$$

which is just the first Born approximation for the phase shift [3].

The standard second Born approximation for the phase shift can be most easily derived using the variable phase equation approach [4];

$$\delta_2 = \frac{1}{k^2} \int_0^\infty W(r) \sin(2kr) dr \int_0^r W(r') \sin^2(kr') dr'. \quad (5.2)$$

This is the same result as we find from equation (3.6) by putting $\delta_0 = 0$ and replacing $\tilde{P}_0(r)$ by its free form.

5.2. The two-potential formula

For the general unperturbed problem, the first-order change must correspond to that given by the two-potential formula of Gell-Mann and Goldberger [3, 5]. They show that the change in the s-wave scattering amplitude f induced by an extra potential $\lambda W(r)$ is

$$f_1 = -e^{2i\delta_0} \lambda \int_0^\infty W(r) \tilde{P}_0(r) dr \quad (5.3)$$

where the non-standard phase factor in front of the integration arises because of the standing-wave boundary conditions.

Now, to order λ , $f_1 = e^{2i\delta_0} \lambda \delta_1/k$ and, equating this to equation (5.3) leads immediately to our first-order expression of equation (2.8).

6. Higher partial waves

The probability equation (1.1) is valid for an arbitrary ℓ th partial wave if the centrifugal barrier contribution is included in an effective potential $U(r)$. Furthermore, apart from an explicit extra $\frac{1}{2}\ell\pi$ term, the boundary condition of equation (2.1) still holds provided that we can let the cut-off radius R go to infinity. In this sense, therefore, we have already treated higher partial waves in the $1/r^2$ example discussed in section 4.2, the limit of $R \rightarrow \infty$ causing no difficulty.

However, the centrifugal barrier term is normally included explicitly when solving the Schrödinger equation in order that the integrations converge quicker at large values of r . We want to show how this can be achieved in the present approach.

For simplicity, suppose that both the unperturbed and perturbed potentials vanish for $r > R_1$. In the region $R_1 < r \leq R$ there is then only the centrifugal barrier contribution and the boundary condition of equation (2.1) is replaced by

$$P(r) = r^2 [\cos \delta_\ell j_\ell(kr) - \sin \delta_\ell n_\ell(kr)]^2 = \tilde{P}_0^{\text{cfb}}(r) \quad \text{for } r \geq R_1 \quad (6.1)$$

$$\rightarrow \frac{1}{k^2} \sin^2 \left(kr + \delta_\ell - \frac{1}{2}\ell\pi \right) \quad \text{as } r \rightarrow \infty. \quad (6.2)$$

Hence the phase shift that we have used so far should be replaced by $\delta \rightarrow \delta_\ell - \pi\ell/2$.

Whereas the formula of equation (3.8) is valid without modification, it is more convenient to split the integration as

$$\delta_2 = \delta_1^2 \cot \delta_0 + \frac{1}{k} \int_0^{R_1} \left\{ \frac{\delta_1(r)^2}{\tilde{P}_0(r)} - \frac{\delta_1^2}{\tilde{P}_0^{\text{free}}(r)} \right\} dr + \Delta^{\text{cfb}} \quad (6.3)$$

where

$$\Delta^{\text{cfb}} = \frac{\delta_1^2}{k} \int_{R_1}^{\infty} \left\{ \frac{1}{\tilde{P}_0^{\text{cfb}}(r)} - \frac{1}{\tilde{P}_0^{\text{free}}(r)} \right\} dr. \quad (6.4)$$

For $r \geq R_1$, only the centrifugal barrier is operative and we have replaced $\tilde{P}_0(r)$ by the large- r form of equation (6.1). The integrations in equation (6.4) can be carried out explicitly to give

$$\Delta^{\text{cfb}} = -\delta_1^2 \left[\frac{\sin \delta_\ell j_\ell(kR_1) + \cos \delta_\ell n_\ell(kR_1)}{\cos \delta_\ell j_\ell(kR_1) - \sin \delta_\ell n_\ell(kR_1)} - \cot(kR_1 + \delta_\ell - \ell\pi/2) \right]. \quad (6.5)$$

The integrations in equation (6.3) are then only over the range where the perturbation is non-vanishing.

7. Extrapolation to bound states

When a system has a loosely bound state, one would hope to be able to extrapolate the perturbation theory results from the scattering domain to the bound state pole in order to retrieve the formulae already established in I. Although this is indeed the case for the first-order corrections, the procedure is not straightforward in second order. To illustrate this, consider the case when the S -matrix has a bound state at $E = -\alpha^2$, i.e. at $k \cot \delta = -\alpha$. In the vicinity of the pole

$$S = e^{2i\delta} = \frac{G(k)}{(\alpha + ik)} \quad (7.1)$$

where $G(k)$ is well behaved. Expanding the pole position in a perturbation series

$$\alpha = \alpha_0 + \lambda \alpha_1 + \lambda^2 \alpha_2 + O(\lambda^3) \quad (7.2)$$

we see that, for $k \approx i\alpha_0$,

$$\alpha_1 = \frac{1}{k}(\alpha_0^2 + k^2) \delta_1 \quad (7.3)$$

$$\alpha_2 = \frac{1}{k}(\alpha_0^2 + k^2) \left(\delta_2 + \frac{\alpha_0}{k} \delta_1^2 \right). \quad (7.4)$$

The consequent changes in the bound state energy are

$$E_1 = -\frac{2\alpha_0}{k}(\alpha_0^2 + k^2) \delta_1 \quad (7.5)$$

$$E_2 = -\frac{2\alpha_0}{k}(\alpha_0^2 + k^2) \left(\delta_2 + \frac{\alpha_0}{k} \delta_1^2 \right) - \frac{E_1^2}{4\alpha_0^2}. \quad (7.6)$$

On the other hand, it was shown in I that bound state perturbation theory gives

$$E_1 = \int_0^\infty W(r) P_0(r) dr \quad (7.7)$$

$$E_2 = - \int_0^\infty \frac{1}{P_0(r)} [Q(r)]^2 dr \quad (7.8)$$

where

$$Q(r) = \int_0^r (W(r') - E_1) P_0(r') dr'. \quad (7.9)$$

Now the probability density $\tilde{P}(r)$ in the scattering domain is normalised by the asymptotic behaviour of equation (2.1), whereas the corresponding $P(r)$ in the bound state case is normalised requiring that the total probability is unity. The two densities are linked by the Fäldt–Wilkin extrapolation theorem [6, 7] which states that, independent of the shape of the potential, as $k \rightarrow i\alpha$

$$P(r) \approx 2\alpha(\alpha^2 + k^2) \tilde{P}(r) + O(\alpha^2 + k^2). \quad (7.10)$$

Inserting equation (2.8) into the first-order shift of equation (7.5) gives

$$E_1 = \frac{2\alpha_0}{k}(\alpha_0^2 + k^2) \frac{1}{2\alpha_0(\alpha_0^2 + k^2)} k \int_0^\infty W(r) P_0(r) dr \quad (7.11)$$

where the limit $k \rightarrow i\alpha_0$ is understood. This leads immediately to the standard result of equation (7.7), as shown already in [7].

However, starting from equation (7.6) to carry out the same procedure for the second order, we find that

$$E_2 = - \int_0^\infty \left\{ \frac{1}{P_0(r)} \left[Q(r) - E_1 \int_0^r P_0(r') dr' \right]^2 - \frac{E_1^2}{P_0^{\text{free}}(r)} \right\} dr - \frac{E_1^2}{4\alpha_0^2}. \quad (7.12)$$

If $E_1 = 0$, then this is just the bound state result of equation (7.8). However, this is no longer true when $E_1 \neq 0$. The discrepancy is due in part to the neglect of higher-order terms in $\alpha^2 + k^2$ in equation (7.10). Such terms, which depend upon the details of the potential [7], give non-vanishing model-dependent contributions in the translation of δ_1^2 to E_1^2 . Corrections of the same order arise from the non-singular part of δ_1 in equation (7.4) and this depends upon the form of $G(k)$ near the pole. Thus, although we have established the major term in the expression for E_2 , further work would be required if one wanted to establish completely the second-order shift in the bound state region from the corresponding formula in the continuum.

Of course, if one knew $\tilde{P}_0(r)$ as a function of k then one could evaluate the phase shift corrections δ_1 and δ_2 , using equations (2.8) and (3.8), and then extrapolate into the bound-state region. This corresponds, however, to knowing the higher-order terms in equation (7.10).

8. Conclusions

The study of time-independent perturbation theory within the framework of the quantum probability equation has been extended from the bound state region to the scattering domain. Formulae for the changes in a phase shift of arbitrary angular momentum, when a spherically symmetric potential is subjected to a spherically perturbation, are derived up to third order in the perturbation.

The results are economic to evaluate; the second-order shift of equation (3.8) requires only a two-dimensional integration mesh. This is very similar to the effort needed to estimate the second-order bound-state energy shift from equation (7.8). Indeed there is a very close relation between the two second-order corrections, though further work is required to derive one unambiguously from the other. In both cases the changes depend purely upon the perturbing potential and the unperturbed probability density; the unperturbed potential does not occur explicitly in our formulae. A soluble example is given illustrating this feature. Unfortunately, most problems of a practical interest have to be solved numerically.

Another soluble problem investigated is that of a centrifugal barrier $\ell(\ell + 1)/r^2$, where the value of ℓ is perturbed slightly. The success here suggests that knowing the probability density and phase shift for one value of the angular momentum might allow one to estimate the phase shift for another value of ℓ using perturbation theory.

We defer to a third publication consideration of problems where one takes the energy as a perturbation. It seems, however, that in principle, knowing the probability density at one energy and angular momentum, it should be possible to evaluate the phase shift at a different energy and angular momentum as a series of quadratures using perturbation theory.

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