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The quantum probability equation: III. Perturbing in the energy

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Abstract

Time-independent perturbation theory in the scattering domain, developed on the basis of the quantum probability equation (Milward G C and Wilkin C 2001 *J. Phys. A: Math. Gen.* **34** 5101), is extended to study the energy dependence of the *S*-wave scattering phase shifts and probability density to second order in the energy change. At low energies, the Bethe formula for the effective range is reproduced and an analogous formula for the shape-dependent term is also derived. The energy dependence of the probability density at short distances is important in final state interaction theory and the method allows the investigation of some of the prescriptions used there. Results from the present approach are illustrated with soluble models.

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1. Introduction

In two earlier papers, we studied time-independent quantum-mechanical perturbation theory for a non-relativistic spherically symmetric single-particle system, with bound states being addressed in paper I [1] and scattering states in paper II [2]. After introducing a small change in the potential energy, $U(r) = U_0(r) + \lambda W(r)$, it was shown that the modification in the binding energy or the scattering phase shift depends only upon the perturbation $\lambda W(r)$ and the probability density of the unperturbed problem $P_0(r)$ but not upon the properties of other states of the system. While our derivation is completely different, the bound state results turned out to be equivalent to those of Bender [3]. However, it has since become clear that these formulae have a much longer history, dating back at least to Zel'dovich [4], though they can be derived on the basis of even earlier methods, such as that proposed by Dalgarno

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and Lewis [5]. Different variants of the formulae have been independently discovered, as for example by Aharonov and Au [6], but with rare exception [7], little emphasis has been placed upon the scattering problem. It is the aim of the present paper to extend the scattering results given in II to the study of their energy dependence by considering a small change in the energy E as a perturbation.

The above authors all worked with the Schrödinger equation but, in a single-channel case, it is always possible to impose real boundary conditions on the wave function $u(r)$. In this case the corresponding probability density $P(r) = [u(r)]^2$ satisfies the quantum probability equation⁴,

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

where units are chosen such that $\hbar = 2m = 1$. At the expense of imposing a second boundary condition at the origin, this second-order non-linear equation can be differentiated to yield a third-order linear form. However, despite the non-linearity, it is in fact easier to derive perturbation theory directly from equation (1.1).

Of course, any result following from the probability equation must also be obtainable from the Schrödinger equation. However, apart from giving a different perspective to standard quantum mechanics [1], the probability approach leads naturally to a perturbation theory that can be applied in similar ways to both the discrete and continuum parts of the spectra. This is because one cannot use the orthogonality between different states and so the sum or integral over intermediate states arising in standard second-order perturbation theory can have no place here.

The formal integral for the energy perturbation of the scattering density has already been given in II, but its application here is very different due to the changed boundary conditions. The procedure is described for S -wave scattering in section 2, where a formula is derived for the shape-dependent term in the effective range expansion that can be considered as an extension of the well-known Bethe formula for the effective range [9]. Expressions for the variation of the probability density to second order in the energy shift are also obtained.

To illustrate the application of the formulae, the Bargmann potential case is described in section 3 before discussing the treatment of a more ad hoc zero-energy density. The energy dependence of the S -wave probability density is of great use when discussing final state interactions in nuclear reactions and in section 4 we compare the standard Watson formula [10] with that obtained by extrapolating to a nearby bound or virtual bound state [11]. Although both prescriptions contain the same pole information, the latter generally gives a somewhat better description than the Watson factor in the important case where there is just one lightly bound state. A summary and conclusions are provided in section 5.

2. Energy dependence of the probability density and phase shift

We consider S -wave scattering in a potential $U(r)$ that vanishes beyond a given range R . It is customary when deriving the effective range expansion to choose a normalization such that, for distances larger than R , the probability density behaves as [12]

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

where δ is the S -wave phase shift at a momentum $k = \sqrt{E}$, in units $2m = 1$. This choice has the advantage that, unlike the conventional density $\tilde{P}(k, r)$ used in II, $\bar{P}(k, r)$ is smooth when extrapolated to any nearby bound state pole of the scattering amplitude $f(k) = e^{i\delta} \sin \delta/k$.

⁴ It has been shown that the restriction to real boundary conditions may in fact be relaxed [8].

However it has to be transformed into $\bar{P}(k, r)$ before using it in physical problems. The boundary condition at the origin is $\bar{P}(k, 0) = 0$.

Expand the density as a power series in k^2 about some point k_0^2 ;

$$\bar{P}(k, r) = \sum_n \frac{1}{n!} (k^2 - k_0^2)^n \bar{P}_n(r). \quad (2.2)$$

Similarly

$$\mathcal{Z}(k) = k \cot \delta = \sum_n \frac{1}{n!} (k^2 - k_0^2)^n \mathcal{Z}_n \quad (2.3)$$

where the conventional scattering length, effective range and shape parameter are given by $a = -1/\mathcal{Z}_0$, $r_0 = 2\mathcal{Z}_1$ and $\mathcal{P} = -\mathcal{Z}_2/r_0^3$ respectively. Though the convergence of the density expansion of equation (2.2) will be very poor at large distances, our results will not in fact be sensitive to this.

The large- r dependence of the first order change in $\bar{P}(k, r)$ is fixed by differentiating equation (2.1) with respect to k^2 ;

$$\bar{P}_1(r) = r \frac{\sin(2kr + 2\delta)}{2k \sin^2 \delta} - \delta' \frac{\sin(kr) \sin(kr + \delta)}{k \sin^3 \delta} \quad \text{for } r \geq R \quad (2.4)$$

where $\delta' = d\delta/dk$.

It follows from the results of II that, when the energy is changed by a small amount $\Delta E = 2k\Delta k$ from its value $E_0 = k_0^2$, the resulting change in the probability density is

$$\bar{P}_1(r) = -2\bar{P}_0(r) \int_R^r \frac{dy}{\bar{P}_0(y)} \int_0^y \bar{P}_0(z) dz + D\bar{P}_0(r) \quad (2.5)$$

where the difference in sign from that in paper II is due to $U(r)$ and E coming in with different signs in equation (1.1). The value of $D = \bar{P}_1(R)/\bar{P}_0(R)$ is fixed by imposing equation (2.4).

After considerable algebraic manipulation, the first order change in $\mathcal{Z}(k)$ becomes

$$\mathcal{Z}_1 = \frac{d(k \cot \delta)}{dk^2} = \bar{Q}_0^{\text{free}}(\infty) - \bar{Q}_0(\infty) \quad (2.6)$$

where the integrated densities are defined by

$$\bar{Q}_n(r) = \int_0^r \bar{P}_n(r') dr'. \quad (2.7)$$

The 'free' superscript in equation (2.6) corresponds to the integral of a density $\bar{P}_0^{\text{free}}(r)$ that is identically equal to the asymptotic form of equation (2.1) for *all* values of r . Because of this cancellation between $\bar{P}_0(r)$ and $\bar{P}_0^{\text{free}}(r)$ at large r , the limit $R \rightarrow \infty$ has been taken in equation (2.6). When evaluated at zero energy, this gives the Bethe formula for the effective range [9], which has a nice pictorial description in terms of the difference between the areas of the free and interacting densities at small distances.

The corresponding expressions for the first order density changes are

$$\begin{aligned} \bar{P}_1(r) &= 2\bar{P}_0(r) \int_r^\infty \frac{\bar{Q}_0(r')}{\bar{P}_0(r')} dr' - 2\bar{P}_0(r) \int_0^\infty \frac{(\bar{Q}_0^{\text{free}}(r') - \mathcal{Z}_1)}{\bar{P}_0^{\text{free}}(r')} dr' \\ \bar{P}_1^{\text{free}}(r) &= -2\bar{P}_0^{\text{free}}(r) \int_0^r \frac{(\bar{Q}_0^{\text{free}}(r') - \mathcal{Z}_1)}{\bar{P}_0^{\text{free}}(r')} dr' \\ \bar{Q}_1(r) &= 2\bar{Q}_0(r) \int_r^\infty \frac{\bar{Q}_0(r')}{\bar{P}_0(r')} dr' - 2\bar{Q}_0(r) \int_0^\infty \frac{(\bar{Q}_0^{\text{free}}(r') - \mathcal{Z}_1)}{\bar{P}_0^{\text{free}}(r')} dr' + 2 \int_0^r \frac{[\bar{Q}_0(r')]^2}{\bar{P}_0(r')} dr' \end{aligned} \quad (2.8)$$

$$\bar{Q}_1^{\text{free}}(r) = -2\bar{Q}_0^{\text{free}}(r) \int_0^r \frac{(\bar{Q}_0^{\text{free}}(r') - \mathcal{Z}_1)}{\bar{P}_0^{\text{free}}(r')} dr' + 2 \int_0^r \bar{Q}_0^{\text{free}}(r') \frac{(\bar{Q}_0^{\text{free}}(r') - \mathcal{Z}_1)}{\bar{P}_0^{\text{free}}(r')} dr'. \quad (2.9)$$

Now the formulae in equations (2.6) and (2.8) are valid for all values of the starting energy E_0 and so we can evaluate the higher order changes by differentiating these results with respect to energy. Formally,

$$\mathcal{Z}_{n+1} = [\bar{Q}_n^{\text{free}}(\infty) - \bar{Q}_n(\infty)] \quad (2.10)$$

where the $\bar{Q}_{n+1}(r)$ is obtained by integrating

$$\bar{P}_{n+1}(r) = \frac{\partial}{\partial E_0} \bar{P}_n(r) \quad (2.11)$$

with respect to r .

The expression for the second order shift in \mathcal{Z} follows immediately from the insertion of equations (2.9) into (2.10);

$$\mathcal{Z}_2 = 2 \int_0^\infty \left\{ \frac{1}{\bar{P}_0^{\text{free}}(r)} (\bar{Q}_0^{\text{free}}(r) - \mathcal{Z}_1)^2 - \frac{1}{\bar{P}_0(r)} (\bar{Q}_0(r))^2 \right\} dr. \quad (2.12)$$

Unlike the \mathcal{Z}_1 case, this result does not have a simple geometric interpretation. It is important to note that, in cases where the densities $\bar{P}_0(r)$ or $\bar{P}_0^{\text{free}}(r)$ have nodes at some point on the real axis, then these are of even order and, as shown in I, these can be avoided by distorting the contour into the complex plane to leave finite integrals.

The second-order change in the density becomes

$$\bar{P}_2(r) = \frac{1}{2} \frac{(\bar{P}_1(r))^2}{\bar{P}_0(r)} + 2\bar{P}_0(r) \int_r^\infty \frac{\bar{Q}_1(r')}{\bar{P}_0(r')} dr' - 2\bar{P}_0(r) \int_0^\infty \frac{(\bar{Q}_1^{\text{free}}(r') - \mathcal{Z}_2)}{\bar{P}_0^{\text{free}}(r')} dr'. \quad (2.13)$$

It is straightforward, but tedious, to extend these formulae to higher orders.

Of importance in final state interaction theory is the energy dependence of the density at short distances. Characterizing this by

$$\gamma_n = \left. \frac{\bar{P}_n(r)}{\bar{P}_0(r)} \right|_{r=0} \quad (2.14)$$

equations (2.8) and (2.13) show that

$$\gamma_1 = 2 \int_0^\infty \left[\frac{\bar{Q}_0(r)}{\bar{P}_0(r)} - \frac{(\bar{Q}_0^{\text{free}}(r) - \mathcal{Z}_1)}{\bar{P}_0^{\text{free}}(r)} \right] dr \quad (2.15)$$

$$\gamma_2 = \frac{1}{2} \gamma_1^2 + 2 \int_0^\infty \left[\frac{\bar{Q}_1(r)}{\bar{P}_0(r)} - \frac{(\bar{Q}_1^{\text{free}}(r) - \mathcal{Z}_2)}{\bar{P}_0^{\text{free}}(r)} \right] dr. \quad (2.16)$$

3. Illustrative examples

The formulae of section 2 can be tested for the delta-shell potential, $\delta(r - R)$, for which the \mathcal{Z}_i and γ_i can be obtained analytically. However, to show the applicability to cases where the potential does not have a sharp cut-off, consider the Bargmann potential [13]

$$U(r) = -\frac{2b^2(b^2 - a^2)}{(b \cosh br + a \sinh br)^2}. \quad (3.1)$$

This case is exceptional in that \mathcal{Z}_2 and all the higher terms in the effective range expansion are identically zero, leaving only $\mathcal{Z}_0 = ab/(b - a)$ and $\mathcal{Z}_1 = 1/(b - a)$.

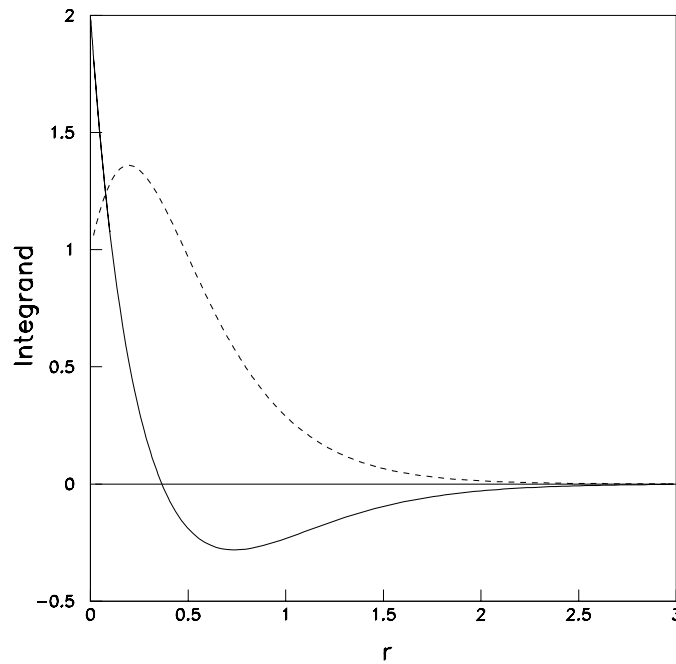


Figure 1. Integrands of equations (2.6) (dashed line) and (2.12) for the effective range and shape parameter terms for the Bargmann potential of equation (3.1) evaluated for $a = 1, b = 2$.

It is typical that the integrand for the Bethe formula of equation (2.6) for \mathcal{Z}_1 converges faster than that for \mathcal{Z}_2 of equation (2.12), with the latter normally having one more oscillation. This is illustrated in figure 1 for parameters $a = 1$ and $b = 2$. The resulting integration can be performed analytically and, in this case, the oscillations for \mathcal{Z}_2 exactly cancel out.

The merit of procedure developed in this paper is that it can be carried out, at least numerically, for an arbitrary zero-energy probability density. As an example of this, consider the case where the density corresponding to a unit scattering length is regularized by an exponential to give the correct boundary condition at the origin.

$$\bar{P}_0(r) = (r + 1 - e^{-r})^2 \quad \bar{P}_0^{\text{free}}(r) = (r + 1)^2. \tag{3.2}$$

The corresponding integrated densities are

$$\begin{aligned} \bar{Q}_0(r) &= -\frac{7}{2} + r + r^2 + \frac{1}{3}r^3 + 2(2 + r)e^{-r} - \frac{1}{2}e^{-2r} \\ \bar{Q}_0^{\text{free}}(r) &= r + r^2 + \frac{1}{3}r^3 \end{aligned} \tag{3.3}$$

and hence, from the Bethe formula of equation (2.6), we see that $\mathcal{Z}_1 = \frac{7}{2}$.

The \mathcal{Z}_2 integrand has the expected oscillation, as shown in figure 2. The corresponding integral cannot be performed analytically but a numerical evaluation shows that $\mathcal{Z}_2 = -4.103$. The variation of the density at short distances is characterized by $\gamma_1 = 4.26$ and $\gamma_2 = 3.17$.

4. Final state interactions

In his seminal work, Watson [10] discussed processes such as pion production in proton–proton scattering, $pp \rightarrow pn\pi^+$, where an enhancement is seen in the excitation energy of the emerging proton–neutron pair caused by their final-state interaction in the 3S_1 and 1S_0 waves.

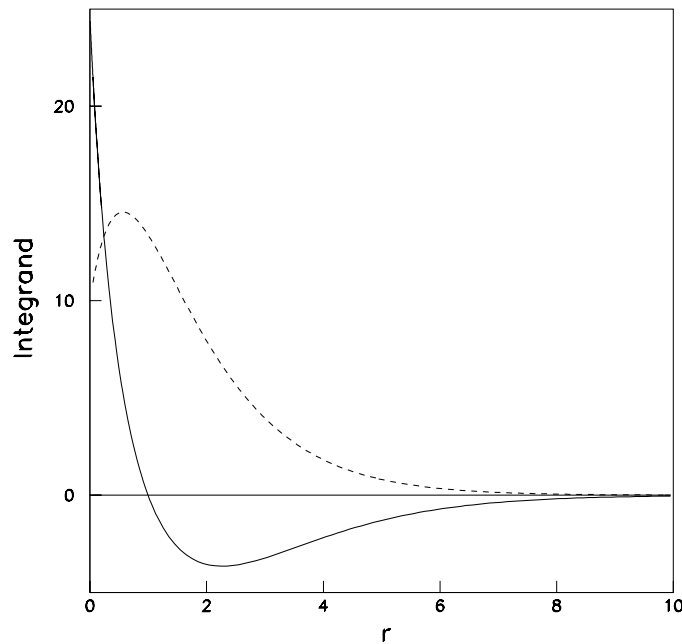


Figure 2. Integrands of equations (2.6) for Z_1 (dashed line) and (2.12) for Z_2 in the case defined by equation (3.2).

It is argued that, due to the large momentum transfer required to produce the pion, the energy dependence of the matrix element may be taken to be proportional the square of the wave function evaluated at $r = 0$;

$$\mathcal{F}(k) \propto |\psi(0)|^2 \propto \tilde{P}(k, 0) = \frac{1}{Z^2 + k^2} \bar{P}(k, 0) \quad (4.1)$$

where we have used equation (2.1) to write the enhancement factor in terms of the density $\bar{P}(r)$ used in this work. What became known as the Watson factor, $1/(Z^2 + k^2)$, corresponds just to neglecting the momentum dependence of $\tilde{P}(k, 0)$. This is a highly successful approach for small k in cases where the scattering amplitude has a nearby pole as, for example, the deuteron bound state in the pn S -wave triplet state or the virtual state in the singlet. It generally decreases too fast at larger values of k and various simple recipes have been proposed to correct this [14].

In an alternative approach, Fäldt and Wilkin [11] have shown that, in the neighbourhood of a loosely bound S -wave state at $k^2 = -\alpha^2$, the probability distribution for the scattering state $\tilde{P}(k, r)$ is linked to that of the normalized bound state density $P(r)$ by the extrapolation theorem,

$$\tilde{P}(k, r) \approx \frac{1}{2\alpha(k^2 + \alpha^2)} P(r) \quad (4.2)$$

the approximation becoming an inequality as $k^2 \rightarrow -\alpha^2$. A similar energy dependence is found for a virtual bound state though there is then no bound state density to set the overall scale in equation (4.2). Since we have seen that the energy dependence of the short range probability density is completely determined by the zero-energy density, we can use this to study which of the approaches gives the better description.

For concreteness and simplicity, consider the case of the spherical well where the potential $U(r) = -U_0\theta(R - r)$ with strength $U_0 = 2.8$ and range $R = 1$ leads to a single bound state

with $\alpha = 0.1587$. By using equations (2.6) and (2.12), or from an algebraic evaluation, the parameters of the effective range expansion are found to be $\mathcal{Z}_0 = -0.1469$, $\mathcal{Z}_1 = 0.4702$ and $\mathcal{Z}_2 = 0.0589$.

It has been shown that the deviation from the extrapolation theorem away from the pole is given by [15]

$$\begin{aligned} 2\alpha(k^2 + \alpha^2) \left. \frac{\tilde{P}(k, r)}{P(r)} \right|_{r=0} &= 1 + \frac{1}{4} \left[\frac{4 + \alpha R}{U_0 - \alpha^2} - \frac{R^2}{1 + \alpha R} \right] (k^2 + \alpha^2) + O((k^2 + \alpha^2)^2) \\ &= 1 + \delta_1 k^2. \end{aligned} \quad (4.3)$$

For the above case the energy variation at short distances is $\approx 1 + 0.159k^2$, to be compared with $1 + \gamma_1 k^2 = 1 + 0.406k^2$. The Fäldt–Wilkin approach therefore gives a slightly better description than the simple Watson factor. However, it must be stressed that in this case these differences are much smaller than the energy dependence arising from the pole factor itself.

The situation is reversed if the potential strength is increased to $U_0 = 22.547$. There is then a deeply bound state as well as a shallow $2S$ level which has the same binding energy as in the previous example. The evaluation of \mathcal{Z}_2 and γ_1 from equations (2.12, 2.15) requires integration in the complex r -plane in order to avoid the node of the $2S$ wave function. The effective range parameters are $\mathcal{Z}_0 = -0.1460$, $\mathcal{Z}_1 = 0.4932$ and $\mathcal{Z}_2 = 0.1332$. Since the value $\gamma_1 = 0.093$ is only half that of $\delta_1 = -0.17$, in this case the Watson model is a little better.

The spherical well example is typical, and numerical studies of other cases suggest that whenever there is just a single bound or virtually bound state close to threshold, the Fäldt–Wilkin approach represents a more robust approach than that given by the Watson formula. It is therefore not surprising that it gives a successful prediction of the total cross section for $pp \rightarrow pn\pi^+$ in terms of that for $pp \rightarrow d\pi^+$ [16].

5. Conclusions

In this series of three papers we have derived time-independent perturbation theory for both scattering and bound states from the probabilistic formulation of quantum mechanics. The seemingly greater complication arising from the use of a non-linear second-order equation rather than the linear Schrödinger equation is balanced by the uniformity of approach afforded by the probability equation in the treatment of the discrete and continuous parts of the spectrum.

In this paper we have concentrated on the study of the energy dependence in the scattering domain, showing how the probability density at one energy uniquely determines that at another energy in terms of quadratures. This allowed us to obtain formulae for the different terms in the effective range expansion, thus generalizing the standard Bethe expression for the effective range. Although we have only considered S -wave scattering, there is no inherent difficulty in considering higher partial waves, as was done in II, but these are generally of lesser importance in final-state-interaction applications.

With the advent of modern fast computers, one has to question the need to resort to perturbation theory. The main advantage of this is its simplicity and transparency. One result of our work is the observation that the shape of the wave function determines its energy dependence and this means that one has to be careful in separating the two in any empirical model. This is important in final-state-interaction theory and we have shown how our technique can be used to investigate different approximations. In particular the extrapolation theorem of equation (4.2) seems to give a better description than the Watson factor for cases where there is just one bound or virtual state pole close to threshold.

The unified approach allows one to combine different elements. Thus it would, in principle, be possible to take the zero-energy S -wave probability density, first perturb in the energy and then introduce the centrifugal barrier potential $\ell(\ell + 1)/r^2$ as a perturbation to provide an estimate for the P -wave scattering amplitude, though the question of convergence would then have to be seriously addressed. Alternatively, since the extrapolation theorem becomes exact at the position of the bound state pole [11], one could then employ the bound state density to derive the terms in an effective range expansion about the pole position.

The probability approach has, of course, its limitations, not being able to handle coupled-channel problems nor time-dependence, where phase information and interference effects are crucial. Nevertheless, we suggest that, in addition to allowing one to derive useful formulae, the probability perturbation approach presents a different and interesting view on some aspects of quantum mechanics.

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