Bound and Unbound Wave Functions at Short Distances

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Abstract

There exists a simple relationship between a quantum-mechanical bound-state wave function and that of nearby scattering states, when the scattering energy is extrapolated to that of the bound state. This relationship is demonstrated numerically for the case of a spherical well potential and analytically for this and other soluble potentials. Provided that the potential is of finite range and that the binding is weak, the theorem gives a useful approximation for the short-distance behaviour of the scattering wave functions. The connection between bound and scattering-state perturbation theory is established in this limit.

I. Introduction

It has recently been shown there is a simple relationship between the normalisations of the scattering and bound-state wave functions when the scattering energy is continued to that of the bound state\(^1\). That the two wave functions become mutually proportional in this limit is known from the standard text books\(^2,3\), but it was unexpected to find that the relative normalisation depended purely upon the binding energy. Though the theorem is valid for arbitrary angular momentum, we wish here to illustrate some of the results for S-wave scattering. Provided the range of the potential is short and the binding is light, it will be seen that the extrapolation
Theorem actually gives useful approximations for scattering wave functions at low energies and short distances.

The $S$-wave Schrödinger equation for the interaction of a particle of mass $m$ in a potential $V(r)$ may be written as

\[
  \begin{align*}
  u''_\alpha(r) - \alpha^2 u_\alpha(r) &= U(r) u_\alpha(r), \\
  v''(k, r) + k^2 v(k, r) &= U(r) v(k, r),
  \end{align*}
\]

(1)

where $U(r) = 2mV(r)/\hbar^2$ and the binding and scattering energies are $-\hbar^2 \alpha^2 / 2m$ and $\hbar^2 k^2 / 2m$ respectively. The corresponding radial wave functions, $u_\alpha(r)$ and $v(k, r)$, vanish at $r = 0$ but satisfy contrasting boundary conditions at large distances. For a potential of finite range the bound-state wave function behaves asymptotically like

\[ u_\alpha(r) \approx N_\alpha e^{-\alpha r} \]

(2)

and is normalised by the integral condition

\[ \int_0^\infty [u_\alpha(r)]^2 dr = 1. \]

(3)

On the other hand the scattering solution normalisation is determined by its asymptotic behaviour and, if we take real boundary conditions (standing waves), then

\[ v(k, r) \to \frac{1}{i k} \sin(kr + \delta(k)) = \frac{1}{2ik} \left( e^{i\delta(k)} e^{ikr} - e^{-i\delta(k)} e^{-ikr} \right) \]

(4)

as $r \to \infty$, where $\delta(k)$ is the $S$-wave phase shift at wave number $k$.

In order that $v(k, r)$ might become an acceptable localisable wave function as $k \to i\alpha$, for which the normalisation condition of Eq.(3) would hold, the S-matrix must have a pole at the position of the bound state and can therefore be written in this region as

\[ S(k) = e^{2i\delta(k)} = N^2(k) \left( \frac{\alpha - ik}{\alpha + ik} \right) \Rightarrow e^{i\delta(k)} = N(k) \frac{(\alpha - ik)}{(\alpha^2 + k^2)^{1/2}}, \]

(5)

where $N(k)$ is well behaved in the vicinity of $k = i\alpha$.

At the bound-state pole the second term in Eq.(4) is eliminated to leave the desired asymptotic behaviour

\[ v(k, r) \approx -\frac{N(i\alpha)}{(\alpha^2 + k^2)^{1/2}} e^{-\alpha r}. \]

(6)
Though this does not establish the relative normalisation of this and the bound-state wave function $u_\alpha(r)$, the presence of the square root in the denominator of Eq.(6) is indicative and this factor is contained within the extrapolation theorem\(^1\), which for potentials of finite range yields

$$\lim_{k \to i\alpha} \left\{ \left[ 2\alpha(\alpha^2 + k^2) \right]^{1/2} v(k, r) \right\} = -u_\alpha(r). \quad (7)$$

It should be noted that this relationship is *independent* of the shape of the potential and is determined purely by the binding energy. It is now easy to see from Eqs.(6) and (7) that, in terms of the asymptotic normalisation constant $N_{as}$ of Eq.(4), the residue at the pole of the $S$-matrix in Eq.(5) equals $-iN_{as}^2$.

As will be seen from the numerical examples given for the spherical well potential discussed in §2, the above extrapolation theorem actually provides useful approximations for scattering wave functions in terms of that of a nearby bound state. Provided that the binding is weak, and that neither $k$ nor $r$ are too large,

$$v(k, r) \approx -\left[ 2\alpha(\alpha^2 + k^2) \right]^{-1/2} u_\alpha(r). \quad (8)$$

The ratio of the scattering to the bound-state wave functions is studied analytically for several exactly soluble potentials in §3, where more precise statements are made on the range of validity of the approximations in Eq.(8) and general trends in the deviations noted. One feature seen for the spherical well potential is that there seems to be a region of $r$ where all the wave functions, scaled by the square root factor as in Eq.(8), come together. A simple understanding of this cross-over effect is also attempted in §3.

The low energy proton-proton system is not quite bound but there is a virtual state with small but negative $\alpha$ situated close to physical energies. Though in such cases there is no bound-state wave function to set the scale, the energy dependence of the scattering wave functions is well approximated by the square-root factor as in Eq.(8). This behaviour is clearly demonstrated by the spherical well and it is seen from these examples that it is the nearest singularity which is dominant.

Though the long range of the Coulomb potential violates the assumptions made when proving the extrapolation theorem of Eq.(4), it nevertheless remains valid for
all the Coulomb bound states, as shown in §4. However the accumulation of bound states in the vicinity of zero energy means that Eq.(8) is of no use in representing the scattering functions even at low energies. There is no nearby dominant pole.

Eq.(8) is of great help in estimating the effects of final state interactions in nuclear processes at large momentum transfers, where the behaviour of the wave function at small distances is important. For example it allows one to estimate the cross section for \( pp \to pm\pi^+ \) in terms of that for \( pp \to d\pi^+ \), where the final neutron-proton triplet pair are fused to become a deuteron. Another simple example discussed in §5 involves the relationship between perturbation theory applied to bound and scattering state problems. A consistent picture is found when using Eq.(8) in the presence of a lightly bound state. A summary of our main conclusions is to be found in §6.

II. Numerical investigation for the spherical well potential

As a first illustration of our ideas, consider the spherical well potential

\[
U(r) = \frac{2m}{\hbar^2} V(r) = \begin{cases} -U_0, & r < a, \\ 0, & r \geq a. \end{cases}
\]

(9)

For \( r \geq a \) the scattering and bound-state wave functions are proportional to \( \sin(kr + \delta) \) and \( e^{-\alpha r} \) respectively, whereas inside the well they are rather \( \sin(kr) \), where \( \kappa^2 = U_0 - \alpha^2 \) or \( \kappa^2 = U_0 + k^2 \). It is trivial to match boundary conditions at \( r = a \) to obtain an implicit equation for the energy eigenvalues and hence the wave functions.

The approximation of Eq.(8) is expected to work best for a loosely bound state, and we start by treating the case where there is just a single 1s state. Taking units where the potential radius \( a = 1 \), a potential strength of \( U_0 = 2.8 \) yields \( \alpha = 0.159 \) and the normalised full bound-state wave function \( \psi_\alpha(r) = u_\alpha(r)/r \) is plotted in fig. 1.1. Also shown there are the corresponding scattering wave functions, modified by the square-root factor of Eq.(8),

\[
\tilde{\psi}(k,r) = -\left[2|\alpha|(<\alpha^2 + k^2>)\right]^{1/2} v(k,r)/r,
\]

(10)

at wave numbers of \( k = 0.1, 0.2, 0.5, \) and 1.0.
At $r = 0$ the agreement between the various functions is very good for low values of $k$, though the scattering ones lie above that of the bound state and steadily increase with $k$. Though the energy dependence of the functions in this region seems to be roughly $\kappa^{1/2}$, too much should not be read into this. The scattering functions must of course be orthogonal to the bound state and this implies that they start to oscillate before the bound state has died out. This is seen clearly in the figure, as is the fact that the oscillations set in earlier for higher $k$-values. What is less evident is why all the curves seem to come close together for $r \approx 0.66$. This has the practical effect however of limiting the deviations between the scattering and bound-state functions over the range of the potential.

If the potential strength is increased in order to generate a deeply bound $1s$ state in addition to a $2s$ state with the same binding as in fig. 1.1, then the latter has the node demonstrated in fig. 1.2. The scattering functions defined by Eq.(9) still fall very close to that of the bound state with the crucial difference that they now lie below for small $r$. A cross-over region still exists but at higher values of $r$.

Fig. 1.3 shows that if the attraction is reduced a little such that the $2s$ state becomes a virtual one with negative $\alpha$ ($\alpha = -0.159$) then, as expected, the scattering wave functions still retain their dominantly $2s$ character, though there is then no bound state to set the scale and $r$-dependence. The wave function of such a virtual state increases like $e^{+|\alpha|r}$ at large distances and hence is non-normalisable. It is therefore clear that it is the nearest singularity of the scattering amplitude which governs the behaviour of the wave function at low $k$. Though Eq.(4) is valid for all the bound states of a problem when extrapolating to the pole, Eq.(8) is only a useful representation for a nearby singularity. An important practical case of this kind is the proton-proton system where the (just) unbound virtual state dominates the low energy wave function and allows us to derive the energy dependence of the $pp \to pp\pi^0$ cross section near threshold\textsuperscript{5}.
III. Analytic expressions for soluble potentials

In addition to the spherical well potential, there are several other potentials for which exact solutions to the Schrödinger equation can be obtained. In such cases it is interesting to study the deviations from the extrapolation theorem analytically in going away from the bound-state pole at $k = i\alpha$ to see the dependence upon the parameters. Define therefore the ratio

$$R(k, r) = -\left[2\alpha(\alpha^2 + k^2)\right]^{1/2} \frac{v(k, r)}{u_\alpha(r)}$$  \hspace{1cm} (11)

In order to satisfy the extrapolation theorem $R(i\alpha, r) = 1$ and, provided that the potential is of finite range, the ratio function can be expanded as a power series in $\alpha^2 + k^2$.

$$R(k, r) = 1 + \sum_{n=1}^{\infty} R_n(r) (\alpha^2 + k^2)^n.$$  \hspace{1cm} (12)

In general this will have a finite radius of convergence since $R(k, r)$ diverges at the position of any other bound state.

A. The Yamaguchi potential

The strength $\lambda$ of the non-local but separable Yamaguchi potential,

$$V(r, r') = -\lambda \left(\frac{e^{-\beta r}}{r} \right) \left(\frac{e^{-\beta r'}}{r'} \right),$$  \hspace{1cm} (13)

can be adjusted to give a solitary bound state at $E = -\hbar^2 \alpha^2 / 2m$.

A straightforward calculation then shows that to second order in $r$

$$R_1(r) = \frac{3}{8\beta(\beta + \alpha)} + \frac{1}{4\beta} r - \frac{(\beta - \alpha)}{8\beta} r^2 + 0(r^3).$$  \hspace{1cm} (14)

B. The Bargmann potential

The Bargmann potential defined by

$$U(r) = \frac{2m}{\hbar^2} V(r) = -2(\beta^2 - \alpha^2) \left(\cosh(\beta r) - \frac{\alpha}{\beta} \sinh(\beta r)\right)^2,$$  \hspace{1cm} (15)

with $\beta > \alpha > 0$, has precisely one bound state with $E = -\hbar^2 \alpha^2 / 2m$. 

6
Taking the ratio of the scattering to bound-state wave functions at low energies and distances then gives

\[ R_1(r) = \frac{1}{2(\beta^2 - \alpha^2)} - \frac{1}{6} r^2 - \frac{1}{90} (2\beta^2 - 3\alpha^2) r^4 + 0(r^6), \]

\[ R_2(r) = -\frac{1}{8(\beta^2 - \alpha^2)^2} - \frac{1}{12(\beta^2 - \alpha^2)} r^2 - \frac{(\beta^2 - 3\alpha^2)}{360(\beta^2 - \alpha^2)} r^4 + 0(r^6). \] \hspace{1cm} (16)

**C. The spherical well potential**

The solutions for the spherical well potential \( U(r) = -U_0 \theta(a - r) \), discussed numerically in §2, also lead to analytic expressions for the ratio function. Thus

\[ R_1(r) = \frac{a^2}{4(1 + aa)} - \frac{(4 + aa)}{4(U_0 - \alpha^2)} - \frac{1}{6} r^2 + 0(r^4), \] \hspace{1cm} (17)

where the binding energy \( E = -\hbar^2 \alpha^2 / 2m \) is determined from the implicit equation

\[ (U_0 - \alpha^2)^{1/2} \cot \left( a(U_0 - \alpha^2)^{1/2} \right) = -\alpha. \] \hspace{1cm} (18)

**D. Conclusions**

It is clear from the examples given above that for a lightly bound state \( (\alpha \ll U(0)) \), the expansion parameter at the origin is proportional to \( \alpha^2 + k^2 \) times the square of the range of the potential, though the coefficient depends upon the shape of the potential. However the \( r \)-dependence of the expansion coefficients \( R_n(r) \) can be obtained directly by expanding the potential in powers of \( r \) and integrating the Schrödinger equation starting from \( r = 0 \). It is therefore no accident that the coefficient of \( r^2 \) in \( R_1(r) \) is the same for the Bargmann case of Eq.(16) as for the square well of Eq.(17). This result is independent of the potential provided that this is finite at the origin. In the Yamaguchi example of Eq.(14) the odd powers of \( r \) arise from the divergence of the potential at short distances.

It was noted in §2 that in the case of the first lightly bound state in a spherical well potential the scattering function lay above the bound-state function, whereas if it were the second bound state then the scattering function lay below. This change
in sign of $R_1(0)$ in Eq.(17) arises because in the first case $U_0 \approx \pi^2/4a^2$, whereas in the second $U_0 \approx 9\pi^2/4a^2$.

In the numerical examples shown in §2, where the deviations from the extrapolation theorem are not too large, a cross-over region was noted where all the functions are very close. That the scattering function cross the bound state, in a region where the latter wave function is large, follows immediately from the condition that the two be orthogonal when integrated over $r$. This position will be stable with respect to changes in $k$ provided that the first term in the power series expansion in $(\alpha^2+k^2)$ in Eq.(12) is dominant and in such an event the cross-over point would be determined by the condition that $R_1(r) = 0$. For $\beta = 1.0$ and $\alpha = 0.1$ in the Bargmann case one would expect that at low energies the cross-over would occur when $r \approx 1.74$ if we keep only the quadratic term in $r^2$ in Eq.(10), but $r \approx 1.68$ with the quartic term. These are to be compared to the numerical value of $r \approx 1.522$. Of course the cross-over point should move to smaller values of $r$ as the energy is increased since the scattering wave functions start to oscillate faster and the node in $r$ is shifted to the left.

The above arguments do not provide any explanation as to the sign of $R_1(0)$ and for this the spherical well case is particularly illuminating. In the case of fig. 1, where one has only one (lightly)-bound state, then $R_1(0)$ is positive. This is also true for the other two potentials discussed in this section. However when the depth of the well is increased so as to make the lightly bound state the second one then $R_1(0)$ changes sign. This is in the right direction to make the extrapolation theorem of Eq.(7) be valid also for the deeply bound state at more negative values of $k^2$ where $R(k,r)$ has to diverge to $+\infty$. On the other hand, when there is only one bound state the only singularities that $R(k,r)$ can be simulating are those associated with the potential itself.
IV. The Coulomb potential

Due to the long range of the Coulomb potential the infinite number of bound-state eigenvalues have an accumulation point at energy zero. Nevertheless it is easy to see explicitly that the extrapolation theorem is still valid for all the bound states.

Define full scattering wave functions as \( \psi(k, r) = v(k, r)/r \), and similarly for the bound state. The value of the square of the real Coulomb wave function at the origin in an \( S \)-wave scattering state is just the Gamow factor

\[
[\psi(k, 0)]^2 = \frac{2\pi \eta}{e^{2\pi \eta} - 1} = \pi \eta [-1 + \coth(\pi \eta)] ,
\]

where in the attractive case the Coulomb parameter \( \eta = -me^2/\hbar^2k \).

The infinite number of bound states correspond to the poles of Eq.(19) when \( \eta = in \), where \( n \) a non-vanishing integer. These can be made explicit by recasting the equation as

\[
[\psi(k, 0)]^2 = -\pi \eta + 1 + 2 \sum_{n=1}^{\infty} \frac{1}{1 + n^2/\eta^2} .
\]

(20)

If we write the virtual momenta of the bound states as \( \alpha_n = me^2/n\hbar^2 \), it is well known that the value of the \( n \)'th bound-state wave function at the origin is

\[
[\psi_n(0)]^2 = 4\alpha_n^3 ,
\]

(21)

so that Eq.(20) may be written as

\[
[\psi(k, 0)]^2 = \frac{\pi me^2}{\hbar^2 k} + 1 + \sum_{n=1}^{\infty} \frac{[\psi_n(0)]^2}{2\alpha_n(\alpha_n^2 + k^2)} .
\]

(22)

Our theorem of Eq.(7) is still formally valid since, in the vicinity of any of the Coulomb bound states, just one term in the sum will be important and for this the residue is clearly correct. Despite this, it is of no practical use in representing the scattering wave function at low energies since no single pole will then dominate and, as can be seen from Eq.(22), the Coulomb potential produces an extra non-trivial term singular at \( k = 0 \). Thus the expansion of \( R(k, r) \) in powers of \( (\alpha^2 + k^2) \) as in Eq.(12) is not valid.
V. The two-potential formula

We here show the relation of our approximation to some of the results of standard perturbation theory. Denote by $f_0$ the S-wave scattering amplitude corresponding to a potential $V_0$. If a small extra potential $V_1$ is added, the change in the amplitude to first order in $V_1$ is given by the two-potential formula

$$\Delta f \approx -\frac{2m}{\hbar^2} e^{2i\delta_0} \langle \chi_k | V_1 | \chi_k \rangle .$$

(23)

The factor involving the phase shift $\delta_0$ for the potential $V_0$ is introduced because $\chi_k$ is the real scattering solution. Note that the integration in the expectation value is only over the radial coordinate $r$.

Assume now the potential $V_1$ to be of short range such that the conditions leading to Eq.(7) are applicable. If the potential $V_0$ has one weakly bound state $\chi_b$, then $\chi_k$ is related to it through the approximate relation of Eq.(8) and this leads to

$$\Delta f \approx -e^{2i\delta_0} \frac{m}{\alpha_0(\alpha_0^2 + k^2)\hbar^2} \langle \chi_b | V_1 | \chi_b \rangle = -e^{2i\delta_0} \frac{m \Delta E}{\alpha_0(\alpha_0^2 + k^2)\hbar^2} .$$

(24)

In the above we have used perturbation theory to identify $\Delta E$ as the change in the binding energy $E_0 = -\alpha_0^2/2m\hbar^2$ of the bound state to first order in $V_1$. In this limit

$$e^{2i\delta} \approx 1 + 2ik(f_0 + \Delta f) = e^{2i\delta_0} \left[ 1 - \frac{2ikm\Delta E}{\alpha_0(\alpha_0^2 + k^2)\hbar^2} \right] .$$

(25)

For a loosely bound state, the S-matrix is given by the scattering length approximation

$$e^{2i\delta} = \frac{\alpha - ik}{\alpha + ik} \quad \text{and} \quad e^{2i\delta} = \frac{\alpha_0 - ik}{\alpha_0 + ik} .$$

(26)

The correction in Eq.(25) is valid only to leading order in $\Delta E$ and introducing this into Eq.(26) and keeping only such terms, we find

$$\alpha = \alpha_0 \left( 1 - \frac{m\Delta E}{\alpha_0^2\hbar^2} \right)$$

(27)

and a binding energy of

$$E = -\frac{\hbar^2 \alpha^2}{2m} = E_0 + \Delta E ,$$

(28)
as expected. This explicitly shows the consistency of first order perturbation theory for bound-state energies and scattering matrices with our approximate wave function.
in the case of a weakly bound state.

VI. Summary and conclusions

We have shown for several soluble examples that it is possible to approximate the real scattering wave function quantitatively in terms of that of a nearby bound state. This goes further than the theorem of Eq.(7) in that it shows that it is a robust extrapolation provided that the binding is weak and that the wave number $k$ and distance $r$ are both small. Though we have worked entirely with real wave functions, this is sufficient for applications in final-state-interaction theory\(^4\).

Provided that the bound-state pole is close, one can use Eq.(5) to obtain the complex scattering wave function with outgoing boundary conditions in the scattering length approximation

$$
\psi^{(+)}(k, r) = \psi(k, r) e^{\delta(k)} \approx -(2\alpha)^{-1/2} \psi_\alpha(r)/(\alpha + ik).
$$

(29)

Though we have a qualitative explanation for the deviations from the approximate relationship of Eq.(8), its magnitude at $r = 0$ must depend upon the structure of the potential and the singularities of the scattering amplitude. Fortunately the cross-over phenomenon, whereby all the functions come very close at some region within the range of the potential, limits the deviations significantly. As explained in §3, this cross-over phenomenon is very general and exists also for realistic nucleon-nucleon potentials, such as that of the Paris group\(^4,9\). It is also demonstrated by numerical resolution of the Schrödinger equation for various finite-range potentials.

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Figure 1: Bound-state (solid line) and scattering wave functions, modified as in Eq. (10), for a spherical well of radius 1.0. The scattering states are evaluated at \( k = 0.1 \) (dot-dashed line), \( k = 0.2 \) (closely spaced dots), \( k = 0.5 \) (dashes), and \( k = 1.0 \) (widely spaced dots). (1) For a depth of \( U_0 = 2.8 \), the resulting 1s bound state has \( \alpha = 0.159 \), and the deviations at \( r = 0 \) are positive and increase with \( k \). (2) A potential of strength \( U_0 = 22.547 \) has a 2s level with the same value of \( \alpha = 0.159 \). The scattering functions now lie below that of the bound state at \( r = 0 \). (3) Reducing the potential strength to \( U_0 = 21.913 \) turns the 2s level into a virtual state with \( \alpha = -0.159 \). Nevertheless the scattering functions retain their dominantly 2s character at short distances and illustrate that it is the nearby singularity, bound or virtual, which governs the energy dependence of the scattering wave functions.