BOUND STATES AND SCATTERING IN AN r^{-2} POTENTIAL

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[*Manuscript received February 15, 1962*]

Summary

The bound-state and scattering wavefunctions for a particle moving in a central r^{-2} potential are investigated. There are no discrete bound states: the discrete states which result when an infinite repulsive core is introduced are specified. The scattering wavefunctions which satisfy physical requirements such as zero net outflow of particles from the scattering region are found. The phase-shifts δ_l are independent of energy and for large l to go to zero as $(2l+1)^{-1}$.

I. Introduction

This paper considers a particle moving in a central r^{-2} potential, or two particles interacting through such a central potential. An r^{-2} potential lies between the long-range Coulomb potential and various short-range potentials, such as Yukawa or square-well, which have been used in nuclear models.

An r^{-2} potential is found not to distort the scattering radial wavefunctions at infinity, as does the Coulomb potential, but it does produce phase-shifts which fall off rather slowly with increasing angular momentum. It is also found that the phase-shifts are independent of system energy (as was noticed in recent work by Spruch, O'Malley, and Rosenberg (1960) and O'Malley, Spruch, and Rosenberg (1961)) so that the simple effective-range theory often used for the analysis of low-energy nuclear scattering data cannot be developed for such a potential. The singularity of r^{-2} at $r=0$ is sufficient to prevent the existence of discrete bound states. (Since this paper was written the author has noticed a treatment of bound states by Landau and Lifshitz (1958) yielding the same conclusion.) The eigenstates which result when this potential is cut off by an infinite repulsive core at $r=0$ are specified.

For a particle moving in a central potential, or two particles interacting through a central potential, of the form

$$V(r)=A\hbar^2/2Mr^2, \tag{1}$$

the Schroedinger equation is separable in spherical polar coordinates and the wavefunction takes the form

$$\psi=R(r)Y_{lm}(\theta),$$

where $R(r)$ satisfies the equation

$$\frac{\mathrm{d}^2R}{\mathrm{d}r^2}+\frac{2}{r}\frac{\mathrm{d}R}{\mathrm{d}r}+\left\{\frac{2M}{\hbar^2}[E-V(r)]-\frac{l(l+1)}{r^2}\right\}R=0.$$

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On writing

$$\rho = r\sqrt{\left(\frac{2ME}{\hbar^2}\right)} = kr, \tag{2}$$

$$R(r) = \frac{1}{\sqrt{\rho}} u(\rho), \tag{3}$$

we obtain

$$\frac{d^2u}{d\rho^2} + \frac{1}{\rho}\frac{du}{d\rho} + \left(1 - \frac{\nu^2}{\rho^2}\right)u = 0, \tag{4}$$

where

$$\nu^2 = A + (l + \tfrac{1}{2})^2. \tag{5}$$

This is simply the equation defining Bessel functions, and the problem is to find linear combinations of these functions of order ν that satisfy the boundary conditions imposed on $R(r)$ by physical requirements of normalization and so on. We will use the notation for Bessel functions defined in Watson (1944).

II. Bound States

For energies $E<0$, $k=i\alpha$ $(\alpha>0)$ is imaginary. The only Bessel function of order ν which vanishes as $\alpha r \to \infty$ is

$$u = K_\nu(\alpha r), \tag{6}$$

which does so exponentially. Now

$$K_\nu(\alpha r) = \frac{\pi}{2 \sin \nu\pi}[I_{-\nu}(\alpha r) - I_\nu(\alpha r)],$$

where

$$I_\nu(\alpha r) = \sum_{n=0}^{\infty} \frac{(\frac{1}{2}\alpha r)^{\nu+2n}}{n!\,\Gamma(\nu+n+1)}.$$

so as $r\to 0$, K_ν will have a singularity of form $r^{-|Rl\,\nu|}$.

For an acceptable wavefunction the normalization integral

$$\int_0^\infty R^2 r^2 dr,$$

must converge: this will require that

$$|Rl\,\nu| < 1. \tag{7}$$

From (5), this restriction means that

$$A < 1 - (l + \tfrac{1}{2})^2. \tag{8}$$

So for wells of depths satisfying (8), equation (6) defines wavefunctions which vanish at infinity, are continuous, and are normalizable. However, they then exist for all values of α: there is therefore a continuum of bound states extending indefinitely downwards in energy. This is an unacceptable model for a physical system.

If we impose the stronger requirement that R remain finite at the origin, then $K_\nu(\alpha r)$ is required to go to zero at least like $\sqrt{(\alpha r)}$ near $r=0$. This is not possible for any values of ν or α. Even if $\nu=0$,

$$K_0(\alpha r) = -I_0(\alpha r) \log \tfrac{1}{2}\alpha r + \sum_{n=0}^{\infty} (\tfrac{1}{2}\alpha r)^{2n} \frac{\psi(n+1)}{(n!)^2},$$

which has a logarithmic infinity at $r=0$. There are then no bound states of the system. We conclude that no physical system having a bound state can be considered to be described at low energies by a potential function Ar^{-2}. However, we are familiar in nuclear theory with the idea of energy-dependent potentials, so for scattering at higher energies such an Ar^{-2} potential need not be ruled out.

(*a*) *Cut-off*

If Ar^{-2} is suitably modified at small r, discrete bound states will exist. If there is an infinite repulsive core at $r=a$, the usual arguments show that the eigenstates are given by (6) for $r>a$, provided that ν and α satisfy

$$K_\nu(\alpha a)=0. \tag{9}$$

Now for any given αa, $K_\nu(\alpha a)$, regarded as a function of ν, has an infinite set of purely imaginary zeros and no other zeros (see Erdélyi *et al.* 1953). Since $K_\nu=K_{-\nu}$, we may specify the solutions of (9), for a given αa, by

$$\nu=\pm i\mu_1,\ \pm i\mu_2, \ldots, \pm i\mu_s, \ldots, \tag{10}$$

where the μ are real and

$$0<\mu_1<\ldots<\mu_s<\ldots \tag{11}$$

These values specify a set of well-depths

$$A_s=-\mu_s^2-(l+\tfrac{1}{2})^2, \tag{12}$$

for a core radius a, for which there is a bound state of energy

$$E=-\frac{\hbar^2}{2M}\alpha^2, \tag{13}$$

and eigenfunction

$$R_{\alpha,a,s}(r)=\frac{1}{\sqrt{(\alpha r)}}K_{i\mu_s}(\alpha r). \tag{14}$$

Conversely, for a given well-depth A and angular momentum l, there will be a set of bound states specified by

$$E_n=-\frac{\hbar^2}{2M}\alpha_n, \tag{15}$$

$$R_n(r)=\frac{1}{\sqrt{(\alpha_n r)}}K_{i\mu}(\alpha_n r), \tag{16}$$

where $\mu^2=-A-(l+\frac{1}{2})^2$ and the α_n satisfy

$$K_{i\mu}(\alpha_n a)=0. \tag{17}$$

In general μ and hence the α_n depend on l: there is no degeneracy between states of different angular momenta. The number of roots of (17) will depend on μ. Starting at $\mu=0$, $(A=-(l+\frac{1}{2})^2)$ there will be no solutions α_n: at a larger μ, one solution α_1 will appear, and so on.

Let these roots be arranged in order:

$$\alpha_1>\alpha_2>\ldots>0. \tag{18}$$

Then α_1 will specify the ground state of the system for the given μ and the wavefunction (16) will be zero only at $r=a$ and as $r\to\infty$. The next state α_2 will be zero at $r_1=a$, $r\to\infty$ but also clearly at

$$r_2=\frac{\alpha_1}{\alpha_2}a\,;$$

similarly, the next state α_3 will have eigenfunction zeros at

$$a,\ \frac{\alpha_2}{\alpha_3}a,\ \frac{\alpha_1}{\alpha_3}a,\ \infty,$$

and so on.

III. Scattering

For positive energies k is real and the only Bessel functions that can remain finite at the origin are

$$\begin{aligned} u=&\mathbf{J}_\nu(kr), && \text{for } \nu \text{ real (positive)},\\ &\mathbf{J}_{\pm\nu}(kr), && \text{for } \nu \text{ imaginary} \end{aligned} \tag{19}$$

(where for convenience ν is the positive or positive imaginary root of ν^2), which functions have the correct oscillating behaviour for r large.

The development which follows differs only slightly from the usual elementary treatment (see e.g. Schiff 1955). We require a solution of the Schroedinger equation possessing polar symmetry:

$$v(r,\theta)=\sum_{l=0}^{\infty} A_l R_l(r) P_l\,(\cos\theta), \tag{20}$$

where the P_l are the Legendre polynomials, which will be identified asymptotically with

$$\mathrm{e}^{ikz}+\frac{1}{r}f(\theta)\mathrm{e}^{ikr}, \tag{21}$$

which represents an incident plane wave plus a scattered spherical wave, in the usual way.

For states of sufficiently large l, ν^2 as defined by (5) will be positive, $\mathbf{J}_\nu$ has the correct behaviour for R_l at $r=0$, and preserves at zero the total outward flux over a sphere about the scattering centre. For states of l low enough to make ν^2 negative (only possible for attractive forces, $A<0$), $\nu=\mathrm{i}\mu$ ($\mu>0$ say), and $\mathbf{J}_\nu$ and $\mathbf{J}_{-\nu}$ both oscillate indefinitely often between finite bounds as $r\to 0$. For small kr,

$$\begin{aligned}\mathbf{J}_{\mathrm{i}\mu}(kr)&\sim(kr)^{\mathrm{i}\mu}\\ &=\cos(\mu\log kr)+\mathrm{i}\sin(\mu\log kr).\end{aligned}$$

The normalization integral about $r=0$ converges. Asymptotically,

$$\begin{aligned}\mathbf{J}_{\mathrm{i}\mu}(kr)&\sim\sqrt{\left(\frac{2}{\pi kr}\right)}\sin\left(kr-\tfrac{1}{2}\mathrm{i}\mu\pi+\tfrac{1}{4}\pi\right)\\ &=\sqrt{\left(\frac{2}{\pi kr}\right)}\sin\left(kr+\tfrac{1}{4}\pi\right)\cosh\tfrac{1}{2}\mu\pi-\mathrm{i}\sqrt{\left(\frac{2}{\pi kr}\right)}\cos\left(kr+\tfrac{1}{4}\pi\right)\sinh\tfrac{1}{2}\mu\pi,\end{aligned}$$

which is not of the usual form, which defines the phase-shift δ_l,

$$\frac{1}{\sqrt{(kr)}} \sin\,(kr-\tfrac{1}{2}l\pi+\delta_l), \tag{22}$$

with δ_l real. The requirement that the total outward flux over a sphere be zero is met if the flux vector

$$\bar{\psi}\,\mathrm{grad}\,\psi-\psi\,\mathrm{grad}\,\bar{\psi} \tag{23}$$

vanishes. If we choose the combination $\mathbf{J}_\nu+\mathbf{J}_{-\nu}$ the asymptotic form is real and the flux vector vanishes. So for ν^2 negative the appropriate form of wave-function to use is

$$R_l=\frac{\text{const.}}{2\sqrt{(kr)}}[\mathbf{J}_\nu(kr)+\mathbf{J}_{-\nu}(kr)].$$

Let l_0 be the lowest positive integer for which

$$\nu^2=A+(l_0+\tfrac{1}{2})^2$$

is positive. Then for $l\geqslant l_0$, we take

$$\begin{aligned} R_l&=\sqrt{\left(\frac{\pi}{2kr}\right)}\mathbf{J}_\nu(kr) \\ &\sim\frac{1}{kr}\sin\,(kr-\tfrac{1}{2}\nu\pi+\tfrac{1}{4}\pi), \end{aligned} \tag{24}$$

while for $l<l_0$ we take

$$\begin{aligned} R_l&=\sqrt{\left(\frac{\pi}{8kr}\right)}\frac{1}{\cosh\,\tfrac{1}{2}\mu\pi}[\mathbf{J}_{i\mu}(kr)+\mathbf{J}_{-i\mu}(kr)] \\ &\sim\frac{1}{kr}\sin\,(kr+\tfrac{1}{4}\pi). \end{aligned} \tag{25}$$

Comparing these asymptotic forms with (22), the phase-shifts are seen to be

$$\begin{aligned} \delta_l&=(l+\tfrac{1}{2})\tfrac{1}{2}\pi && \text{for } l<l_0, \\ &\left.\begin{aligned}&=(l+\tfrac{1}{2}-\nu)\tfrac{1}{2}\pi \\ &=(l+\tfrac{1}{2})\{1-\sqrt{[1+A/(l+\tfrac{1}{2})^2]}\}\tfrac{1}{2}\pi\end{aligned}\right\}, && \text{for } l\geqslant l_0. \end{aligned} \tag{26}$$

For l large, the phase-shift is

$$\delta_l\sim-\frac{A}{2l+1}\cdot\tfrac{1}{2}\pi, \tag{27}$$

which goes to zero rather slowly as l increases. A potential Ar^{-2} does not distort the radial wave function at infinity, as does the longer range Coulomb potential, but it is not like a short-range force and affects states of high angular momentum. It is notable that δ_l is independent of the energy.

We require (20) to equal (21) asymptotically :

$$\begin{aligned} \sum_{l=0}^{\infty} A_l R_l P_l\,(\cos\theta)&\sim e^{ikr\cos\theta}+\frac{1}{r}f(\theta)e^{ikr} \\ &=\sum_{l=0}^{\infty}(2l+1)i^l j_l(kr)P_l\,(\cos\theta)+\frac{1}{r}e^{ikr}\sum_{l=0}^{\infty}f_l P_l\,(\cos\theta). \end{aligned}$$

Since the $P_l(\cos\theta)$ are orthogonal, this requires that

$$A_l R_l \sim (2l+1)\mathrm{i}^l j_l(kr) + \frac{1}{r}\mathrm{e}^{\mathrm{i}kr} f_l. \tag{28}$$

Substituting asymptotic forms in (28) and equating coefficients of e^{ikr} and e^{-ikr} leads to the usual results

$$f_l = \frac{2l+1}{2\mathrm{i}k}(\mathrm{e}^{2\mathrm{i}\delta_l}-1),$$

$$\sigma(\theta) = |f(\theta)|^2 = \frac{1}{k^2} \left| \sum_{l=0}^{\infty} (2l+1)\mathrm{e}^{\mathrm{i}\delta_l} \sin\delta_l P_l(\cos\theta) \right|^2,$$

$$\sigma = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1)\sin^2\delta_l.$$

The wavefunction S_l asymptotically orthogonal as $kr\to\infty$ to R_l for $l<l_0$, (as given by (25)) is clearly

$$S_l = \sqrt{\left(\frac{\pi}{8kr}\right)} \cdot \frac{\mathrm{i}}{\sinh\frac{1}{2}\mu\pi}[\mathbf{J}_{\mathrm{i}\mu} - \mathbf{J}_{-\mathrm{i}\mu}] \tag{29}$$

$$\sim \frac{1}{kr}\cos(kr+\tfrac{1}{4}\pi),$$

which is real and for which the flux (23) again vanishes. If a hard core at $r=a$ is introduced, the appropriate wavefunctions are of the form, for any l,

$$R_l = \frac{b_l}{\sqrt{kr}}[\mathbf{J}_\nu(kr) + \mathbf{J}_{\nu^*}(kr)] + \frac{\mathrm{i}c_l}{\sqrt{kr}}[\mathbf{J}_\nu(kr) - \mathbf{J}_{\nu^*}(kr)], \tag{30}$$

with b_l, c_l real and chosen so that $R_l(ka)=0$.

IV. References

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