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1993 J. Phys. A: Math. Gen. 26 L825

(http://iopscience.iop.org/0305-4470/26/17/013)

J. Phys. A: Math. Gen. 26 (1993) L825–L830. Printed in the UK

LETTER TO THE EDITOR

A solvable non-separable quantum two-body problem

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Received 5 May 1993

Abstract. We present a non-separable one-dimensional two body problem. It describes the reflection of a two-particle bound state off a discontinuity across which there is a steplike change in the interparticle potential. The model can be used as a primitive description of a pick-up or stripping reaction at an interface and also describes the diffusion of a particle in a plane containing an extended finite depth trap. The reflection coefficient for the discontinuity is obtained in closed form.

The only known quantum mechanical two-body problem, which is not separable in centre of mass coordinates, is the reflective half-plane barrier system [1]. It is presented in [1] in terms of the diffusion of a point mass in the x–y-plane with an infinitely repulsive barrier along the line $x=y$, $x\geqslant 0$, but can be reformulated as a two-particle system having the Hamiltonian

$$\mathcal{H}=\frac{P^2}{2M_0}+\frac{p^2}{2m}+\Theta(X)v(X-x) \tag{1}$$

where

$$\Theta(x)=\begin{cases}1 & x>0\\ 0 & x<0\end{cases} \tag{2}$$

and v is a repulsive potential. As shown in [1], the problem can be mapped onto Sommerfield's half-plane diffraction problem.

The model presented in this note is also of the form (1), but with the variable strength attractive potential

$$v(X-x)=-\lambda\delta(X-x) \tag{3}$$

with $\lambda>0$. It is similarly equivalent to the diffusion of a point in the plane but the half-line barrier is now a finite depth extended trap. In this form the problem will be discussed elsewhere; here we treat it as a two-particle scattering problem. In a primitive way this model describes the possible decomposition of an atom as it passes from a vacuum into a medium where the atomic potential is screened. The method of solution is to map the problem onto the two-dimensional diffraction problem considered by Bazer and Karp [2].

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0305-4470/93/170825+06 $07.50

Calculation. By transforming to centre of mass coordinate R and relative coordinate $r=X-x$ (total mass M and reduced mass μ), we arrive at the two-particle Schrödinger equation

$$\left(-\frac{\hbar^2}{2M}\partial_R^2-\frac{\hbar^2}{2\mu}\partial_r^2-\lambda\Theta(R)\delta(r)\right)\psi(R,r)=E\psi(R,r). \tag{4}$$

For $R>0$ we have the Schrödinger equation for the 'one-dimensional hydrogen atom'. By setting $\psi(R,r)=\rho(R)\phi(r)$ the equation separates giving

$$\rho''+\frac{M}{\hbar^2}(E+E_0)\rho=0 \tag{5}$$

$$-\frac{\hbar^2}{2\mu}\phi''-\lambda\delta(r)\phi=-E_0\phi. \tag{6}$$

The incoming and outgoing solutions to (5) are

$$\rho_{\pm}(R)=N\exp(\pm \mathrm{i}KR) \tag{7}$$

$$K^2=\frac{2M}{\hbar^2}(E+E_0). \tag{8}$$

There is only one bound state solution to (6), which is

$$\phi(r)=a\,\mathrm{e}^{-\kappa|r|} \tag{9}$$

$$\kappa^2=\frac{2\mu}{\hbar^2}E_0$$

$$E_0=\mu\lambda^2/2\hbar^2 \qquad \kappa=\mu\lambda/\hbar^2.$$

The incoming part of the solution to (4) with $E\geqslant 0$ is therefore

$$N\exp[-\mathrm{i}KR-\kappa|r|]$$

$$E=\frac{\hbar^2K^2}{2M}-\frac{\mu\lambda^2}{2\hbar^2}. \tag{10}$$

To obtain the remainder of the wavefunction, we note that (4) simplifies to the Helmholtz equation

$$\frac{\partial^2\psi}{\partial R^2}+\frac{M}{\mu}\frac{\partial^2\psi}{\partial r^2}+k_0^2\psi=0 \tag{11}$$

with the mixed boundary conditions

$$\frac{\partial\psi}{\partial r}(R,0^+)=\begin{cases}-\kappa\psi(R,0) & R>0\\ 0 & R<0\end{cases} \tag{12}$$

By introducing new coordinates

$$x=R \qquad y=(\mu/M)^{1/2}r \tag{13}$$

our problem has been reformulated as the wave propagation problem

$$\begin{aligned}&\psi_{xx}+\psi_{yy}+k_0^2\psi=0 \qquad -\infty<x<\infty, \qquad y>0\\ &\psi_y(x,0^+)=\begin{cases}-\alpha\psi(x,0^+) & x>0\\ 0 & x<0\end{cases}\\ &\psi_{\text{inc}}=\exp[-\mathrm{i}Kx-ay]\end{aligned} \tag{14}$$

where $k_0^2=2ME/\hbar^2$, $a=(M/\mu)^{1/2}\kappa$, $K=(k_0^2+a^2)^{1/2}$. In this form it is identical to the problem of diffraction of a ground wave at the linear shoreline of a planar land–sea interface treated by Bazer and Karp [2]. To apply their solution, we take k_0 and a as primary parameters subject to $\operatorname{Im} k_0>0$, $Im\, a>0$ (for technical reasons). Then $\operatorname{Im} K>0$ and we introduce the quantity

$$\delta=\min[\operatorname{Im} k_0, \operatorname{Im} K]>0. \tag{15}$$

With minor changes in notation, the solution from equation (2.9) in [1]

$$\psi(x,y)=\begin{cases}\exp[-\mathrm{i}Kx-ay]+\dfrac{\alpha\sigma^+(k)}{2\pi\mathrm{i}}\displaystyle\int_{-\infty}^{\infty}\frac{\exp[\mathrm{i}kx-y\sqrt{k^2-k_0^2}]}{(k+K)(k^2-k_0^2)}\sigma^-(k)\,\mathrm{d}k\\ \exp[-\mathrm{i}kx-ay]-\dfrac{\alpha\sigma^-(K)}{2\pi\mathrm{i}}\displaystyle\int_{-\infty}^{\infty}\frac{\exp[\mathrm{i}kx-y\sqrt{k^2-k_0^2}]}{(k+K)(a-\sqrt{k^2-k_0^2})}\sigma^+(k)\,\mathrm{d}k.\end{cases} \tag{16}$$

The branch of the square root is specified by $\sqrt{k^2-k_0^2}|_{k=0}=-\mathrm{i}k_0$, with hyperbolic branch cuts extending from $k_0(-k_0)$ and asymptotic to the positive (negative) $\operatorname{Im} k$ axis. (This specification differs slightly from [2] and is chosen such that $\operatorname{Re}\sqrt{k^2-k_0^2}\geqslant 0$). The functions $\sigma^\pm(k)$ enter into the Wiener–Hopf factorization

$$\sigma(k)=1-\frac{a}{\sqrt{k^2-k_0^2}}=\frac{\sigma^+(k)}{\sigma^-(k)} \tag{17}$$

where $\sigma(k)$ vanishes at $k=\pm K$ and is analytic and non-zero for $-\delta<\operatorname{Im} k<\delta$. The factors $\sigma^+(k)$ and $\sigma^-(k)$ are analitic, non-zero and bounded in the upper and lower half-planes $\operatorname{Im} k>-\delta$, $\operatorname{Im} k<\delta$, respectively. This factorization can be carried out explicitly [3], yielding

$$\sigma^+(k)=\exp\left[\frac{1}{2\pi\mathrm{i}}\int_{-\infty}^{\infty}\frac{\log[1-a(\eta^2-k_0^2)^{-1/2}]}{\eta-k}\mathrm{d}\eta\right.\qquad \operatorname{Im} k\geqslant 0 \tag{18a}$$

$$\sigma^-(k)=\exp\left[\frac{1}{2\pi\mathrm{i}}\int_{-\infty}^{\infty}\frac{\log[1-a(\eta^2-k_0^2)^{-1/2}]}{\eta-k}\mathrm{d}\eta\right.\qquad \operatorname{Im} k\leqslant 0 \tag{18b}$$

where the path of integration in (18*a*) is indented below, and that in (18*b*) is indented above $\eta = k$, when k is real.

An alternative representation for $\psi(x, y)$ is found by closing the contour of integration in (16) into the upper or lower half-plane, as appropriate. For $x<0$, the contour can be closed into the lower half-plane, enclosing the simple pole $k=-K$ and encircling the branch cut. Since $\sigma^-(-K) = 1/\sigma^+(K)$, the incident wave is cancelled by the residue term and we have

$$\psi(x, y) = \frac{a\sigma^+(K)}{2\pi i} \oint \frac{\exp[ikx - y\sqrt{k^2 - k_0^2}]}{(k+K)\sqrt{k^2 - k_0^2}} \sigma^-(k)\,dk \qquad x<0 \qquad y>0. \tag{19}$$

Similarly, for $x>0$

$$\psi(x, y) = \exp[-iKx - ay] + \frac{a^2[\sigma^+(K)]^2}{2K^2} \exp[iKx - ay]$$

$$-\frac{a\sigma^+(K)}{2\pi i} \oint \frac{\exp[ikx - y\sqrt{k^2 - k_0^2}]}{(k+K)[a - \sqrt{k^2 - k_0^2}]} \sigma^+(k)\,dk \qquad x>0, y>0 \tag{20}$$

where in (19) and (20) the path of integration encircles the appropriate branch cut.

Reflection coefficient. The reflection amplitude ξ can be read immediately from (20):

$$\xi = \frac{a^2[\sigma^+(K)]^2}{2K^2} = \frac{1}{2}\left(1 - \frac{k_0^2}{K^2}\right) [\sigma^+(K)]^2 \tag{21}$$

where

$$\sigma^+(K) = \exp\left[\frac{1}{2\pi i} \int_{-\infty}^{\infty} \log\left(1 - \sqrt{\frac{K^2 - k_0^2}{\eta^2 - k_0^2}}\right) \frac{d\eta}{\eta - K}\right] \tag{22}$$

with the path of integration along the real axis indented above $-K$, $-k_0$ and below k_0, K, which are taken to be real and positive with $0<k_0<K$.

The integral in (22) is easily transformed into $G(k_0/K)$ where

$$G(u) = \frac{1}{\pi i} \int_0^{\infty} \log\left[1 - \sqrt{\frac{1-u^2}{z^2-u^2}}\right] \frac{dz}{z^2-1} \tag{23}$$

with the path of integration indented below $z=1$, u. The path of integration is next moved to the imaginary axis by setting $z=-\mathrm{i}y$, where

$$G(u)=\frac{1}{\pi}\int_0^\infty \log\left(1-\mathrm{i}\sqrt{\frac{1-u^2}{y^2+u^2}}\right)\frac{\mathrm{d}y}{y^2+1}. \tag{24}$$

One easily finds the special value

$$G(0)=\frac{1}{\pi}\int_0^\infty \frac{\log(1-\mathrm{i}y)}{1+y^2}\,\mathrm{d}y=\tfrac{1}{2}\ln(2)-\frac{\pi\mathrm{i}}{8} \tag{25}$$

and the derivative

$$\begin{aligned}G'(u)&=-\frac{u}{\pi}\int_0^\infty \frac{\mathrm{d}y}{(y^2+1)(y^2+u^2)}+\frac{\mathrm{i}}{\pi}\frac{u}{\sqrt{1-u^2}}\int_0^\infty \frac{\mathrm{d}y}{(y^2+1)\sqrt{y^2+u^2}}\\ &=-\frac{1}{2(1+u)}+\frac{\mathrm{i}}{2\pi}\frac{u}{1-u^2}\log\left(\frac{1+\sqrt{1-u^2}}{1-\sqrt{1-u^2}}\right).\end{aligned} \tag{26}$$

By integrating (26) we obtain

$$G(u)=-\tfrac{1}{2}\log\left(\frac{1+}{2}\right)-\frac{\pi\mathrm{i}}{8}+\frac{\mathrm{i}}{2\pi}\int_0^u \frac{t}{1-t^2}\log\left(\frac{1+\sqrt{1-t^2}}{1-\sqrt{1-t^2}}\right)\mathrm{d}t \tag{27}$$

and by the substitution $s=\sqrt{1-t^2}$ the integral in (27) reduces to simply

$$\int_{\sqrt{1-u^2}}^1 \log\left(\frac{1+s}{1-s}\right)\frac{\mathrm{d}s}{s} \tag{28}$$

which may be expressed in terms of the Euler dilogarithm [4]. Therefore,

$$G(u)=-\frac{1}{2}\log\left(\frac{1-u}{2}\right)-\frac{\mathrm{i}}{2\pi}[Li_2(\sqrt{1-u^2})-Li_2(-\sqrt{1-U^2})]. \tag{29}$$

It follows now from (22) that ($u=k_0/K=[E/(E+E_0)]^{1/2}$)

$$\sigma^+(K)=\sqrt{\frac{2K}{K+k_0}}\exp\left\{-\frac{\mathrm{i}}{2\pi}\left[Li_2\left(\frac{\sqrt{K^2-k_0^2}}{K}\right)-Li_2\left(-\frac{\sqrt{K^2-k_0^2}}{K}\right)\right]\right\} \tag{30}$$

and the reflection coefficient is

$$R=|\xi|^2=\frac{(\sqrt{E+E_0}-\sqrt{E})^2}{E+E_0} \tag{31}$$

which depends only on the dimensionless energy E/E_0.

Discussion. The reflection coefficient for the model presented in (1–3) has been calculated exactly and shown to depend only on the dimensionless energy $\varepsilon=E/E_0$. As $\varepsilon\to 0$ there is total reflection, while R drops off monotonically as ε increases and decays asymoptotically as $(2\varepsilon)^{-2}$. The much simpler case of a single electron scattering from a delta potential at fixed distance from a potential step was treated by Lapidus [5], who found $R\sim(4\varepsilon)^{-1}$.

Examining equations (19) and (20) for the two-particle wavefunction on either side of the discontinuity shows that there is damped oscillatory, square integrable behaviour contained in the contour integrals. This interesting feature must arise from quantum interference between the bound state and free particle channels, and does not appear to have been investigated previously. An asymptotic and numerical study of these terms is under way [6].

Equations (1)–(3) appear to represent the simplest non-trivial two body problem in an external potential and it is surprising to find how difficult it is to solve and the complexity of the results. Nevertheless, there are a number of ways by which it could be modified, yet remain tractible. For example, the inclusion of a second potential step might serve as a model for an exciton in a quantum well.

The author thanks Professor J Boersma for pointing out how the original calculation could be reformulated in terms of [2].

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