Irregular solutions and completeness

1982 J. Phys. A: Math. Gen. 15 L161

(http://iopscience.iop.org/0305-4470/15/4/003)

J. Phys. A: Math. Gen. **15** (1982) L161–L164. Printed in Great Britain

LETTER TO THE EDITOR

Irregular solutions and completeness

V J Menon and A V Lagu

Department of Physics, Banaras Hindu University, Varanasi 221005, India

Received 10 December 1981

Abstract. It is pointed out that the bound and scattering states generated by a short-range two-body potential form a complete set even in the space of irregular solutions. Working with the relevant Wronskian relations an explicit eigenfunction expansion for the outgoing Jost solution is obtained. The formalism reduces to an interesting integral of spherical Bessel functions for the case of free particles.

By making use of the analytic properties of the Green function, it has been shown (Newton 1966) that the scattering states $|\psi^{\pm}\rangle$ together with the bound states $|\psi_b\rangle$ of fixed angular momentum l for two non-relativistic spinless particles of reduced mass $\mu\,(\hbar=c=1)$ form a complete set in the space of vectors $|F\rangle$ whose squared norm $\langle F|F\rangle$ is either finite or exists at least in the delta function sense for the class of two-body central potentials $V(r)$ for which the first and second absolute moments are finite. In most physical applications one encounters wavefunctions $F(r)=\langle r|F\rangle$ which are regular at $r=0$ and the expansion

$$|F\rangle=\int_0^\infty \frac{dk'}{2\pi^2}k'^2|\psi_{k'}^-\rangle\langle\psi_{k'}^-|F\rangle+\sum_b|\psi_b\rangle\langle\psi_b|F\rangle \qquad \langle F|F\rangle<\infty \tag{1}$$

is employed to deal with such regular functions.

The usual literature (see, for example, Newton 1966, Goldberger and Watson 1964, Sitenko 1971) has not investigated the question whether equation (1) also holds for vectors $|f\rangle$ whose wavefunction $f(r)=\langle r|f\rangle$ is not regular at $r=0$, or for which $\langle f|f\rangle=\infty$. In this letter we have chosen for investigation a particular example of such functions, namely the irregular Jost solution $|f_k^+\rangle$ of the radial Schrödinger equation, and find that because $\langle\psi_{k'}^-|f_k^+\rangle$ and $\langle\psi_b|f_k^+\rangle$ exist, the extension of equation (1) is possible. This we achieve, without using analyticity in any way, simply by utilising Wronskian relationships. These irregular solutions are of paramount importance in the formal development of the potential scattering theory and there is no need to re-emphasise their role. However, in most physical applications the irregular solutions are discarded owing to the blowing up of the probability density like $r^{-(2l+2)}$ near $r=0$. Therefore, it may be thought that the validity of the completeness relation (1) in the space of the Jost solutions is a purely mathematical property devoid of much physical significance; however, we may refer to the work of Kim and Vasavda (1972) who have pictured a two-body resonance state as being described by an irregular solution $f^-(r,k_j)=\langle r|f_{k_j}^-\rangle$ of the Schrödinger equation belonging to a *complex* energy eigenvalue $E_j=k_j^2/2\mu$, $\operatorname{Im}E_j<0$. It is clear that if such a state is produced in some multiparticle reaction, and one wishes to apply perturbation theory to it, one would like to expand the total wavefunction in a complete set of *regular* eigenfunctions; in this light the eigenfunction expansion derived below assumes special significance. As a mathematical by-product of the present investigation, we seem to have obtained a new integral relationship between the spherical Bessel and Hankel functions for general integer l.

To demonstrate this contention, we first recall the small and large r behaviour of the Jost, scattering and bound-state solutions respectively,

$$f^+(r,k) \underset{r\to 0}{\longrightarrow} \frac{AL^+(k)(2l-1)!!}{(kr)^{l+1}} \qquad k>0$$

$$\underset{r\to\infty}{\longrightarrow} \frac{A\exp[\mathrm{i}(kr-l\pi/2)]}{kr} \tag{2a}$$

$$\psi^+(r,k) \underset{r\to 0}{\longrightarrow} \frac{A}{L^+(k)}\frac{(kr)^l}{(2l+1)!!} \qquad k>0$$

$$\underset{r\to\infty}{\longrightarrow} \frac{A}{2\mathrm{i}kr}\{S^+(k)\exp[\mathrm{i}(kr-l\pi/2)]-\exp[-\mathrm{i}(kr-l\pi/2)]\} \tag{2b}$$

$$\psi_b(r) \underset{r\to 0}{\longrightarrow} \frac{N_bA}{L^+(-k_b)}\frac{(k_br)^l}{(2l+1)!!}$$

$$\underset{r\to\infty}{\longrightarrow} \frac{N_bA}{2i}\frac{\exp[\mathrm{i}(k_br-l\pi/2)]}{k_br} \tag{2c}$$

where $L^+(k)$ is the Jost function for the problem, $S^+(k)=L^+(-k)/L^+(k)$ is the partial-wave S matrix, k_b is a pure positive imaginary momentum corresponding to the bth bound state at which $L^+(k_b)=0$, and $N_b=(-)^lN_b^*$ is a normalisation constant. The constants $A=(4\pi)^{1/2}$ and N_b are, of course, chosen to be consistent with the normalisation conditions

$$\langle\psi_{k'}^+|\psi_k^+\rangle = 2\pi^2\,\delta(k'-k)/k'k \qquad \text{and} \qquad \langle\psi_{b'}|\psi_b\rangle=\delta_{b'b}. \tag{3}$$

Employing the usual procedure for obtaining Wronskians from the differential equations, we find

$$\lim_{\substack{r_0\to 0\\ R\to\infty}}\int_{r_0}^{R}\mathrm{d}r\,r^2\psi^+(r,k')f^+(r,k)=\lim_{\substack{r_0\to 0\\ R\to\infty}}\mathrm{P}\frac{1}{k'^2-k^2}[W(r;k',k)]_{r_0}^{R} \tag{4}$$

where we have introduced a Wronskian

$$W(r;k',k)=r\psi^+(r,k')\frac{\mathrm{d}}{\mathrm{d}r}(rf^+(r,k))-rf^+(r,k)\frac{\mathrm{d}}{\mathrm{d}r}(r\psi^+(r,k')) \tag{5}$$

and the Cauchy principal value part P because we have taken both k' and k real positive. In the same way inserting the bound-state wavefunction $\psi_b(r)$ in place of $\psi^+(r,k')$ we can deduce

$$\lim_{\substack{r_0\to 0\\ R\to\infty}}\int_{r_0}^{R}\mathrm{d}r\,r^2\psi_b(r)f^+(r,k)=\lim_{\substack{r_0\to 0\\ R\to\infty}}\frac{1}{k_b^2-k^2}[W_b(r;k)]_{r_0}^{R} \tag{6}$$

with the Wronskian defined by

$$W_b(r; k) = r\psi_b(r)\frac{\mathrm{d}}{\mathrm{d}r}(rf^+(r, k)) - rf^+(r, k)\frac{\mathrm{d}}{\mathrm{d}r}(r\psi_b(r)) \tag{7}$$

and the principal value symbol P is omitted in equation (6) remembering that $k_b^2 < 0$ and $k^2 > 0$.

The left-hand side of equation (4) is obviously equal to the overlap $\langle\psi_{k'}^-|f_k^+\rangle$ which should exist (at least in a delta-function sense) because the integrand behaves like $r^2 \cdot r^l \cdot r^{-(l+1)} \sim r$ as $r \to 0$ and as undamped oscillations as $r \to \infty$. The right-hand side of equation (4) can be evaluated using the boundary conditions (2a) and (2b), yielding

$$\langle\psi_{k'}^-|f_k^+\rangle = \lim_{R\to\infty} \mathrm{P}\frac{1}{k'^2 - k^2}\bigg(\frac{A^2}{2k'k}\{(k-k')S^+(k')\exp[\mathrm{i}(k'R - l\pi/2)]$$

$$-(k+k')\exp[-\mathrm{i}(k'R - l\pi/2)]\}\exp[\mathrm{i}(kR - l\pi/2)] + \frac{A^2k'^l}{k^{l+1}}\frac{L^+(k)}{L^+(k')}\bigg) \tag{8a}$$

where the last term arises from the $r_0 \to 0$ limit. To simplify the right-hand side of equation (8a), we find that the piece

$$\lim_{R\to\infty} \mathrm{P}\frac{1}{k'^2 - k^2}\frac{A^2}{2k'k}\{-(k+k')\exp[-\mathrm{i}(k'R - l\pi/2)]\}\exp[\mathrm{i}(kR - l\pi/2)]$$

$$= \lim_{R\to\infty}\frac{2\pi}{kk'}P\frac{\exp[\mathrm{i}(k-k')R]}{k-k'}$$

$$= \frac{2\pi}{kk'}\{\mathrm{i}\pi\,\delta(k-k')\}$$

$$= \frac{4\mathrm{i}\pi^2}{k}\delta(k^2 - k'^2).$$

In the same way we can show that the remaining piece containing $\exp[\mathrm{i}(k+k')R]$ gives rise to $\delta(k+k')$ which *vanishes* in the region of positive k and k'. Hence equation (8a) simplifies to

$$\langle\psi_{k'}^-|f_k^+\rangle = -\frac{4\pi k'^l}{k^{l+1}}\frac{L^+(k)}{L^+(k')}\frac{1}{k^2 - k'^2 + \mathrm{i}\varepsilon} \qquad k, k' > 0. \tag{8b}$$

Next, the left-hand side of equation (6) is clearly equal to the overlap $\langle\psi_b|f_k^+\rangle$ which should exist because the integrand goes like r near $r = 0$ and as damped oscillations as $r \to \infty$. The right-hand side of equation (6) can be evaluated using the boundary conditions (2a) and (2c) and we obtain

$$\langle\psi_b|f_k^+\rangle = \lim_{R\to\infty}\frac{1}{k_b^2 - k^2}\bigg(\frac{A^2N_b}{2k_bk}(k-k_b)\exp[\mathrm{i}(k_bR - l\pi/2)]$$

$$\times\exp[\mathrm{i}(kR - l\pi/2)] + \frac{N_bA^2k_b^l}{k^{l+1}}\frac{L^+(k)}{L^+(-k_b)}\bigg)$$

$$= -\frac{4\pi k_b^l}{k^{l+1}}\frac{L^+(k)}{L^+(-k_b)}\frac{N_b}{k^2 - k_b^2} \tag{9}$$

because the $\exp(ik_bR)$ term vanishes as $R\to\infty$ and the last term arises from the $r_0\to 0$ limit.

We have thus obtained the explicit values for the coefficients which, upon substitution in equation (1), yield the desired expansion for $f^+(r,k)$ as

$$f^+(r,k)=-\frac{4\pi}{k^{l+1}}L^+(k)\left(\int_0^\infty \frac{dk'\,k'^{l+2}}{2\pi^2}\,\frac{\psi^-(r,k')}{L^+(k')(k^2-k'^2+i\varepsilon)}+\sum_b\frac{N_bk_b^l\psi_b(r)}{L^+(-k_b)(k^2-k_b^2)}\right). \tag{10}$$

The correctness of equation (10) can also be checked by starting from the right-hand side, evaluating the k' integral explicitly by making use of the analytic properties of the integrand in the k' plane (for fixed r), and finally showing that the result reduces to $f^+(r,k)$.

Finally, to obtain the integral relationship between the spherical Hankel and Bessel functions for any l, we go over to the case of free particles ($V(r)=0$), for which we must do the following replacements: $L^+(k)\to 1$, $\psi_b(r)\to 0$, $f^+(r,k)\to Ah_l^+(kr)$ and $\psi^-(r,k)\to Aj_l(kr)$ where h_l and j_l are spherical Hankel and Bessel functions, respectively. Thus, equation (10) reduces to

$$h_l^+(kr)=-\frac{2}{\pi k^{l+1}}\int_0^\infty \frac{dk'\,k'^{l+2}j_l(k'r)}{k^2-k'^2+i\varepsilon}. \tag{11a}$$

This appears to be a new integral involving spherical Bessel functions, not tabulated in the usual tables (Gradshteyn and Ryzhik 1973, Abramowitz and Stegun 1968) at least for general integral l. In the special case of $l=0$, however, the real part of equation (11a) reads

$$\cos kr=-\frac{2}{\pi}\,\mathrm{P}\int_0^\infty dk'\,\frac{k'\sin k'r}{k^2-k'^2} \tag{11b}$$

which is a standard result (Gradshteyn and Ryzhik 1973).

This work has been supported in part by the DAE, Government of India.

References

Abramowitz M and Stegun I A 1968 *Handbook of Mathematical Functions* (New York: Dover) p 488
Goldberger M L and Watson K M 1964 *Collision Theory* (New York: John Wiley) p 278
Gradshteyn I S and Ryzhik I M 1973 *Table of Integrals, Series and Products* (New York: Academic) pp 407, 685, 690
Kim Y S and Vasavda K V 1972 *Phys. Rev.* D **5** 1002–11
Newton R G 1966 *Scattering Theory of Waves and Particles* (New York: McGraw-Hill) pp 368–73
Sitenko A G 1971 *Lectures in Scattering Theory* (Oxford: Pergamon) p 93