Kapur-Peierls, Wigner-Eisenbud And All That

by

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1 Introduction

These methods are used in the expression of the solution of

$$(E - H)\phi = 0 \tag{1}$$

in a finite volume in terms of a set of states satisfying the same equation within the volume and satisfying a set of boundary conditions at the edge of the volume. We study s-wave scattering in a potential $V(r)$ as an example. The scattering wavefunction $\phi(r)$ ($\equiv r\Psi(r)$) satisfies

$$(E - H)\phi = 0, \qquad \text{for all } r \tag{2}$$

$$\phi = e^{-ikr} - Se^{ikr}, \qquad r > r_0. \tag{3}$$

S is the scattering matrix required.

The radius r_0 is such that

$$H \rightarrow \frac{-\hbar^2}{2\mu}\frac{d^2}{dr^2} \text{ for } r > r_0. \tag{4}$$

Also,

$$E = \frac{\hbar^2 k^2}{2\mu}. \tag{5}$$

A suitable complete set is defined by

$$(\tilde{\epsilon}_i - H)\tilde{\phi}_i = 0, r < r_0, \tag{6}$$

$$\left(\frac{1}{\tilde{\phi}_i}\frac{d\tilde{\phi}_i}{dr}\right)_{r=r_0} = b, \tilde{\phi}_i(0) = 0 \tag{7}$$

where b may be complex. Assuming

$$H = \frac{-\hbar^2}{2\mu}\frac{d^2}{dr^2} + V(r), \tag{8}$$

with $V(r)$ real for simplicity, we easily show that (note no complex conjugate)

$$\int_0^{r_0} dr \tilde{\phi}_i(r)\tilde{\phi}_j(r) = 0, i \neq j \tag{9}$$

$$= 1, i = j \text{ (normalisation)} . \tag{10}$$

The idea is to use the expansion

$$\phi(r) = \sum_i a_i \tilde{\phi}_i(r), r \leq r_0. \tag{11}$$

If the $\tilde{\phi}_i$'s are complete we can assume that at $r = r_0$

$$\phi(r_0) = \sum_i a_i \tilde{\phi}_i(r_0) \tag{12}$$

and by matching using equation (3) we can obtain

$$e^{-ikr_0} - Se^{ikr_0} = \sum_i a_i \tilde{\phi}_i(r_0). \tag{13}$$

But note that we can <u>not</u> match derivatives at $r = r_0$ because equation (11) gives

$$\begin{aligned} \left(\frac{d\phi}{dr}\right)_{r=r_0} &= \sum_i a_i \left(\frac{d\tilde{\phi}_i(r)}{dr}\right)_{r=r_0} = \sum_i a_i b \tilde{\phi}_i(r_0) \\ &= b\phi(r_0) \end{aligned} \tag{14}$$

which is certainly not generally true.

The trick is to note that the coefficients a_i are determined entirely by ϕ and its derivative at $r = r_0$:

From equations (9) and (11)

$$\begin{aligned} a_i &= \int_0^{r_0} dr \tilde{\phi}_i \phi \\ &= \int_0^{r_0} dr \frac{(H\tilde{\phi}_i)\phi - \tilde{\phi}_i(H\phi)}{\tilde{\epsilon}_i - E} \\ &= \frac{-\hbar^2}{2\mu} \int_0^{r_0} dr \frac{\left[\frac{d}{dr}\left(\tilde{\phi}_i'\phi - \tilde{\phi} - i\phi'\right)\right]}{\tilde{\epsilon}_i - E} \\ &= \frac{-\hbar^2}{2\mu} \frac{1}{\tilde{\epsilon}_i - E} \left[\frac{\tilde{\phi}_i'}{\tilde{\phi}_i}\phi - \phi'\right]_{r=r_0} \tilde{\phi}_i(r_o) \\ &= \frac{-\hbar^2}{2\mu} \frac{1}{\tilde{\epsilon}_i - E} \tilde{\phi}_i(r_0) \left[b\phi - \phi'\right]_{r=r_0} \end{aligned} \tag{15}$$

so that

$$\boxed{a_i = \frac{-\hbar^2}{2\mu} \frac{1}{\tilde{\epsilon}_i - E} \tilde{\phi}_i(r_0) \left[b\phi - \phi'\right]_{r=r_0}} \tag{16}$$

Using equation (3) this can be written

$$a_i = \frac{-\hbar^2}{2\mu} \frac{1}{\tilde{\epsilon}_i - E} \tilde{\phi}(r_0) \left[e^{-ikr_0}(b + ik) - Se^{ikr_0}(b - ik)\right]. \tag{17}$$

Substituting into equation (13) gives

$$e^{-ikr_0} - Se^{ikr_0} = \sum_i \frac{-\hbar^2}{2\mu} \frac{1}{\tilde{\epsilon}_i - E} \left(\tilde{\phi}_i(r_0)\right)^2 \left[e^{-ikr_0}(b + ik) - Se^{ikr_0}(b - ik)\right] \tag{18}$$

and solving for S

$$S = e^{-2ikr_0} \frac{[1 + R(E)(b + ik)]}{[1 + R(E)(b - ik)]} \tag{19}$$

where

$$R(E)=\frac{\hbar^2}{2\mu}\sum_i\frac{\left(\tilde{\phi}_i(r_0)\right)^2}{\tilde{\epsilon}_i-E}. \tag{20}$$

2 The Choice of b

2.1 Choose b to be Real: "R-matrix Theory"

For this choice, the $\tilde{\phi}$'s can be chosen to be real the $\tilde{\epsilon}_i$'s will be real automatically if H is Hermitian. This has two advantages that $R(E)$ is real and S of equation (19) is obviously unitary, i.e. $|S|^2=1$.

2.2 Choose $b=ik$: "Kapur-Peierls Theory"

The obvious advantage of this choice is that it simplifies the denominator of equation (19) so that

$$S=e^{-2ikr_0}\left[1+2ikR_{KP}(E)\right]. \tag{21}$$

Now unitarity is not at all obvious, but equation (21) is deceptively simple. Note that the E dependence is now not just in the energy denominator of $R_{KP}(E)$, but also through the $\tilde{\phi}$'s themselves because the boundary conditions (equation (7)) now depends on E.

The proof of unitarity in this case follows from the following identity, which is easily proved from equations (6) and (7)

$$\begin{aligned}\left(\tilde{\epsilon}_i-\tilde{\epsilon}_j^*\right)\int_0^{r_0}dr\tilde{\phi}_j^*(r)\tilde{\phi}_i(r) &= \frac{-\hbar^2}{2\mu}\int_0^{r_0}dr\frac{d}{dr}\left(\tilde{\phi}_j^*\frac{d\tilde{\phi}_i}{dr}-\left(\frac{d\tilde{\phi}_j^*}{dr}\right)\tilde{\phi}_i\right)\\ &= \frac{-\hbar^2}{2\mu}2ik\tilde{\phi}_j^*(r_0)\tilde{\phi}_i(r_0)\end{aligned} \tag{22}$$

ie:

$$\boxed{\int_0^{r_0}dr\tilde{\phi}_j^*\tilde{\phi}_i=\frac{\hbar^2}{2\mu}2ik\frac{\tilde{\phi}_j^*(r_0)\tilde{\phi}_i(r_0)}{\tilde{\epsilon}_j^*-\tilde{\epsilon}_i}} \tag{23}$$

and hence

$$|R_{KP}|^2=\left(\frac{\hbar^2}{2\mu}\right)^2\sum_{i,j}\frac{\tilde{\phi}_i(r_0)\tilde{\phi}_i(r_0)\tilde{\phi}_j^*(r_0)\tilde{\phi}_j^*(r_0)}{(\tilde{\epsilon}_i-E)(\tilde{\epsilon}_i^*-E)} \tag{24}$$

$$=\left(\frac{\hbar^2}{2\mu}\right)^2\sum_{i,j}\tilde{\phi}_i\tilde{\phi}_i\tilde{\phi}_j^*\tilde{\phi}_j^*\left[\frac{1}{(\epsilon_j^*-\epsilon_i)}\frac{1}{(\epsilon_i-E)}-\frac{1}{(\epsilon_j^*-\epsilon_i)}\frac{1}{(\epsilon_j^*-E)}\right] \tag{25}$$

$$=\left(\frac{\hbar^2}{2\mu}\right)^2\sum_{i,j}\left[\tilde{\phi}_i(r_0)\tilde{\phi}_j^*(r_0)\left(\frac{2\mu}{\hbar^2}\frac{1}{2ik}\int_0^{r_0}dr\tilde{\phi}_j^*(r)\phi_i(r)\right)\right.$$

$$\times\left(\frac{1}{\epsilon_i - E} - \frac{1}{\epsilon_j^* - E}\right)\Bigg] \tag{26}$$

$$= \frac{\hbar^2}{2\mu}\frac{1}{2ik}\left(\sum_i \tilde{\phi}_i(r_0)\int_0^{r_0} dr\delta(r-r_0)\tilde{\phi}_i(r)\frac{1}{\epsilon_i - E}\right.$$

$$\left.-\sum_j \tilde{\phi}_j^*(r_0)\int_0^{r_0} dr\delta(r-r_0)\tilde{\phi}_j^*(r_0)\frac{1}{\epsilon_j^* - E}\right) \tag{27}$$

$$= \frac{1}{2ik}\left(\frac{\hbar^2}{2\mu}\sum_i \frac{\tilde{\phi}_i(r_0)\tilde{\phi}_i(r_0)}{\epsilon_i - E} - \frac{\hbar^2}{2\mu}\sum_j \frac{\tilde{\phi}_j^*(r_0)\tilde{\phi}_j^*(r_0)}{\epsilon_k^* - E}\right) \tag{28}$$

$$= \frac{1}{2ik}\left(R_{KP} - R_{KP}^*\right) \tag{29}$$

Equation (27) follows from the "completeness relationship",

$$\sum_i \tilde{\phi}_i(r)\tilde{\phi}_i(r_0) = \delta(r-r_0). \tag{30}$$

We have thus proven that

$$\left(R_{KP}(E) - R_{KP}^*\right) = 2ik|R_{KP}|^2, \tag{31}$$

and hence

$$|S(E)|^2 = \left(1 + 2ikR_{KP}\right)\left(1 - 2ikR_{KP}^*\right), \tag{32}$$

$$= 1 + 2ik\left(R_{KP} - R_{KP}^*\right) + 4k^2|R_{KP}|^2, \tag{33}$$

$$= 1. \tag{34}$$

3 Connection with Green's functions

Suppose the Green function, $G(r, r')$, satisfies

$$(E - H)G(r', r) = \delta(r - r'). \tag{35}$$

Using this function we can write

$$\phi(r) = \int_0^{r_0} dr'\delta(r-r')\phi(r'), r \le r_0 \tag{36}$$

$$= \int_0^{r_0} dr'\left((E-H)G(r',r)\right)\phi(r') \tag{37}$$

$$= \int_0^{r_0} dr'\left((H\phi(r'))G(r',r) - (HG(r',r))\phi(r')\right)$$

$$+ \int_0^{r_0} dr' G(r',r)\left((E-H)\phi(r')\right) \tag{38}$$

$$= \frac{-\hbar^2}{2\mu}\left[\frac{d\phi(r')}{dr'}G(r',r) - \frac{dG(r',r)}{dr'}\phi(r')\right]_{r'=r_0}$$

$$+ \int_0^{r_0} dr' G(r',r)(E-H)\phi(r') \tag{39}$$

Where we have assumed

$$\underline{G(0,r) = 0 = \phi(0)} \tag{40}$$

If in addition ϕ satisfies

$$(E - H)\phi = 0 \tag{41}$$

then we have

$$\boxed{\phi(r) = \frac{-\hbar^2}{2\mu}\left[\phi'(r_0)G(r_0,r) - \frac{dG(r_0,r)}{dr_0}\phi(r_0)\right]_{r<r_0}} \tag{42}$$

Substituting $r = r_0$ into equation (42) gives

$$\underline{1 = \frac{-\hbar^2}{2\mu}\left[\frac{\phi'(r_0)}{\phi(r_0)}G(r_0,r_0) - \left(\frac{dG(r,r_0)}{dr}\right)_{r=r_0}\right].} \tag{43}$$

In terms of the $\tilde{\phi}$ we can write

$$G(r',r) = \sum_i \frac{\tilde{\phi}_i(r')\tilde{\phi}_i(r)}{(E-\epsilon_i)} \text{ where } r, r' < r_0 \tag{44}$$

Using the "completeness relation" it is easy to show that this G satisfies equation (35). So we have

$$G(r_0,r_0) = \sum_i \frac{\left(\tilde{\phi}_i(r_0)\right)^2}{E - \tilde{\epsilon}_i} = \frac{-2\mu}{\hbar^2}R \tag{45}$$

$$\left(\frac{dG(r,r_0)}{dr}\right)_{r=r_0} = bG = \frac{-2\mu}{\hbar^2}bR \tag{46}$$

and so (43) gives

$$1 = \frac{-\hbar^2}{2\mu}\left[\frac{\phi'(r_0)}{\phi(r_0)} - b\right]\left(\frac{-2\mu}{\hbar^2}R\right) \tag{47}$$

ie:

$$\underline{\frac{\phi'(r_0)}{\phi(r_0)} - b = \frac{1}{R}} \tag{48}$$

If

$$\phi(r_0) = e^{-ikr_0} - Se^{ikr_0} \tag{49}$$

$$\phi' = ik\left(-e^{ikr_0} - Se^{ikr_0}\right) \tag{50}$$

$$\frac{\phi'}{\phi} = ik\left(\frac{-e^{ikr_0} - Se^{ikr_0}}{e^{-ikr_0} - Se^{ikr_0}}\right) \tag{51}$$

$$S = e^{-2ikr_0} \left(\frac{\phi'/\phi + ik}{\phi'/\phi - ik} \right) \tag{52}$$

so that equation (48) gives

$$S = e^{-2ikr_0} \left(\frac{b + \frac{1}{R} + ik}{b + \frac{1}{R} - ik} \right) \tag{53}$$

$$= e^{-2ikr_0} \left(\frac{1 + R(b + ik)}{1 + R(b - ik)} \right) \tag{54}$$

which is in agreement with equation 19.