Physics 601, B-matrix

Wave functions for the square well potential:

Potential:

$$V(r) = -V_0, \ r \le r_0$$
$$V(r) = 0. \ r > r_0 \tag{1}$$

More generally $V(r) =$ `any function` for $r \le r_0$.

The S-eq for $\phi(r)$ is

$$\left(-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{2\mu r^2} + V(r)\right)\phi = E\phi \tag{2}$$

For $r \le r_0$ set $\phi = \phi_{in}(r)$ and assume the equation is solved. For $r > r_0$ set $k^2 = 2\mu E/\hbar^2$ and define

$$u_\ell(kr) = j_\ell(kr)kr \tag{3}$$
$$v_\ell(kr) = n_\ell(kr)kr \tag{4}$$

Define the logarithmic derivative matrix $B(E)$ as

$$B(E) = \left.\frac{d\log\phi_{in}(r)}{dr}\right|_{r=r_0} \tag{5}$$

[Note: Here I use log to denote $\log_e$ that is log to the base e. This is the notation, common in mathematics, used in most computer programs. It is identical to ln function commonly used in engineering.] and define

$$u'_\ell(kr) = \frac{du_\ell(kr)}{d(kr)} \tag{6}$$
$$v'_\ell(kr) = \frac{dv_\ell(kr)}{d(kr)} \tag{7}$$

Notice that u' and v' are defined as derivatives with respect to the argument kr not r. This is done because the functions u' and v' are then functions only of kr. This differs from the derivative used to define $B(E)$ since $\phi_{\rm in}(r)$ depends upon both r and E, not the combination $\sqrt[2\mu E]{r}$ as for $u(kr)$ and $v(kr)$.

The solution for $r > r_0$ is

$$\phi(r) = A(u_\ell(kr) + K_\ell v_\ell(kr)) \tag{8}$$

where A is a normalization constant and K_ℓ is a constant to be determined by matching functions and derivatives at $r = r_0$. Alternatively, we can match logarithmic derivatives. Matching logarithmic derivatives and recalling the definition of $B(E)$ gives:

$$B(E) = k\frac{u'_\ell + K_\ell v'_\ell}{u_\ell + K_\ell v_\ell} \tag{9}$$

and all functions are evaluated at $r = r_0$. From the asymptotic forms of u_ℓ and v_ℓ namely

$$\lim_{r\to\infty} u_\ell(kr) \to \quad \sin(kr - \ell\pi/2) \tag{10}$$

$$\lim_{r\to\infty} v_\ell(kr) \to \quad \cos(kr - \ell\pi/2) \tag{11}$$

we see that

$$\lim_{r\to\infty} \phi \to A\sin(kr - \ell\pi/2 + \delta_\ell) \tag{12}$$

if we set

$$K_\ell = \tan\delta_\ell. \tag{13}$$

The quantity δ_ℓ is the phase shift for the ℓ' th partial wave. This quantity has physical significance therefore we solve for K_ℓ.

Using the Wronskian relation

$$u'_\ell v_\ell - u'_\ell v_\ell = 1 \tag{14}$$

we have

$$K_\ell = -\frac{u_\ell}{v_\ell} + \frac{k/v_\ell^2}{B(E) - kv'_\ell/v_\ell} \tag{15}$$

For simplicity we will drop the subscripts ℓ and suppose that the value of ℓ is known from context.

Instead of solving for K we could solve for $1/K = \cot\delta$. Then

$$K_\ell^{-1} = K^{(\mathrm{inv})} = \cot\delta = -\frac{v}{u} - \frac{k/u^2}{B(E) - ku'/u} \tag{16}$$

This quantity does not have a special name, however the closely related quantity namely

$$M = k^{2\ell+1}\cot\delta_\ell \tag{17}$$

does. It is called the M-matrix. Its importance derives from the property that it is an analytic function of k^2 and can be expanded in a power series about $k^2 = 0$ according to

$$M = -\frac{1}{a_\ell^{2\ell+1}} + \frac{1}{2}\frac{1}{\tilde{r}_\ell^{2\ell-1}}k^2 + \dots. \tag{18}$$

where the first two terms define the quantities a_ℓ called the *scattering lengths* and r_ℓ the *effective ranges*. Often the terms "scattering length" and "effective range" refer to the $\ell = 0$ quantities only. [Note: do not confuse the cutoff distance r_0 with the effective range $\tilde{r}_0$. Determine the meaning from context.].

The phase shift is the main physical quantity extracted for $E > 0$. For $E < 0$ we define $k = i\kappa$, $\kappa > 0$ and seek wave functions that are physically acceptable even though the wave vector $k = i\kappa$ is complex.

For $E < 0$ we know that there are no physically acceptable solutions, *i. e* ones that decrease as $e^{-\kappa r}$ except at special value of E called the eigenenergies or eigenvalues of the hamiltonian H. To find these values we rewrite Eq. (12) as

$$\lim_{r\to\infty} \phi \to \frac{Ae^{-i\delta}}{2i}\left(S^{-1}e^{-(ikr-\ell\pi/2)} - e^{i(kr-\ell\pi/2)}\right) \tag{19}$$

where

$$S = e^{2i\delta}$$

is the *scattering matrtix* or S-matrix. Now if we write Eq. (19) for $E < 0$ using $k \to i\kappa$ we see that ϕ diverges exponentially as $r \to \infty$ unless $S^{-1} = 0$ We can write the equation $S^{-1} = 0$ in terms of K as

$$S^{-1} = \frac{e^{-i\delta}}{e^{i\delta}} = \frac{\cos\delta - i\sin\delta}{\cos\delta + \sin\delta} = \frac{\cot\delta - i}{\cot\delta + i} = \frac{i + \tan\delta}{1 - i\tan\delta} = \frac{i + K}{i - K} = 0. \tag{20}$$

This gives the equation

$$K(E) + i = 0 \tag{21}$$

as the equation determining the eigenvalues.

A plot of $\Im[K(E) + i]$ or $\Im[K^{(inv)}(E) - i]$ locates the bound states at energies where the curve crosses 0.

Problem: 1a. Compute the s-wave ($\ell = 0$) scattering length for a square well potential with $V_0 = 2$ au, $\mu = m_e = 1$ au and cutoff distance $r_0 = 2.33$ au. Recall that atomic units (au) take $e = \hbar = m_e = 1$. How many $\ell = 0$ bound states does this potential have? Give the eigenenergies of the bound states.