Problems Chapter 13

Quantum Mechanics
K. Konishi, G. Paffuti

Problem 1

Write the Green function for a free particle in one dimension by solving the equation (E-H)G=1 in the x representation. Verify the result by writing G as a sum over eigenstates of H.

Solution

x representation

With $E = (\hbar k)^2 / 2m$ the equation for the Green function in one dimension is

$$\left(\frac{\hbar^2 k^2}{2m} + \frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right) G[x-y] = \delta[x-y]. \tag{1.1}$$

The solution with a divergent (i.e. expanding) wave as boundary condition is

$$G[k; x, y] = G[k; x-y] = \frac{1}{2\,i\,k}\frac{2m}{\hbar^2}\,\mathrm{Exp}[i\,k\,|x-y|]; \tag{1.2}$$

with

$$k = i\frac{1}{\hbar}\sqrt{-2mE}\,;\quad k>0 \text{ for } E>0.$$

To check the result first we remember that

$$\epsilon[x] \equiv \mathrm{Sign}[x] = \begin{cases} +1; & x>0 \\ -1; & x<0 \end{cases}\;;\quad \epsilon'[x] = 2\,\delta[x].$$

The first derivatives of G are (we omit the k argument as it is kept fixed below)

$$G'[x] = \frac{1}{2\,i\,k}\frac{2m}{\hbar^2}\,i\,k\,\epsilon[x]\,e^{i\,k\,|x|};$$

$$G''[x] = \frac{1}{2\,i\,k}\frac{2m}{\hbar^2}\left(-k^2\,\epsilon[x]^2 + 2\,i\,k\,\delta[x]\right)e^{i\,k\,|x|} = -k^2\,G[x];\ \text{c.v.d.}$$

k representation

The computation can be performed also in Fourier transform. From eq.(1) using the known prescription $i\epsilon$ on poles (with $\epsilon \to 0$)

$$G[x] = \frac{2m}{\hbar^2}\int\frac{dk'}{2\pi}\frac{e^{i\,k'\,x}}{k^2 + i\epsilon - k'^2} = -\frac{2m}{\hbar^2}\int\frac{dk'}{2\pi}\frac{e^{i\,k'\,x}}{(k'-k_+)\,(k'-k_-)}. \tag{1.3}$$

Where $k_\pm$ are the poles with positive and negative imaginary part, respectively. The integral can be evaluated by closing the contour in the complex plane with a half-circle at infinity and applying the Cauchy theorem. With $x>0$ the path must be closed in the half plane $\mathrm{Im}[k]>0$ while for $x<0$ in the region $\mathrm{Im}[k]<0$. The integral gives immediately (Res is the residue of the integrand)

$$G[x] = 2\pi\,i\,\theta[x]\,\mathrm{Res}[k_+]\,e^{i\,k_+\,x} - 2\pi\,i\,\theta[-x]\,\mathrm{Res}[k_-]\,e^{i\,k_-\,x}. \tag{1.4}$$

Using the values of the poles (remember that $\epsilon \to 0$ in all expressions)

$$k_\pm == \pm\sqrt{k^2 + i\epsilon} = \pm(k + i\epsilon)$$

we have

$$\text{Res}[k_+] = -\frac{2m}{\hbar^2}\frac{1}{2\pi}\frac{1}{k_+ - k_-} = -\frac{2m}{\hbar^2}\frac{1}{2\pi}\frac{1}{2k}; \quad \text{Res}[k_-] = -\frac{2m}{\hbar^2}\frac{1}{2\pi}\frac{1}{k_- - k_+} = +\frac{2m}{\hbar^2}\frac{1}{2\pi}\frac{1}{2k};$$

and by substitution in (4) we recover the previous result

$$G[x] = i\theta[x]\left(-\frac{2m}{\hbar^2}\frac{1}{2k}\right)e^{ikx} - i\,\theta[-x]\frac{2m}{\hbar^2}\frac{1}{2k}e^{-ikx} = \frac{2m}{\hbar^2}\frac{1}{2ik}e^{ik|x|}.$$

- **Analyticity**

Let us note that the analyticity properties (a cut for $E > 0$) and by definition of the adjoint we must have both

$$\langle y \mid G^\dagger[E] \mid x \rangle = \langle y \mid G[e^{2\pi i}E] \mid x \rangle; \quad \langle y \mid G^\dagger[E] \mid x \rangle = \langle x \mid G[E] \mid y \rangle^*. \qquad (1.5)$$

As for $E \to e^{2\pi i}E$ one has $k \to -k$ the above relations imply

$$G[k; x, y]^* = G[-k; y, x]$$

which is indeed verified with our solution (2).

Problem 2

Write the Green function for a free particle in any dimension solving the equation (E-H)G=1 in the x representation.

Solution

We are looking for a (radial symmetric) solution of

$$(\Delta + k^2)\,G = \frac{2m}{\hbar^2}\delta^{(d)}[x]. \qquad (2.1)$$

In dimension d the Laplacian operator has the form

$$\Delta = \frac{1}{r^{d-1}}\frac{\partial}{\partial r}r^{d-1}\frac{\partial}{\partial r} + \text{angular terms};$$

eq.(1) has the form

$$\frac{1}{r^{d-1}}\frac{\partial}{\partial r}r^{d-1}\frac{\partial}{\partial r}G[r] + k^2 G[r] = \frac{2m}{\hbar^2}\delta^{(d)}[x]. \qquad (2.2)$$

In $x \neq 0$ by the change of variables

$$z = k\,r; \quad G = A\,z^{1-\frac{d}{2}}f[z]$$

eq.(2) becomes

$$f''[z] + \frac{1}{z}f'[z] + \left(1 - \frac{\left(\frac{d}{2}-1\right)^2}{z^2}\right)f[z] = 0. \qquad (2.3)$$

This is a Bessel equation of order d/2-1. The request of outgoing waves selects as a solution the Hankel function $H^{(1)}_{\frac{d}{2}-1}$:

$$H^{(1)}_\nu[x] = J_\nu[x] + i\,Y_\nu[x];$$

J, Y being Bessel function of first and second kind. The Green function then has the form

$$G[r] = A\,(k\,r)^{1-\frac{d}{2}}H^{(1)}_{\frac{d}{2}-1}[k\,r].$$

The small x behavior of the Hankel function is

$$H^{(1)}_\nu[x] \sim i\,Y_\nu[x] \sim -i\frac{1}{\text{Sin}[\pi\nu]}\left(\frac{x}{2}\right)^{-\nu}\frac{1}{\Gamma[1-\nu]} = -i\frac{\Gamma[\nu]}{\pi}\left(\frac{x}{2}\right)^{-\nu},$$

where we used the identity

$$\Gamma[x]\,\Gamma[1-x] = \frac{\pi}{\text{Sin}[\pi x]}.$$

The small r behavior of G follows

$$G \sim -i A \frac{\Gamma\left[\frac{d}{2}-1\right]}{\pi} 2^{\frac{d}{2}-1} (k r)^{2-d}. \tag{2.4}$$

To fix A we use Gauss theorem for a small sphere S of radius R enclosing the origin

$$\int_S \nabla^2 r^{2-d} = \int_{\partial S} \frac{\partial}{\partial r} r^{2-d} = \Omega_d R^{d-1} (2-d) R^{1-d} = -(d-2)\Omega_d.$$

Ω_d is the solid angle in d dimensions

$$\Omega_d = \frac{2\pi^{d/2}}{\Gamma\left[\frac{d}{2}\right]}.$$

Using the Gauss theorem on the equation (1) one sees that the singular term in G must be

$$G \sim \frac{2m}{\hbar^2}\left(-\frac{1}{(d-2)\Omega_d}\right) r^{2-d}.$$

One gets easily

$$A = \frac{1}{i}\frac{2m}{\hbar^2}\frac{k^{d-2}}{\pi^{\frac{d}{2}-1} 2^{\frac{d}{2}+1}}; \qquad G[r] = \frac{1}{i}\frac{2m}{\hbar^2}\frac{k^{d-2}}{\pi^{\frac{d}{2}-1} 2^{\frac{d}{2}+1}} (k r)^{1-\frac{d}{2}} H^{(1)}_{\frac{d}{2}-1}[k r]. \tag{2.5}$$

In particular for d = 3, using

$$H^{(1)}_{\frac{1}{2}}[x] = -i\sqrt{\frac{2}{\pi x}}\, e^{i x};$$

one recovers the known result

$$G[r] = -\frac{m}{2\pi\hbar^2}\frac{e^{i k r}}{r}. \tag{2.6}$$

Problem 3

Compute the Green function for a particle in one dimension in a potential V[x] = g δ[x] solving (E-H)G=1 in the x representation and verify the result by considering H eigenstates. Compute the spectral density g[E]. Verify the relation between g[E] and scattering phases by computing the transmission and reflection coefficients.

Solution

The Hamiltonian for the problem is

$$H = \frac{p^2}{2m} + g\,\delta[x]. \tag{3.1}$$

The equation for the Green function G is

$$\left(\frac{d^2}{dx^2} + q^2\right) G = \frac{2m}{\hbar^2}\delta(x-y) + \frac{2 m g}{\hbar^2}\delta[x]\, G[0]; \quad \text{with } E = \frac{\hbar^2 q^2}{2m}. \tag{3.2}$$

Note that the equation is not translation invariant. In the free particle case a function Exp[i q |x-y|] gave rise to a singularity δ[x-y]. The equation (2) has two δ singularities in x=y and x=0. It is then natural to look for solutions in the form

$$G[x, y] = A\, e^{i q |x-y|} + B\, e^{i q |x|}. \tag{3.3}$$

The derivatives give

$$\left(\frac{d^2}{dx^2} + q^2\right) G[x, y] = 2 i q A\, \delta[x-y] + 2 i q B\, \delta[x].$$

By substitution in (2) we see that the equation is satisfied for

$$A = \frac{m}{i \hbar^2 q}; \; B = \frac{2 \beta A}{2 (i q - \beta)} e^{i q |y|}; \quad \beta \equiv \frac{m g}{\hbar^2}.$$

β plays the role of a momentum scale. The final form of G is

$$G[x, y] = \frac{m}{i \hbar^2 q} \left(e^{i q |x-y|} + \frac{e^{i q (|x|+|y|)}}{i \frac{q}{\beta} - 1} \right). \quad (3.4)$$

■ Analytic properties

Our conventions for the cut in the square root function are

$$\hbar q = -i \sqrt{-2 m E}; \; E = \frac{q^2}{2 m}; \quad \text{physical sheet: } \mathrm{Im}[q] > 0 \text{ (first Riemann sheet in E)}. \quad (3.5)$$

The function G is expressed through q then has a cut in the complex plane E. The cut is for Re[E] > 0.

The function G in (4) has a pole at $q = -i\beta$.

- **a.** If $\beta > 0$ (repulsive potential) the pole is in the second sheet of complex plane E (Im[q] < 0)
- **b.** If $\beta < 0$ (attractive potential) the pole is in the physical sheet and corresponds to a bound state with energy

$$E_0 = \frac{\hbar^2 q^2}{2 m} = -\frac{\hbar^2 \beta^2}{2 m}.$$

For attractive potential near the pole, (4) becomes

$$G[x, y] \sim \frac{m}{i \hbar^2} \frac{e^{-|\beta| (|x|+|y|)}}{q + i \beta} \simeq \frac{|\beta| \, e^{-|\beta| (|x|+|y|)}}{E - E_0}. \quad (3.6)$$

The residue at the pole gives the wave function of the bound state (see below).

■ Spectral density

Spectral density is defined by

$$g[E] = -\frac{1}{\pi} \mathrm{Im}[\mathrm{Tr}[G[E]]] \equiv g_0[E] + \delta g[E] \quad (3.7)$$

g_0 is the density of states for a free particle. The operation Tr means x=y and integration of (4).

The integration of the first term in (4) gives the known result for g_0 (see also the text):

$$g_0[E] = V \frac{m}{\pi \hbar^2 q} = V \frac{\sqrt{m}}{\hbar} \frac{1}{\pi \sqrt{2 E}}. \quad (3.8)$$

The second term can be integrated with $q \to q + i \epsilon$ (upper side of the cut in the first sheet of E-plane) and then taking the limit $\epsilon \to 0$:

$$\int_{-\infty}^{+\infty} dx \, e^{i 2 (q + i \epsilon) |x|} = \frac{i}{q}.$$

Substitution in δg gives

$$\delta g[E] = -\frac{1}{\pi} \mathrm{Im}\left[-\frac{m}{\hbar^2 q^2} \frac{1}{1 - i \frac{q}{\beta}}\right] = \frac{m}{\pi \hbar^2 q \beta} \frac{1}{1 + \frac{q^2}{\beta^2}}. \quad (3.9)$$

■ Scattering phases and spectral density

In the text it has been shown that the scattering phases δ[E] are related to δg by

$$\delta g[E] = \frac{1}{\pi} \frac{d \delta[E]}{dE}. \quad (3.10)$$

To compute δ[E] we can consider the regular solution of the equation or compute the transmission and reflection coefficients.

▫ Regular solutions

In the text it is shown that even and odd solutions have respectively the asymptotic forms

$$\psi_e[x] \to \mathrm{Cos}[q x + \delta_e]; \qquad \psi_o[x] \to \mathrm{Sin}[q x + \delta_o]. \quad (3.11)$$

By imposing the continuity of ψ and the correct discontinuity in x=0, $\psi'[0]_+ - \psi'[0]_- = \hbar^2\, 2\, m\, g$ one easily obtains

$$-2\, q\, \mathrm{Sin}[\delta_e] = 2\, \beta\, \mathrm{Cos}[\delta_e]; \quad \mathrm{Sin}[\delta_o] = 0; \;\Rightarrow\; \delta_o = 0; \;\; \mathrm{Tan}[\delta_e] = -\frac{\beta}{q}.$$

By a derivative

$$\delta g_o[E] = 0; \quad \delta g_e[E] = \frac{1}{\pi}\frac{m}{\hbar^2 q}\frac{d\delta_e}{dq} = \frac{m}{\pi\hbar^2 q\beta}\frac{1}{1+\frac{q^2}{\beta^2}},$$

in agreement with eq.(9).

Transmission and reflection coefficients

The transmission and reflection coefficients A_T and A_R are found by solving the Schrödinger equation with the boundary conditions

$$x < 0 : e^{i q x} + A_R\, e^{-i q x}; \quad x > 0 : A_T\, e^{i q x}.$$

Imposing the continuity of ψ and the discontinuity of $2\beta\psi[0]$ on the derivative, it is found

$$A_T = \frac{i q}{i q - \beta}; \quad A_R = \frac{\beta}{i q - \beta}. \tag{3.12}$$

The potential is even, and in the text it has been shown that in this case one has

$$\delta g_e = -i\frac{m}{2\hbar^2 q}\frac{1}{A_T + A_R}\frac{d}{dq}(A_T + A_R); \quad \delta g_o = -i\frac{m}{2\hbar^2 q}\frac{1}{A_T - A_R}\frac{d}{dq}(A_T - A_R). \tag{3.13}$$

By substitution we get

$$\delta g_o[E] = 0; \quad \delta g_e[E] = \frac{m}{\pi\hbar^2 q\beta}\frac{1}{1+\frac{q^2}{\beta^2}}.$$

in agreement with the previous results.

As expected only the density of even states is changed. For odd states vanishing at x=0 the perturbation g δ[x] has no effects.

Sum of eigenfunctions

One can obtain the result (4) also by a more complex computation, from the knowledge of the eigenfunctions of the problem.

A set of eigenfunctions for our problem is (see text)

$$\psi^R_k[x] = \frac{1}{\sqrt{2\pi}}\left(e^{i k x} - F[k]\, e^{i k |x|}\right); \quad \psi^L_k[x] = \frac{1}{\sqrt{2\pi}}\left(e^{-i k x} - F[k]\, e^{i k |x|}\right). \tag{3.14}$$

where

$$F[k] = \frac{1}{1 - i\frac{k}{\beta}}; \quad F[-k] = F^*[k]; \quad F + F^* = \frac{2}{1+\frac{k^2}{\beta^2}} = 2\,|F|^2. \tag{3.15}$$

These functions are normalized to $\delta[k - k']$ and $k > 0$.

1. If $g > 0$ the spectrum is continuous, and (14) are a complete set.
2. If $g < 0$there is a bund state with energy and eigenvalue

$$E_0 = -\frac{\hbar^2\beta^2}{2 m}; \quad \psi_0[x] = \sqrt{|\beta|}\, e^{-|\beta||x|}.$$

The Green function by definition is

$$\begin{aligned} G[x, y] &= \sum \frac{\psi_\alpha[x]\,\psi^*_\alpha[y]}{E + i\epsilon - E'} = \\ &= \frac{2 m}{\hbar^2}\int_0^\infty dk\, \frac{\psi^R_k[x]\,\overline{\psi^R_k}[y] + \psi^L_k[x]\,\overline{\psi^L_k}[y]}{q^2 + i\epsilon - k^2} - \frac{2 m\,|\beta|}{\hbar^2}\frac{e^{-|\beta|(|x|+|y|)}}{\beta^2 + q^2}\,\Theta[-\beta]. \end{aligned} \tag{3.16}$$

The last term gives a contribution only for $g < 0$ and in this case it reproduces the result (6).

In expanding the products in (16) it is convenient to consider several cases

- **x, y > 0, or x, y < 0**

$$\psi_k^R[x]\,\overline{\psi_k^R}[y] + \psi_k^L[x]\,\overline{\psi_k^L}[y] = \frac{1}{2\pi}\left(e^{i k (x-y)} + e^{-i k (x-y)} - F[k]\, e^{i k (x+y)} - F^*[k]\, e^{-i k (x-y)}\right).$$

Due to properties (15) of F[k] this expression is symmetric in $k \to -k$ then the integral in (16) can be extended to the whole k-axis. The continuum contribution is

$$G_{cont} = -\frac{2m}{\hbar^2}\int_0^\infty \frac{dk}{2\pi}\left(\frac{e^{i k (x-y)}}{k^2 - q^2 + i\epsilon} - \frac{1}{1 - i\frac{k}{\beta}}\,\frac{e^{i k (x+y)}}{k^2 - q^2 + i\epsilon}\right).$$

The first integral has poles in $k = \pm q \pm i\epsilon$ with residues $\pm 1/2q$ respectively. The integration path is closed in the region Im[k]>0 or Im[k]<0 if the sign of x-y is ± 1. One has in any case, as the reader can easily check

$$\int_0^\infty \frac{dk}{2\pi}\,\frac{e^{i k (x-y)}}{k^2 - q^2 + i\epsilon} = \frac{i}{2q}\, e^{i q |x-y|}. \tag{3.17}$$

This term is the free propagator. The second term has an additional pole in $k = -i\beta$ which contributes only for $x + y < 0$ if $\beta > 0$, otherwise it gives a contribution also for $x + y > 0$. The second contribution to the continuum part of G is then

$$\beta > 0: \quad -i\,\frac{1}{1 - i\frac{q}{\beta}}\, e^{i q (x+y)}$$

$$\beta < 0: \quad -i\,\frac{1}{1 - i\frac{q}{\beta}}\, e^{i q (x+y)} - |\beta|\,\frac{e^{-|\beta|(x+y)}}{\beta^2 + q^2}$$

The whole expression for the continuum part becomes

$$G_{cont} = \frac{m}{i\hbar^2 q}\left(e^{i q |x-y|} + \frac{e^{i q (|x|+|y|)}}{i\frac{q}{\beta} - 1}\right) + \frac{2m\,|\beta|}{\hbar^2}\,\frac{e^{-|\beta|(|x|+|y|)}}{\beta^2 + q^2}\,\Theta[-\beta]$$

For x, y < 0 the computation is identical. By summing the possible contribution of the bound state we cancel the last term above and get

$$G[x, y] = \frac{m}{i\hbar^2 q}\left(e^{i q |x-y|} + \frac{e^{i q (|x|+|y|)}}{i\frac{q}{\beta} - 1}\right)$$

- **x,>0>y > 0, or y>0>x**

We leave to the reader the exercise to show that by using the relations (15) the same expression holds in this region, reproducing (4).

Problem 4

Compute the Green function for a particle in one dimension in a potential V[x] = g δ[x-a] + g δ[x+a] solving (E-H)G=1 in the x representation. Verify the analyticity properties in the complex E plane and compute the parameters for resonant states. Compare the results with the Gamow Siegert approach. Compute the spectral density g[E] from G and verify the result by using the scattering phases.

Solution

The Hamiltonian of our problem is

$$H = \frac{p^2}{2m} + g\,\delta[x-a] + g\,\delta[x+a] \tag{4.1}$$

The equation for the Green function reads

$$\left(\frac{d^2}{dx^2} + k^2\right) G = \frac{2m}{\hbar^2}\,\delta(x-y) + \frac{2mg}{\hbar^2}\left(\delta[x-a]\,G[a] + \delta[x+a]\,G[-a]\right). \tag{4.2}$$

We write

$$E = \frac{\hbar^2 k^2}{2m}; \quad \beta \equiv \frac{mg}{\hbar^2}.$$

We look for a solution in the form

$$G[x,\ y] = A\, e^{i k |x-y|} + B_1\, e^{i k |x+a|} + B_2\, e^{i k |x-a|}.$$

Using

$$\partial_x\ |x| = \epsilon[x]; \quad \partial_x \epsilon[x] = 2\,\delta[x];$$

substitution in (2) gives

$$A = \frac{m}{i\,\hbar^2\, k};$$
$$B_1 = -i\,\beta\, A\, e^{-2 i k a} \frac{\left(e^{i k |y+a|}\ (\beta - i\, k) - \beta\, e^{2 i k a}\, e^{i k |y-a|}\right)}{\left(2\,\beta\, \mathrm{Sin}[k\, a] + k\, e^{-i k a}\right)\ \left(2\,\beta\, \mathrm{Cos}[k\, a] - i\, k\, e^{-i k a}\right)}; \tag{4.3}$$
$$B_2 = -i\,\beta\, A\, e^{-2 i k a} \frac{\left(e^{i k |y-a|}\ (\beta - i\, k) - \beta\, e^{2 i k a}\, e^{i k |y+a|}\right)}{\left(2\,\beta\, \mathrm{Sin}[k\, a] + k\, e^{-i k a}\right)\ \left(2\,\beta\, \mathrm{Cos}[k\, a] - i\, k\, e^{-i k a}\right)};$$

■ Analytic properties

The propagator has singularities in the k-plane at the origin, and at zeros in the denominators in (3), poles in E.

In the E-plane there is a cut on the real positive axis and poles at

$$\begin{aligned} &2\,\beta\, \mathrm{Cos}[k\, a] - i\, k\, e^{-i k a} = 0 \ \Rightarrow\ (2\,\beta - i\, k)\ \mathrm{Cos}[k\, a] - k\, \mathrm{Sin}[k\, a] = 0; \\ &2\,\beta\, \mathrm{Sin}[k\, a] + k\, e^{-i k a} = 0 \ \Rightarrow\ (2\,\beta - i\, k)\ \mathrm{Sin}[k\, a] + k\, \mathrm{Cos}[k\, a] = 0. \end{aligned} \tag{4.4}$$

With $k\, a = x + i\, y$ the two equations for the poles can be written as

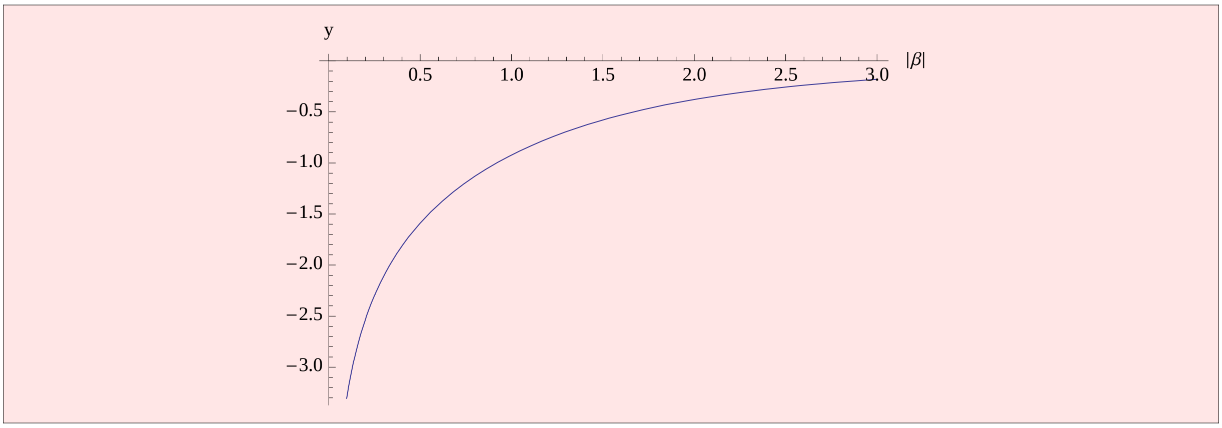
$$\begin{cases} y = -\beta\, a\ \left(1 + e^{-2 y}\, \mathrm{Cos}[2\, x]\right) \\ x = \beta\, a\, \mathrm{Sin}[2\, x]\ e^{-2 y} \end{cases} ; \begin{cases} y = \beta\, a\ \left(e^{-2 y}\, \mathrm{Cos}[2\, x] - 1\right) \\ x = -\beta\, a\, \mathrm{Sin}[2\, x]\ e^{-2 y} \end{cases} . \tag{4.5}$$

Let us consider the attractive and the repulsive case.

1. For $\beta > 0$ (repulsive potentials) the solutions do not have solutions for $y > 0$. In fact, if $y > 0$ then $\left| e^{-2 y}\, \mathrm{Cos}[2\, x] \right| < 1$and the equations imply $y < 0$. G has no pole in the physical sheet Im[k]>0.
2. For $\beta < 0$ there are solutions with x=0 and y>0, y is given by

   $$y = |\beta|\ a\ \left(1 + e^{-2 y}\right); \quad y = |\beta|\ a\ \left(1 - e^{-2 y}\right).$$

   These solutions with purely imaginary k correspond to negative energies, i.e. poles on the negative real axis in the E plane. As y>0 the solutions are on the first Riemann sheet.
3. For x≠0 we note that if x is a solution, then also -x is. To look for solutions is enough to consider positive x. Instead of a long discussion let us give a graph of the solution for the first of eq.(5).



It is apparent that y < 0 for all β. In conclusion

1. For $\beta > 0$ G has no singularity on the physical sheet $\mathrm{Im}[k] > 0$ and for $\beta < 0$ the only singularities are poles on the axis $\mathrm{Re}[k] = 0$, i.e. bound states with negative energy.
2. In the non physical sheet $\mathrm{Im}[k] < 0$there are singularities, corresponding to metastable states. The position of these singularities is the same as that found in solving the same problem with Gamow-Siegert method (see prob.6 in chap11, [prob6Chap11]). We refer to that problem for a more detailed analysis of the metastable states.

The spectral density

The spectral density is defined by

$$g[E] = -\frac{1}{\pi}\,\mathrm{Im}[\mathrm{Tr}[G[E]]] \equiv g_0[E] + \delta g[E] \tag{4.6}$$

g_0 is the density of states for a free particle. The operation Tr means x=y and integration in (2). The first term gives the free particle contribution, see also the previous problem. V is the volume:

$$g_0[E] = V\,\frac{m}{\pi\,\hbar^2\,q} = V\,\frac{\sqrt{m}}{\hbar}\,\frac{1}{\pi\sqrt{2\,E}}. \tag{4.7}$$

The second term can be integrated by writing $k \to k + i\epsilon$ (upper side of the cut) and then taking the limit $\epsilon \to 0$. Using

$$I_1 = \lim_{\epsilon\to 0}\int_{-\infty}^{+\infty} dx\, e^{i\,2\,(k+i\,\epsilon)\,|x\pm a|} = \frac{i}{k};$$

$$I_2 = \lim_{\epsilon\to 0}\int_{-\infty}^{+\infty} dx\, e^{i\,(k+i\,\epsilon)\,(|x+a|+|x-a|)} = e^{2\,i\,k\,a}\,\frac{i+2\,k\,a}{k}.$$

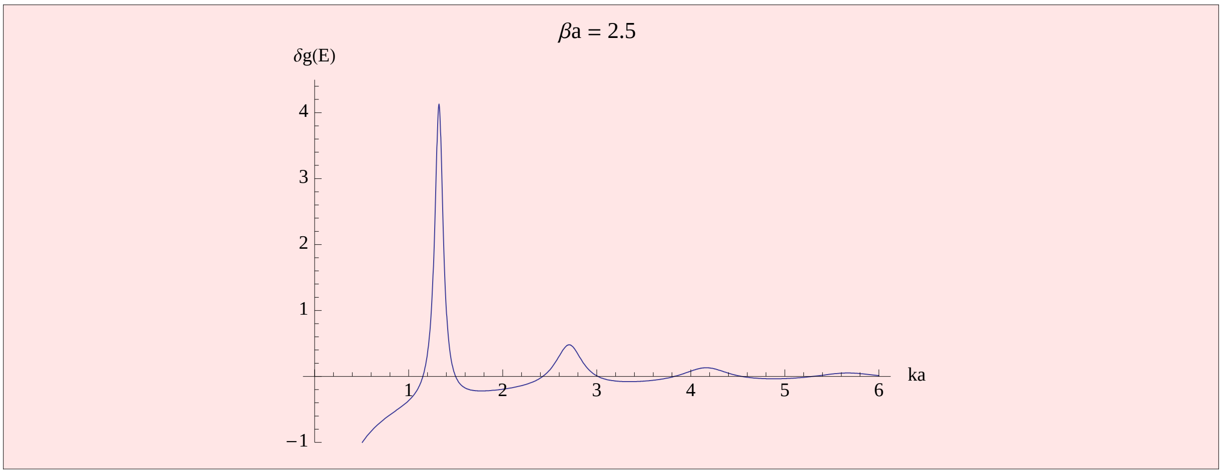
one gets easily

$$\mathrm{Tr}[\delta G[E]] = \frac{2\,m\,\beta}{i\,\hbar^2\,k^2}\,\frac{\left(i\,(\beta - i\,k) - e^{4\,i\,a\,k}\,(2\,a\,k + i)\,\beta\right)}{e^{4\,i\,a\,k}\,\beta^2 - (\beta - i\,k)^2}$$

and finally after some simplifications

$$\delta g[E] = -\frac{1}{\pi}\,\mathrm{Im}[\mathrm{Tr}[\delta G[E]]] = \frac{2\,m\,\beta}{\pi\,\hbar^2\,k}\,\frac{\left(-2\,a\,\beta^3 + \beta^2 - \left(\beta + 2\,a\,\left(k^2-\beta^2\right)\right)\mathrm{Cos}[4\,a\,k]\,\beta - k\,(4\,a\,\beta - 1)\,\mathrm{Sin}[4\,a\,k]\,\beta + k^2\right)}{k^4 + 2\,\beta^2\,k^2 + 4\,\beta^3\,k\,\mathrm{Sin}[4\,k\,a] + 2\,\beta^4 + 2\,\beta^2\,\left(k^2-\beta^2\right)\mathrm{Cos}[4\,a\,k]} \tag{4.8}$$

A typical behavior of δg with peaks corresponding to resonant states is shown in the figure below.



Scattering phases

In the text it has been shown that the scattering phases δ[E] are related to δg by

$$\delta g[E] = \frac{1}{\pi}\,\frac{d\,\delta[E]}{dE}. \tag{4.9}$$

To compute δ[E] we can consider the regular solutions of the equation.

In the text it is shown that even and odd solutions have respectively the asymptotic form

$$\psi_e[x] \to \mathrm{Cos}[q\,x + \delta_e]; \qquad \psi_o[x] \to \mathrm{Sin}[q\,x + \delta_o]. \tag{4.10}$$

It is sufficient to consider the positive values of x. In the two regions $0 < x < a$ and $x > a$ the two solutions have the form

$$\psi_e = \begin{cases} A\,\text{Cos}[k\,x] \\ \text{Cos}[k\,x + \delta_e] \end{cases} ; \quad \psi_o = \begin{cases} A\,\text{Sin}[k\,x] \\ \text{Sin}[k\,x + \delta_o] \end{cases} ;$$

By imposing the continuity of ψ at x=a and the correct discontinuity $2\beta\,\psi[a]$ for the derivative one easily obtains

$$\delta_e = -a\,k + \text{ArcTan}\left[\frac{-2\,\beta + k\,\text{Tan}[a\,k]}{k}\right]; \quad \delta_o = -a\,k + \text{ArcTan}\left[\frac{k}{2\,\beta + k\,\text{Cot}[a\,k]}\right]. \qquad (4.11)$$

The spectral density is written as

$$\delta g[E] = \frac{1}{\pi}\frac{d\,\delta_e[E]}{dE} + \frac{1}{\pi}\frac{d\,\delta_o[E]}{dE} =$$
$$= \frac{2\,m\,\beta}{\pi\,\hbar^2\,k}\left(\frac{-2\,a\,\beta + 2\,a\,k\,\text{Tan}[a\,k] + 1}{\text{Tan}[a\,k]^2\,k^2 + k^2 - 4\,\beta\,k\,\text{Tan}[a\,k] + 4\,\beta^2} - \frac{2\,a\,\beta + 2\,a\,k\,\text{Cot}[a\,k] - 1}{\text{Cot}[a\,k]^2\,k^2 + k^2 + 4\,\beta\,k\,\text{Cot}[a\,k] + 4\,\beta^2}\right).$$

After some (boring) simplifications this expression is shown to be equal to equal to (8).

Problem 5

Compute the eigenvalues for a free particle in a volume bounded by a parallelepiped with edges (a,b,c) and verify the form of the Weyl expansion.

Solution

In three dimensions Weyl's formula gives for the asymptotic number of the eigenvalues of a free particle

$$\frac{dN}{dE} = g[E] = \frac{1}{4\,\pi^2}\left(\frac{2\,m}{\hbar^2}\right)^{3/2} V\,\sqrt{E} - \frac{S}{16\,\pi}\left(\frac{2\,m}{\hbar^2}\right) + \frac{C}{12\,\pi^2}\left(\frac{2\,m}{\hbar^2}\right)^{1/2}\frac{1}{\sqrt{E}} + \ldots \qquad (5.1)$$

V is the volume, S the surface and C the mean curvature. The last term changes if cusps are present, so we shall not consider it.

The definition of g[E] is

$$g[E] = \sum \delta[E - E_i].$$

It is convenient to work with the Laplace transformation of g (see text)

$$Z[\beta] = \int_0^\infty \text{Exp}[-\beta\,E]\,g[E]\,dE = \sum \text{Exp}[-\beta\,E_i]. \qquad (5.2)$$

Z is the statistical partition function of the system, and the high energy behavior of g[E] is related to the small β behavior of Z[β].

The eigenstates can be classified by three integers n_1, n_2, n_3 and the eigenvalues of H are

$$E_{n_1,n_2,n_3} = \frac{\hbar^2}{2\,m}\left(\frac{\pi^2\,n_1^2}{a^2} + \frac{\pi^2\,n_2^2}{b^2} + \frac{\pi^2\,n_3^2}{c^2}\right). \qquad (5.3)$$

Using the definition of multiplication of two series it follows from (2) :

$$Z[\beta] = \sum_{n_1,n_2,n_3} \text{Exp}[-\beta\,E_{n_1,n_2,n_3}] = Z_1[a, \beta]\,Z_1[b, \beta]\,Z_1[c, \beta]; \qquad (5.4)$$

where

$$Z_1[a, \beta] = \sum_1^\infty \text{Exp}\left[-\beta\,\frac{\hbar^2}{2\,m}\,\frac{\pi^2\,n^2}{a^2}\right] = \sum_0^\infty \text{Exp}\left[-\beta\,\frac{\hbar^2}{2\,m}\,\frac{\pi^2\,n^2}{a^2}\right] - 1. \qquad (5.5)$$

The sum in (5) can be estimated with the Euler-McLaurin formula:

$$\sum_0^n f[n] = \int_0^\infty f[x]\,dx + \frac{1}{2}\,f[0] + \ldots O\,(f')$$

In our case f[x]~ Exp[-$\beta\,x^2$] and the correction terms are depressed by powers of β. A trivial integration gives

$$Z_1[a, \beta] \simeq \int_0^\infty dn\,\text{Exp}\left[-\beta\,\frac{\hbar^2}{2\,m}\,\frac{\pi^2\,n^2}{a^2}\right] - \frac{1}{2} = \left(\frac{2\,m}{\hbar^2}\right)^{1/2}\frac{a}{\pi\,\beta^{1/2}}\,\frac{\sqrt{\pi}}{2} - \frac{1}{2}. \qquad (5.6)$$

Inserting this result in (4) we get, at first two orders at low β:

$$Z[\beta] \simeq \left(\frac{2\,m}{\hbar^2}\right)^{3/2} \frac{a\,b\,c}{\left(2\sqrt{\pi}\right)^3}\beta^{-3/2} - \frac{1}{2}\left(\frac{2\,m}{\hbar^2}\right)\frac{1}{\left(2\sqrt{\pi}\right)^2}(a\,b + a\,c + b\,c)\,\beta^{-1}. \tag{5.7}$$

As

$$V = a\,b\,c; \quad S = 2\,(a\,b + a\,c + b\,c);$$

we have

$$Z[\beta] \simeq \left(\frac{2\,m}{\hbar^2}\right)^{3/2} \frac{V}{\left(2\sqrt{\pi}\right)^3}\beta^{-3/2} - \frac{1}{2}\left(\frac{2\,m}{\hbar^2}\right)\frac{1}{\left(2\sqrt{\pi}\right)^2}\frac{S}{2}\beta^{-1}. \tag{5.8}$$

To get g[E] from Z[β] we have to take the inverse Laplace transform of this result. This is easily done by noticing that

$$\mathcal{L}_\beta\left[E^{\alpha-1}\right] = \int dE\, e^{-\beta E} E^{\alpha-1} = \beta^{-\alpha}\,\Gamma[\alpha] \;\Rightarrow\; \mathcal{L}_E^{-1}[\beta^{-\mu}] = \frac{E^{\mu-1}}{\Gamma[\mu]}. \tag{5.9}$$

In particular

$$\mathcal{L}_E^{-1}\left[\beta^{-3/2}\right] = \frac{E^{1/2}}{\Gamma\left[\frac{3}{2}\right]} = \frac{2}{\sqrt{\pi}}\sqrt{E}\;; \qquad \mathcal{L}_E^{-1}\left[\beta^{-1}\right] = 1.$$

Taking the inverse Laplace transform in (8)

$$g[E] \simeq \left(\frac{2\,m}{\hbar^2}\right)^{3/2} E^{1/2}\frac{V}{4\,\pi^2} - \left(\frac{2\,m}{\hbar^2}\right)\frac{S}{16\,\pi} + \ldots \tag{5.10}$$

in agreement with Weyl's formula.

The number of states is

$$N[E] = \int_0^E g[x]\,dx = \left(\frac{2\,m}{\hbar^2}\right)^{3/2}\frac{2}{3}E^{3/2}\frac{V}{4\,\pi^2} - \left(\frac{2\,m}{\hbar^2}\right)\frac{S}{16\,\pi}E. \tag{5.11}$$

Problem 6

Show that in the pole approximation for a decay state χ for all t

$$P_{\chi\chi}[t] + \sum_s P_{s\chi}[t] = 1. \tag{6.1}$$

Solution

We use the notation of the text. The survival probability is

$$P_{\chi\chi}[t] = \mathrm{Exp}[-\Gamma\,t/\hbar]; \tag{6.2}$$

where the line width Γ is given by

$$\Gamma = \sum_s \left|\langle s \mid R[E_R] \mid \chi\rangle\right|^2 2\,\pi\,\delta[E_R - E_s]. \tag{6.3}$$

E_R is the resonance energy and R[E] is the decay matrix.

The states are classified by energy and some other quantum numbers, α and

$$\sum_s \equiv \sum_\alpha \int g[\alpha, E]\,dE$$

where g[α,E] is the density of states in dE around E. Then Γ is written explicitly as

$$\Gamma = \sum_\alpha \left|\langle \alpha, E_R \mid R[E_R] \mid \chi\rangle\right|^2 2\,\pi\,g[\alpha, E_R]. \tag{6.4}$$

In the text it is shown that

$$P_{s\chi}[t] = |\langle s \,|\, R[E] \,|\, \chi \rangle|^2 \left(\frac{1 + e^{-\Gamma t/\hbar} - 2\, e^{-\Gamma t/2\hbar} \cos[(E_R - E)\, t/\hbar]}{(E - E_R)^2 + \frac{\Gamma^2}{4}} \right). \tag{6.5}$$

This expression has poles in $E = E_R \pm i\,\Gamma/2$. In the pole approximation we can write (with $\Gamma \ll E$)

$$\sum_s P_{s\chi}[t] = \sum_\alpha g[\alpha, E_R]\, |\langle \alpha, E_R \,|\, R[E_R] \,|\, \chi \rangle|^2 \int dE \left(\frac{1 + e^{-\Gamma t/\hbar} - 2\, e^{-\Gamma t/2\hbar} \cos[(E_R - E)\, t/\hbar]}{(E - E_R)^2 + \frac{\Gamma^2}{4}} \right). \tag{6.6}$$

The first two terms in the integral can be computed with Jordan lemma as integrals in the complex E-plane closing the contour at infinity

$$\int dE \left(\frac{1 + e^{-\Gamma t/\hbar}}{(E - E_R)^2 + \frac{\Gamma^2}{4}} \right) = \left(1 + e^{-\Gamma t/\hbar}\right) 2\pi i \frac{1}{2 i \frac{\Gamma}{2}} = \frac{2\pi}{\Gamma} \left(1 + e^{-\Gamma t/\hbar}\right). \tag{6.7}$$

The third integral can be written

$$\int dE \frac{2\cos[(E_R - E)\, t/\hbar]}{(E - E_R)^2 + \frac{\Gamma^2}{4}} = \int dE \frac{1}{(E - E_R)^2 + \frac{\Gamma^2}{4}} \left(e^{i (E - E_R)\, t/\hbar} + e^{-i (E - E_R)\, t/\hbar}\right).$$

In applying Jordan lemma for $t > 0$ the first integral must be closed in the upper half plane (Im[E]>0) while the second in the lower half plane, then

$$\int dE \frac{2\cos[(E_R - E)\, t/\hbar]}{(E - E_R)^2 + \frac{\Gamma^2}{4}} = 2\pi i \left(\frac{e^{-\Gamma t/2\hbar}}{2 i \frac{\Gamma}{2}} \right) - 2\pi i \left(\frac{e^{-\Gamma t/2\hbar}}{-2 i \frac{\Gamma}{2}} \right) = -\frac{4\pi}{\Gamma} e^{-\Gamma t/2\hbar} \tag{6.8}$$

Inserting (7) and (8) in eq.(6) we have, using (4)

$$\sum_s P_{s\chi}[t] = \sum_\alpha g[\alpha, E_R]\, |\langle \alpha, E_R \,|\, R[E_R] \,|\, \chi \rangle|^2 \frac{2\pi}{\Gamma} \left(1 + e^{-\Gamma t/\hbar} - 2\, e^{-\Gamma t/\hbar}\right) = \left(1 - e^{-\Gamma t/\hbar}\right). \tag{6.9}$$

This and (2) verify eq.(1).