E837: Resolvent for a particle in box

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The problem:

(1) Find the resolvent for a particle inside one-dimensional potential well with infinite depth.
(2) Find the energy eigenvalues and the wave eigenfunctions.
(3) Show that in the case of potential well with infinite width ($(b-a) \to \infty$), $G(x|x')$ satisfies outgoing-waves boundary conditions in the source region.

The solution:

(1) *The resolvent for a particle inside one-dimensional potential well with infinite depth.*

Potential energy of a particle inside one-dimensional potential well with infinite depth can be written as:

$$V(x) = \begin{cases} \infty, & x < a \\ 0, & a \le x \le b \\ \infty, & x > b \end{cases} \tag{1}$$

The Shrödinger equation for a particle in such potential is written as

$$\mathcal{H}\Phi = -\frac{\hbar^2}{2\mathsf{m}}\frac{d^2\Phi}{dx^2} = E\Phi \tag{2}$$

The operator-valued function $G(z)$ of complex variable z, called as resolvent of operator $\mathcal{H}$ is defined as

$$G(z) = \frac{1}{z-\mathcal{H}} \tag{3}$$

The resolvent $G(z)$ can be represented as an integral transform of the wave functions. That is,

$$G(z) = \frac{1}{z-\mathcal{H}} = \sum_k \frac{|k\rangle\langle k|}{z-E_k} \tag{4}$$

where

$$|k\rangle = \Phi_k(x). \tag{5}$$

One can define the Green's function $G(x,x')$ as

$$G(x,x') = \sum_k \frac{\Phi_k(x)\Phi_k^*(x')}{z-E_k} \tag{6}$$

Consider now the formal relation

$$(z-\mathcal{H})G(z) = (z-\mathcal{H})\frac{1}{z-\mathcal{H}} = 1 \tag{7}$$

Corresponding to this we have

$$\left(\frac{d^2}{dx^2} + k_E^2\right)G(x,x') = \frac{2\mathsf{m}}{\hbar^2}\delta(x-x') \tag{8}$$

where $k_E = \sqrt{\frac{2\mathsf{m}E}{\hbar^2}}$.

This Green's function $G(x,x')$ is the kernel for a resolvent. It is the solution of the homogeneous differential equation corresponded to Eq.(8), which satisfies the boundary conditions of the problem (see (1)) since it may be expressed in an expansion of basis vectors satisfying the boundary conditions Eq.(2). For a potential well (1) the boundary conditions are

$$G(x=a,x') = G(x=b,x') = 0 \tag{9}$$

The homogeneous differential equation corresponded to the equation (8) is rewritten as

$$\left(\frac{d^2}{dx^2}+k_E^2\right)G(x,x')=0 \tag{10}$$

The general solution of equation (10) is

$$G(x,x')=\begin{cases} A_1\sin k_E x+B_1\cos k_E x, & a\le x<x' \\ A_2\sin k_E x+B_2\cos k_E x, & x'<x\le b\end{cases} \tag{11}$$

Therefore the boundary conditions (9) satisfy

$$\begin{array}{l} A_1\sin k_E a+B_1\cos k_E a=0 \\ A_2\sin k_E b+B_2\cos k_E b=0\end{array} \tag{12}$$

By using the boundary conditions (12) equation (11) can be deduced to

$$G(x,x')=\begin{cases} \frac{A_1}{\cos k_E a}\sin k_E(x-a), & x<x' \\ \frac{A_2}{\cos k_E b}\sin k_E(x-b), & x>x'\end{cases} \tag{13}$$

Integrating equation (8) from $x'-\varepsilon$ to $x'+\varepsilon$, where ε is an infinitesimal value one obtains

$$\left.\frac{\partial G}{\partial x}\right|_{x'-\varepsilon}^{x'+\varepsilon}=\frac{2\mathsf{m}}{\hbar^2} \tag{14}$$

By integrating again one obtains

$$G|_{x'-\varepsilon}^{x'+\varepsilon}=0 \tag{15}$$

Substituting equation (13) in (15) gives

$$\frac{A_1}{\cos k_E a}\sin k_E(x'-a)=\frac{A_2}{\cos k_E b}\sin k_E(x'-b) \tag{16}$$

Substituting equation (13) in (14) gives

$$\frac{2\mathsf{m}}{\hbar^2}+\frac{A_1 k_E}{\cos k_E a}\cos k_E(x'-a)=\frac{A_2 k_E}{\cos k_E b}\cos k_E(x'-b) \tag{17}$$

Solving equations (16) and (17) gives the following constants

$$A_1=\frac{2\mathsf{m}}{\hbar^2}\frac{\cos k_E a}{k_E\sin k_E(b-a)}\sin k_E(x'-b) \qquad A_2=\frac{2\mathsf{m}}{\hbar^2}\frac{\cos k_E b}{k_E\sin k_E(b-a)}\sin k_E(x'-a) \tag{18}$$

Substituting the constants A_1 and A_2 in equations (13) gives the following expression of the resolvent for a particle inside one-dimensional potential well with infinite depth:

$$G(x,x')=\frac{2\mathsf{m}}{\hbar^2}\begin{cases} \frac{\sin k_E(x-a)\sin k_E(x'-b)}{k_E\sin k_E(b-a)}, & x<x' \\ \frac{\sin k_E(x-b)\sin k_E(x'-a)}{k_E\sin k_E(b-a)}, & x>x'\end{cases} \tag{19}$$

Last expression can be also obtained by looking for solution of Eq.(8) in following form

$$G(x,x')=\frac{\mathsf{m}}{\hbar^2 k_E}\sin k_E|x-x'|+\alpha\cos(k_E x+\beta) \tag{20}$$

as was noted in QM Lecture Notes. This way one can omit the step of matching the solutions as was done above by using Eqs.(14), (15) and solve two equations representing Eq.(20) at boundary points.

(2) *The energy eigenvalues and the wave eigenfunctions.*

The energy eigenvalues of the problem correspond to poles of the resolvent, which require the following:

$$k_E = \frac{\pi n}{b-a}, \quad n = \pm 1, \pm 2, \pm 3, ... \tag{21}$$

Therefore the energy eigenvalues are

$$E_n = \frac{\hbar^2 k_E^2}{2\mathsf{m}} = \frac{\hbar^2 \pi^2 n^2}{2\mathsf{m}(b-a)^2}, \quad n = 1, 2, 3, ... \tag{22}$$

The wave eigenfunctions can be found from residues of the resolvent. That is,

$$\Phi_n(x)\Phi_n(x')^* = \frac{1}{2\pi i}\oint_{C_n} G(z)dz = \lim_{z\to E_n}(z-E_n)G(x,x') = \frac{2\mathsf{m}}{\hbar^2}\lim_{z\to E_n}(z-E_n)\begin{cases} \frac{\sin k_E(x-a)\sin k_E(x'-b)}{k_E \sin k_E(b-a)}, & x < x' \\ \frac{\sin k_E(x-b)\sin k_E(x'-a)}{k_E \sin k_E(b-a)}, & x > x' \end{cases} \tag{23}$$

here C_n is a contour around a pole on z-plane which corresponds to n-th eigenvalue.
One can consider the following limit

$$\begin{aligned} \frac{2\mathsf{m}}{\hbar^2}\lim_{z\to E_n}\left[\frac{z-E_n}{k_E \sin k_E(b-a)}\right] &= \frac{2\mathsf{m}}{\hbar^2}\frac{b-a}{\pi n}\lim_{z\to E_n}\left[\frac{z-E_n}{\sin\sqrt{\frac{2\mathsf{m}z}{\hbar^2}}(b-a)}\right] = \{L'H\hat{o}spital's\ Rule\} = \\ &= \frac{2\mathsf{m}}{\hbar^2}\frac{b-a}{\pi n}\lim_{z\to E_n}\left[\frac{2\sqrt{z}}{\sqrt{\frac{2\mathsf{m}}{\hbar^2}}(b-a)\cos\sqrt{\frac{2\mathsf{m}z}{\hbar^2}}(b-a)}\right] = (-1)^n\frac{2}{b-a}, \end{aligned} \tag{24}$$

and

$$\sin k_E(x'-b) = \sin k_E(x'-a+a-b) = \sin k_E(x'-a)\cos k_E(b-a) = (-1)^n \sin k_E(x'-a) \tag{25}$$

Therefore the product $\Phi_n(x)\Phi_n(x')^*$ in region $x < x'$ is rewritten as

$$\Phi_n(x)\Phi_n(x')^* = \frac{2}{b-a}\sin k_E(x-a)\sin k_E(x'-a) \tag{26}$$

As one can see the product $\Phi_n(x)\Phi_n(x')^*$ in region $x > x'$ is similar to (26) when using (25) with replacing $x' \to x$. Then Eq. (26) yields

$$\Phi_n(x) = \sqrt{\frac{2}{b-a}}\sin k_E(x-a) \tag{27}$$

Notice that Eq.(23) can be rewritten also as

$$\Phi_n(x) = Const \cdot \oint_{C_n} G(z)dz = Const \cdot \lim_{z\to E_n}(z-E_n)G(x,x') = Const \cdot \sin k_E(x-a) \tag{28}$$

In this case the $Const$ have to be found from normalization of $\Phi_n(x)$, i.e.

$$\int_{-\infty}^{\infty}|\Phi_n(x)|^2 dx = Const^2 \cdot \int_a^b \sin^2 k_E(x-a)dx = 1 \tag{29}$$

From Eqs.(28) and (29) one obtains $\Phi_n(x)$ similar to one obtained in (27).

As one can see the eigenvalues (22) and eigenstates (27) obtained by method of resolvent coincide with eigenvalues and eigenstates obtained from direct solving of the Shrödinger equation (2).

(3) *The case of potential well with infinite width ($(b-a) \to \infty$).*

Since, we are looking for solution of Schrödinger equation corresponding to outgoing waves, which means that outgoing waves decay to zero, while ingoing waves grow exponentially, the boundary conditions imply that the outgoing waves should have exponentially small weight that goes to zero in the $a \to -\infty, b \to \infty$ limits. In this case we have to consider energies in the upper complex plane. To do this, we use approach $k_E = \tilde{k}_E + \imath\alpha$, where $\alpha > 0$.

We wish to take the limit $a \to -\infty, b \to \infty$ on the Green's function (19).

To do this, consider,

$$\sin k_E(x-a) = \sin(\tilde{k}_E + \imath\alpha)(x-a) = \frac{1}{2\imath}\left[e^{\imath(\tilde{k}_E+\imath\alpha)(x-a)} - e^{-\imath(\tilde{k}_E+\imath\alpha)(x-a)}\right] = -\frac{1}{2\imath}e^{-\imath k_E(x-a)} \tag{30}$$

$$\sin k_E(x'-b) = \sin(\tilde{k}_E + \imath\alpha)(x'-b) = \frac{1}{2\imath}\left[e^{\imath(\tilde{k}_E+\imath\alpha)(x'-b)} - e^{-\imath(\tilde{k}_E+\imath\alpha)(x'-b)}\right] = \frac{1}{2\imath}e^{\imath k_E(x'-b)} \tag{31}$$

$$\sin k_E(x'-a) = \sin(\tilde{k}_E + \imath\alpha)(x'-a) = \frac{1}{2\imath}\left[e^{\imath(\tilde{k}_E+\imath\alpha)(x'-a)} - e^{-\imath(\tilde{k}_E+\imath\alpha)(x'-a)}\right] = -\frac{1}{2\imath}e^{-\imath k_E(x'-a)} \tag{32}$$

$$\sin k_E(x-b) = \sin(\tilde{k}_E + \imath\alpha)(x-b) = \frac{1}{2\imath}\left[e^{\imath(\tilde{k}_E+\imath\alpha)(x-b)} - e^{-\imath(\tilde{k}_E+\imath\alpha)(x-b)}\right] = \frac{1}{2\imath}e^{\imath k_E(x-b)} \tag{33}$$

$$\sin k_E(b-a) = \sin(\tilde{k}_E + \imath\alpha)(b-a) = \frac{1}{2\imath}\left[e^{\imath(\tilde{k}_E+\imath\alpha)(b-a)} - e^{-\imath(\tilde{k}_E+\imath\alpha)(b-a)}\right] = -\frac{1}{2\imath}e^{-\imath k_E(b-a)} \tag{34}$$

Therefore substituting Eqs.(30)-(34) in Eq.(19) one can obtain the Green's function in 1D, which satisfies the "outgoing waves" boundary conditions:

$$G(x,x') = -\imath\frac{\mathsf{m}}{\hbar^2 k_E}\left\{\begin{array}{ll} e^{-\imath k_E(x-x')}, & x < x' \\ e^{\imath k_E(x-x')}, & x > x' \end{array}\right. = -\imath\frac{\mathsf{m}}{\hbar^2 k_E}e^{\imath k_E|x-x'|} \tag{35}$$