Physics 631 Homework 5

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Problem 1. Let $\psi(x,t)$ be a normalized solution to the free particle Schrödinger equation in one dimension. We claim that

$$\check{\psi}(x,t) := \eta \sum_{j=-\infty}^{\infty} [\psi(x+2jL,t) - \psi(2jL-x,t)] \tag{1}$$

is a solution to the infinite-square-well on $[0,L]$, where η is a normalization factor assuming $\psi(x,t)$ is not even about $2Ln$ for some integer n.
We will plug $\check{\psi}(x,t)$ into the Schrödinger equation and check that it satisfies the boundary conditions. Since we are only interested in the region $[0,L]$, the only boundary conditions we must check are $\check{\psi}(0,t) = \check{\psi}(L,t) = 0$. Additionally, since $\psi(x,t)$ is a solution to the free particle Schrödinger equation for all $x \in \mathbb{R}$, then it must be continuous and Observe that $\psi(x,t)$ satisfies

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi(x,t)}{\partial x^2} \tag{2}$$

Since we have a second derivative in x on the right hand side of (2), $\psi(x+2jL,t)$ and $\psi(2jL-x,t)$ are also solutions to (2).

$$\begin{aligned}
i\hbar\frac{\partial\check{\psi}}{\partial t} &= \eta \sum_{j=-\infty}^{\infty}\left[i\hbar\frac{\partial\psi(x+2jL,t)}{\partial t} - i\hbar\frac{\partial\psi(2jL-x,t)}{\partial t}\right] \\
i\hbar\frac{\partial\check{\psi}}{\partial t} &= \eta \sum_{j=-\infty}^{\infty}\left[-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x+2jL,t)}{\partial x^2} + \frac{\hbar^2}{2m}\frac{\partial^2\psi(2jL-x,t)}{\partial x^2}\right] \\
i\hbar\frac{\partial\check{\psi}}{\partial t} &= \eta \sum_{j=-\infty}^{\infty} -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}[\psi(x+2jL,t) + \psi(2jL-x,t)] \\
i\hbar\frac{\partial\check{\psi}}{\partial t} &= -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\eta \sum_{j=-\infty}^{\infty}[\psi(x+2jL,t) + \psi(2jL-x,t)] \\
i\hbar\frac{\partial\check{\psi}}{\partial t} &= -\frac{\hbar^2}{2m}\frac{\partial^2\check{\psi}}{\partial x^2}
\end{aligned} \tag{3}$$

Therefore, $\check{\psi}(x,t)$ satisfies (2) on $[0,L]$.
At $x=0$, clearly

$$\check{\psi}(0,t) = \eta \sum_{j=-\infty}^{\infty}[\psi(2jL,t) - \psi(2jL,t)] = 0 \tag{4}$$

At $x = L$ we have

$$\begin{aligned}
\check{\psi}(L,t) &= \eta \sum_{j=-\infty}^{\infty} \left[\psi((2j+1)L,t) - \psi((2j-1)L,t)\right] \\
\check{\psi}(L,t) &= \eta \left(\sum_{j=-\infty}^{\infty} \psi((2j+1)L,t) - \sum_{j=-\infty}^{\infty} \psi((2j-1)L,t) \right)
\end{aligned} \tag{5}$$

But the index of each sum in (5) maps both $2j+1$ and $2j-1$ bijectively to $\mathbb{Z}_{odd}$. So we can rewrite (5) as follows

$$\check{\psi}(L,t) = \eta \left(\sum_{n\in\mathbb{Z}_{odd}} \psi(nL,t) - \sum_{n\in\mathbb{Z}_{odd}} \psi(nL,t) \right) = 0 \tag{6}$$

Therefore, $\check{\psi}(x,t)$ is a solution to the infinite square well Schrödinger equation on $[0, L]$.

Problem 2.

(a) Let

$$\psi_c(x) = \int_{-\infty}^{\infty} dx' K(x-x')\psi(x') \tag{7}$$

We claim that

$$\phi_c(p) = \sqrt{2\pi\hbar}\tilde{K}(p)\phi(p) \tag{8}$$

Where

$$\begin{aligned}
\phi(p) &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-ipx/\hbar}\psi(x)dx \\
\phi_c(p) &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-ipx/\hbar}\psi_c(x)dx \\
\tilde{K}(p) &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-ipx/\hbar}K(x)dx
\end{aligned} \tag{9}$$

We can show this by taking the Fourier transform of (7). This yields

$$\begin{aligned}
\phi_c(p) &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-ipx/\hbar} \int_{-\infty}^{\infty} K(x-x')\psi(x')dx'dx \\
\phi_c(p) &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x') \int_{-\infty}^{\infty} K(x-x')e^{-ipx/\hbar}dxdx' \\
\phi_c(p) &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x') \int_{-\infty}^{\infty} K(u)e^{-ip(u+x')/\hbar}dudx' \\
\phi_c(p) &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x')e^{-ipx'/\hbar}dx' \int_{-\infty}^{\infty} K(u)e^{-ipu/\hbar}du \\
\phi_c(p) &= \frac{1}{\sqrt{2\pi\hbar}} (\sqrt{2\pi\hbar}\phi(p))(\sqrt{2\pi\hbar}\tilde{K}(p)) \\
\phi_c(p) &= \sqrt{2\pi\hbar}\tilde{K}(p)\phi(p)
\end{aligned} \tag{10}$$

(b) Now suppose

$$\phi_c(p) = \int_{-\infty}^{\infty} \tilde{L}(p-p')\phi(p')dp' \tag{11}$$

Where

$$L(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{ipx/\hbar}\tilde{L}(p)dp \tag{12}$$

We claim that

$$\psi_c(x) = \sqrt{2\pi\hbar}L(x)\psi(x) \tag{13}$$

To show this we can again just take the (inverse) Fourier transform of both sides of (11):

$$\begin{aligned}
\psi_c(x) &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{ipx/\hbar} \int_{-\infty}^{\infty} \tilde{L}(p-p')\phi(p')dp'dp \\
\psi_c(x) &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{ipx/\hbar}\tilde{L}(p-p')\phi(p')dp'dp \\
\psi_c(x) &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{i(\omega+p')x/\hbar}\tilde{L}(\omega)\phi(p')dp'd\omega \\
\psi_c(x) &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \tilde{L}(\omega)e^{i\omega x/\hbar}d\omega \int_{-\infty}^{\infty} \phi(p')e^{ip'x/\hbar}dp' \\
\psi_c(x) &= \frac{1}{\sqrt{2\pi\hbar}}(\sqrt{2\pi\hbar}L(x))(\sqrt{2\pi\hbar}\psi(x)) \\
\psi_c(x) &= \sqrt{2\pi\hbar}L(x)\psi(x)
\end{aligned} \tag{14}$$

(c) Suppose $\psi(x)$ is normalized. We would like to find a condition on $K(x)$ such that $\psi_c(x)$ is normalized whenever $\psi(x)$ is normalized. To do this, we will suppose that

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1 \tag{15}$$

And require that

$$\int_{-\infty}^{\infty} |\psi_c(x)|^2 dx = 1 \tag{16}$$

If (16) is true then

$$\begin{aligned}
1 &= \int_{-\infty}^{\infty} |\psi_c(x)|^2 dx \\
&= \int_{-\infty}^{\infty} |\int_{-\infty}^{\infty} K(x-z)\psi(z)dz|^2 dx \\
&= \int_{-\infty}^{\infty} (\int_{-\infty}^{\infty} K(x-z)\psi(z)dz)(\int_{-\infty}^{\infty} K(x-y)\psi(y)dy)^* dx \\
&= \int_{-\infty}^{\infty} (\int_{-\infty}^{\infty} K(x-z)\psi(z)dz)(\int_{-\infty}^{\infty} K^*(x-y)\psi^*(y)dy)dx \\
&= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} K(x-z)K^*(x-y)\psi(z)\psi^*(y)dzdydx
\end{aligned} \tag{17}$$

Define

$$f(y,z) := \int_{-\infty}^{\infty} K(x-z)K^*(x-y)dx \tag{18}$$

Then we have

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f(y,z)\psi(z)\psi^*(y)dzdy = 1 \tag{19}$$

But we can write the normalization condition on $\psi(x)$ in the following way

$$\begin{aligned} 1 &= \int_{-\infty}^{\infty} |\psi(y)|^2 dy \\ &= \int_{-\infty}^{\infty} \psi(y)\psi(y)^* dy \\ &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \delta(y-z)\psi(z)\psi(y)^* dzdy \end{aligned} \tag{20}$$

But equations (19) and (20) must be equal for all $\psi(x)$, so we must have

$$f(y,z) = \delta(y-z) \tag{21}$$

Therefore, if $\psi(x)$ is normalized, $\psi_c(x)$ is also normalized provided

$$\delta(y-z) = \int_{-\infty}^{\infty} K(x-z)K^*(x-y)dx \tag{22}$$

Problem 3.

(a) The goal here will be to solve for E in terms of k. We first write equation (2.66) in the dimensionless units

$$x = \frac{kL}{2}$$

and

$$\alpha^2 = \frac{mL^2V_0}{2\hbar^2}$$

From equations (2.29) and (2.70) we can see that if $\alpha \to 0$ then we have one even solution and zero odd solutions. Therefore, in order to solve for k, we need only solve for x in the equation

$$\cot(x) = \frac{x}{\sqrt{\alpha^2 - x^2}} \tag{23}$$

We will make a series of approximations in the limit where both $\alpha \to 0$ and $x \to 0$.

$$
\begin{aligned}
\cot(x) &= \frac{x}{\sqrt{\alpha^2 - x^2}} \\
\tan(x) &= \frac{\sqrt{\alpha^2 - x^2}}{x} \\
x \approx \tan(x) &= \frac{\sqrt{\alpha^2 - x^2}}{x} \\
x^2 &= \sqrt{\alpha^2 - x^2} \\
x^4 + x^2 - \alpha^2 &= 0 \\
(x^2)^2 + x^2 - \alpha^2 &= 0 \\
x^2 &= -\frac{1}{2} + \frac{1}{2}\sqrt{1 + 4\alpha^2} \approx -\frac{1}{2} + \frac{1}{2}(1 + 2\alpha^2 - 2\alpha^4) \\
x^2 &= \alpha^2 - \alpha^4 \\
k^2 &= \frac{2mV_0}{\hbar^2} - \frac{m^2L^2V_0^2}{2\hbar^4} \\
\frac{2m(V_0 - |E|)}{\hbar^2} &= \frac{2mV_0}{\hbar^2} - \frac{m^2L^2V_0^2}{2\hbar^4} \\
E &= -\frac{m\beta^2}{2\hbar^2}
\end{aligned} \tag{24}
$$

Since $L \to 0$, the solution in region II disappears and since we only have one solution which is even, we must have $a_{\mathrm{I}} = a_{\mathrm{III}}$. And the bound state looks like

$$
\begin{aligned}
\psi_E(x) &= \begin{cases} a_{\mathrm{I}} e^{k_I x} & x < 0 \\ a_{\mathrm{I}} e^{-k_I x} & x > 0 \end{cases} \\
\psi_E(x) &= a_{\mathrm{I}} e^{-m\beta|x|/\hbar^2}
\end{aligned} \tag{25}
$$

To normalize $\psi_E(x)$ we will just require that

$$a_{\mathrm{I}}^2 \int_{-\infty}^{\infty} e^{-2m\beta|x|/\hbar^2} dx = 1$$

Which implies that

$$\psi_E(x) = \sqrt{\frac{m\beta}{\hbar^2}} e^{-m\beta|x|/\hbar^2}$$

(b) We can also solve this using the "direct" method. The time independent Schrödinger equation becomes

$$\frac{\partial^2 \psi_E}{\partial x^2} = -\frac{2m}{\hbar^2}(E + \beta\delta(x))\psi_E \tag{26}$$

Observe that

$$\frac{\partial^2 |x|}{\partial x^2} = 2\delta(x) \quad \text{and} \quad \left(\frac{\partial |x|}{\partial x}\right) = 1 \tag{27}$$

This leads us to postulate a solution

$$\tilde{\psi}(x) = Ce^{-A|x|} \tag{28}$$

Differentiating $\tilde{\psi}$ twice yields

$$\begin{aligned}
\frac{\partial^2 \tilde{\psi}}{\partial x^2} &= \frac{\partial}{\partial x}\left(-ACe^{A|x|}\frac{\partial |x|}{\partial x}\right) \\
&= A^2 Ce^{-A|x|}\left(\frac{\partial |x|}{\partial x}\right)^2 - 2ACe^{-A|x|}\delta(x) \\
&= A^2 Ce^{-A|x|} - 2ACe^{-A|x|}\delta(x) \\
&= (A^2 - 2A\delta(x))\tilde{\psi}
\end{aligned} \tag{29}$$

Therefore, if $\tilde{\psi}$ is to solve (26) we must have

$$A = \frac{m\beta}{\hbar^2} \quad \text{and} \quad E = -\frac{m\beta^2}{2\hbar^2} \tag{30}$$

Thus, our postulated solution was in fact a solution to (26) so

$$\psi_E(x) = Ce^{-m\beta|x|/\hbar^2}$$

Normalizing $\psi_E(x)$ yields the final form of the single bound state of the delta function potential

$$\psi_E(x) = \sqrt{\frac{m\beta}{\hbar^2}}e^{-m\beta|x|/\hbar^2} \tag{31}$$

Problem 4.

We start with the general solution to the Schrödinger equation given the potential.

$$\psi_E(x) = \begin{cases} e^{ikx} + re^{-ikx} & \text{(region I)} \\ ae^{-\kappa x} + be^{\kappa x} & \text{(region II)} \\ \tau e^{ikx} & \text{(region III)} \end{cases} \tag{32}$$

We can solve for r and τ using the boundary conditions and requiring that $\psi_E(x)$ and $\psi_E'(x)$ are continuous everywhere.

$$\begin{aligned}
\psi_E(\pm L/2 + 0^+) &= \psi_E(\pm L/2 + 0^-) \\
\psi_E'(\pm L/2 + 0^+) &= \psi_E'(\pm L/2 + 0^-)
\end{aligned} \tag{33}$$

Which yields the following system of equations

$$\begin{aligned}
e^{-ikL/2} + re^{ikL/2} &= ae^{\kappa L/2} + be^{-\kappa L/2} \\
ae^{-\kappa L/2} + be^{\kappa L/2} &= \tau e^{ikL/2} \\
ike^{-ikL/2} - ikre^{ikL/2} &= -a\kappa e^{\kappa L/2} + b\kappa e^{-\kappa L/2} \\
-a\kappa e^{-\kappa L/2} + b\kappa e^{\kappa L/2} &= ik\tau e^{ikL/2}
\end{aligned} \tag{34}$$

We can solve these as two matrix equations

$$
\begin{aligned}
\begin{bmatrix} e^{-ikL/2} & e^{ikL/2} \\ i\frac{k}{\kappa}e^{-ikL/2} & -i\frac{k}{\kappa}e^{ikL/2} \end{bmatrix} \begin{bmatrix} 1 \\ r \end{bmatrix} &= \begin{bmatrix} e^{\kappa L/2} & e^{-\kappa L/2} \\ -e^{\kappa L/2} & e^{-\kappa L/2} \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} \\
\begin{bmatrix} e^{-\kappa L/2} & e^{\kappa L/2} \\ -e^{-\kappa L/2} & e^{\kappa L/2} \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} &= \tau \begin{bmatrix} e^{ikL/2} \\ i\frac{k}{\kappa}e^{ikL/2} \end{bmatrix}
\end{aligned} \tag{35}
$$

We can invert the top matrix on the right hand side and the bottom matrix on the left hand side to solve these for the a, b vector. This yields

$$
\frac{1}{2} \begin{bmatrix} e^{-\kappa L/2} & e^{\kappa L/2} \\ -e^{-\kappa L/2} & e^{\kappa L/2} \end{bmatrix} \begin{bmatrix} e^{-\kappa L/2} & -e^{-\kappa L/2} \\ e^{\kappa L/2} & e^{\kappa L/2} \end{bmatrix} \begin{bmatrix} e^{-ikL/2} & e^{ikL/2} \\ i\frac{k}{\kappa}e^{-ikL/2} & -i\frac{k}{\kappa}e^{ikL/2} \end{bmatrix} \begin{bmatrix} 1 \\ r \end{bmatrix} = \tau \begin{bmatrix} e^{ikL/2} \\ i\frac{k}{\kappa}e^{ikL/2} \end{bmatrix} \tag{36}
$$

We can shamelessly plug this into Mathematica to solve to r and τ, arriving at the following solutions

$$
\begin{aligned}
r &= \frac{e^{-ikL}(e^{2L\kappa}-1)(k^2+\kappa^2)}{(e^{2L\kappa}-1)k^2 + 2ik\kappa(1+e^{2L\kappa}) - (e^{2L\kappa}-1)\kappa^2} \\
\tau &= \frac{4ik\kappa e^{-ikL}e^{L\kappa}}{(e^{2L\kappa}-1)k^2 + 2ik\kappa(1+e^{2L\kappa}) - (e^{2L\kappa}-1)\kappa^2}
\end{aligned} \tag{37}
$$

Which again simplify slightly to

$$
\begin{aligned}
r &= \frac{e^{ikL}(k^2+\kappa^2)}{k^2-\kappa^2+2ik\kappa\coth(L\kappa)} \\
\tau &= \frac{2ik\kappa e^{-ikL}}{2ik\kappa\cosh(L\kappa)+(k-\kappa)(k+\kappa)\sinh(L\kappa)}
\end{aligned} \tag{38}
$$

By defining

$$
\tau_1 = -\frac{2ik}{\kappa - ik} \quad \tau_1' = \frac{2\kappa}{\kappa - ik} \quad r_1 = -\frac{\kappa + ik}{\kappa - ik} \tag{39}
$$

we can simplify (32) by putting r and τ over the common denominator $1 - r_1^2 e^{-2L\kappa}$. This reduces (32) to

$$
\begin{aligned}
r &= \frac{\tau_1\tau_1' e^{-L\kappa}e^{-ikL}}{1-r_1^2e^{-2L\kappa}} \\
\tau &= \frac{r_1(1-e^{-2L\kappa})e^{-ikL}}{1-r_1^2e^{-2L\kappa}}
\end{aligned} \tag{40}
$$