Assignment 2

OPTI 570 Quantum Mechanics

University of Arizona

Nicolás Hernández Alegría

September 3, 2025
Total time: 8 hours

1 Exercise 1

A particle under a delta function potential has the following hamiltonian:

$$H = -\frac{\hbar}{2m}\frac{d^2}{dx^2} - \alpha\delta(x),$$

where $\delta(x)$ is the potential to be analyzed which is centered at $x = 0$.

(a) (a.1) The integration of the eigenvalue equation

$$\begin{aligned} H\varphi(x) &= E\varphi(x) \\ -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\varphi(x) - \alpha\delta(x)\varphi(x) &= E\varphi(x) \end{aligned}$$

in the range $x \in [-\epsilon, \epsilon]$ is

$$\int_{-\epsilon}^{\epsilon} \left[-\frac{\hbar^2}{2m}\frac{d^2\varphi}{dx^2}(x) - \alpha\delta(x)\varphi(x)\right] \, dx = \int_{-\epsilon}^{\epsilon} E\varphi(x) \, dx,$$

where in this infinitesimal region around $x = 0$ different things will happen:

- By property of the delta function, we will have

$$\int_{-\infty}^{\infty} \alpha\delta(x)\varphi(x) \, dx = \alpha\varphi(0).$$

- The integration of the second derivative will become a substraction of two first derivatives:

$$\int_{-\epsilon}^{\epsilon} \left[-\frac{\hbar^2}{2m}\frac{d^2\varphi}{dx^2}(x)\right] \, dx = -\frac{\hbar^2}{2m}\left[\frac{d\varphi}{dx}(\epsilon) - \frac{d\varphi}{dx}(-\epsilon)\right].$$

- The right-hand term will be zero, as the function cannot change abruptly (to be physically realizable) in an infinitesimal range:

$$\int_{-\epsilon}^{\epsilon} E\varphi(x) \, dx = 0.$$

Putting all in the eigenvalue equation yields

$$-\frac{\hbar^2}{2m}\left[\frac{d\varphi}{dx}(\epsilon)-\frac{d\varphi}{dx}(-\epsilon)\right]-\alpha\varphi(0)=0, \quad x\in[-\epsilon,\epsilon]. \tag{1}$$

(a.2) Recall that continuity of a function $f(x)$ at $x=x_0$ needs that both lateral limits be equal as they approach to the point, and that the value be equal to the function evaluated at that point: $f(x_0^-)=f(x_0^+)=f(x_0)$.
Taking the limit $\epsilon\to 0$ in a rearranged version of the equation (1) allow us to construct the difference of the derivative used to prove continuity in the first derivate of $\varphi(x)$:

$$\lim_{\epsilon\to 0}\left[\frac{d\varphi}{dx}(\epsilon)-\frac{d\varphi}{dx}(-\epsilon)\right]=-\frac{2m\alpha}{\hbar^2}\varphi(0).$$

We can see that lateral derivatives are not equal, but rather there is a finite jump of $-\frac{2m\alpha}{\hbar^2}\varphi(0)$ at $x=0$. Therefore, we conclude that $\varphi'(x)$ is not continue at that point.

(b) (b.1) We will assume that $E<0$ but we will not replace the minus sign in the derivation to maintain the generalization of the equations. If one wants to put a particular value, then it has to come with the minus sign. That said, to obtain an expression for ρ we replace the wavefunctions

$$\begin{aligned} x<0: &\quad \varphi(x)=A_1e^{\rho x}+A_1'e^{-\rho x}\\ x>0: &\quad \varphi(x)=A_2e^{\rho x}+A_2'e^{-\rho x}.\end{aligned}$$

into the eigenvalue problem. These solutions must be stable, so we evaluate them at $-\infty$ and $+\infty$ to see if any term blows up:

$$\begin{aligned}\varphi(-\infty)&=A_1e^{\rho(-\infty)}+\cancel{A_1'e^{-\rho(-\infty)}}^{\text{blows up}},\\ \varphi(+\infty)&=\cancel{A_2e^{\rho(\infty)}}^{\text{blows up}}+A_2'e^{-\rho(\infty)}.\end{aligned}$$

Therefore, to have a stable and normalizable wavefunction we redefine the above:

$$\varphi(x)=\begin{cases}A_1e^{\rho x}, & x<0\\ A_2'e^{-\rho x}, & x>0\end{cases}.$$

Now, we can proceed. In order to obtain an expression for ρ, we will study each domain separately.
For $x<0$, the function has not passed through the delta potential yet so the hamiltonian reduces to the derivative term only.

$$\begin{aligned} H\varphi(x)&=E\varphi(x)\\ -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\left[A_1e^{\rho x}\right]&=E\left[A_1e^{\rho x}\right]\\ -\frac{\hbar^2}{2m}\frac{d}{dx}\left[\rho A_1e^{\rho x}\right]&=EA_1e^{\rho x}\\ -\frac{\hbar^2}{2m}\rho^2\cancel{A_1e^{\rho x}}&=E\cancel{A_1e^{\rho x}}\\ \rho&=\sqrt{-\frac{2mE}{\hbar^2}}\end{aligned}$$

For $x > 0$, despite that the delta function is not active, it has imposed initial conditions on the function in the first derivative.

First, we know that the function must be continuous throught the whole domain. Matematically, that means that

$$\varphi(0^-) = \varphi(0^+) = \varphi(0) \Longrightarrow A_1 = A_2' = A.$$

Then, again

$$\varphi(x) = Ae^{-\rho|x|} = \begin{cases} Ae^{\rho x}, & x < 0 \\ Ae^{-\rho x}, & x > 0 \end{cases}.$$

Now, if we look at the equation of discontinuity we have derived in (a.2) and replace the function above we can solve for ρ.

$$\begin{aligned} \varphi'(0^+) - \varphi(0^+) &= -\frac{2m\alpha}{\hbar^2}\varphi(0) \\ -\rho Ae^{-\rho(0)} - \rho Ae^{\rho(0)} &= -\frac{2m\alpha}{\hbar^2}\left[Ae^{-\rho(0)}\right] \\ -2\rho &= -\frac{2m\alpha}{\hbar^2} \\ \rho &= \frac{m\alpha}{\hbar^2}. \end{aligned}$$

Because the variable ρ must be equal in either region, we conclude that

$$\rho = \sqrt{-\frac{2mE}{\hbar^2}} = \frac{m\alpha}{\hbar^2}. \tag{2}$$

The dimension of α can now be found easily. We know that ρ must have dimensions of $[L]^{-1}$ in order to have a dimensionless quantity in the argument of the exponential of the wave $\varphi(x)$. Knowing also that the mass have dimension of $[M]$ and $\hbar^2$ of $[M^2L^4T^{-2}]$, doing dimensional analysis with the last equation yields

$$[L^{-1}] = [M][M^2L^4T^{-2}]^{-1}[\alpha] \longrightarrow [\alpha] = [L]^{-1}[M]^{-1}[M^2L^4T^{-2}] = [ML^3T^{-2}].$$

(b.2) Above we have already limited the general equation to only terms that dont blow up when x goes to $\pm\infty$, meaning that they are square-interable over the space. We have also implicitly set continuity in $\varphi(x)$ when assigned the same coefficient A for both wavefunctions.

The energy possible upon these constraints is obtained solving for E in the equation (2)

$$\sqrt{-\frac{2mE}{\hbar^2}} = \frac{m\alpha}{\hbar^2} \longrightarrow E = -\frac{m\alpha^2}{2\hbar^2}.$$

The wavefunction must be normalized in order to satisfy the normalization condition and be interpreted as a probability density function:

$$\int_{-\infty}^{\infty} |\varphi(x)|^2 \, dx = 1.$$

For that, we will separate the domain in two regions, one for $x < 0$ and other for $x > 0$ and in each subdomain we will use the respective wavefunction.

$$\begin{aligned}
\int_{-\infty}^{0} |Ae^{\rho x}|^2 \, dx + \int_{0}^{\infty} |Ae^{-\rho x}|^2 &= 1 \\
\int_{-\infty}^{0} A^2 e^{2\rho x} \, dx + \int_{0}^{\infty} A^2 e^{-2\rho x} \, dx &= \\
\frac{A^2}{2\rho} \left[e^{2\rho x}\right]\Big|_{-\infty}^{0} - \frac{A^2}{2\rho} \left[e^{-2\rho x}\right]\Big|_{0}^{\infty} &= \\
\frac{A^2}{2\rho} [1 - 0] - \frac{A^2}{2\rho} [0 - 1] &= \\
\frac{A^2}{\rho} &= 1 \\
A &= \sqrt{\rho} \quad [L]^{-1/2}.
\end{aligned}$$

Therefore, the normalized wavefunctions are:

$$\varphi(x) = \sqrt{\rho} e^{-\rho|x|} = \begin{cases} \sqrt{\rho} e^{\rho x}, & x < 0 \\ \sqrt{\rho} e^{-\rho x}, & x > 0 \end{cases}.$$

(c) The plot of the $\varphi(x)$ is illustrated below, where we can see that is symmetric.

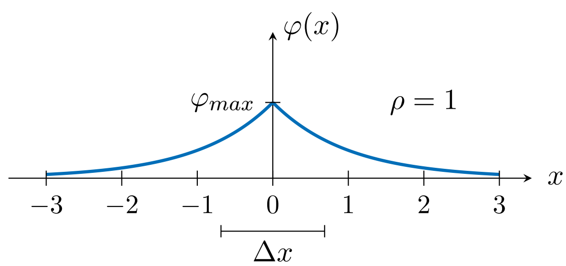

Figure 1: Normalized wavefunction $\varphi(x)$ with its respective Δx.

We are going to use the Full Width at Half Maximum to define Δx. It is defined as the diameter (full width) at which half of the peak is reached. We will use the $x > 0$ function and the value of x obtained will be multiplied by two because of symmetry.

$$\begin{aligned}
\varphi(x) &= \frac{\varphi_{max}}{2} \\
\sqrt{\rho} e^{-\rho x} &= \frac{\sqrt{\rho}}{2} \Big/ \ln(\cdot) \\
-\rho x &= -\ln 2 \\
x &= \frac{\ln 2}{\rho} \longrightarrow \Delta x = \frac{2 \ln 2}{\rho}.
\end{aligned}$$

The order of magnitude of Δx would be something proportional to the inverse of ρ as the other terms are constant:

$$\Delta x \sim \frac{1}{\rho}.$$

(d) The Fourier transform applied to our wavefunction is:

$$
\begin{aligned}
\tilde{\varphi}(p) &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \varphi(x) \exp\left\{-i\frac{p}{\hbar}x\right\}\, dx \\
&= \frac{\sqrt{\rho}}{\sqrt{2\pi\hbar}} \left[\int_{-\infty}^{0} \exp\left\{\rho x - i\frac{p}{\hbar}x\right\}\, dx + \int_{0}^{\infty} \exp\left\{-\rho x - i\frac{p}{\hbar}x\right\}\, dx\right] \\
&= \sqrt{\frac{\rho}{2\pi\hbar}} \left[\int_{-\infty}^{0} \exp\left\{\left(\frac{\rho\hbar - ip}{\hbar}\right)x\right\}\, dx + \int_{0}^{\infty} \exp\left\{\left(-\frac{\rho\hbar + ip}{\hbar}\right)x\right\}\, dx\right] \\
&= \sqrt{\frac{\rho}{2\pi\hbar}} \left[\frac{\hbar}{\rho\hbar - ip} \exp\{u\}\Big|_{-\infty}^{0} - \frac{\hbar}{\rho\hbar + ip} \exp\{u\}\Big|_{0}^{-\infty}\right] \\
&= \sqrt{\frac{\rho}{2\pi\hbar}} \left[\frac{\hbar}{\rho\hbar - ip} + \frac{\hbar}{\rho\hbar + ip}\right] \\
\tilde{\varphi}(p) &= \sqrt{\frac{\rho}{2\pi\hbar}} \frac{2\hbar^2\rho}{\rho^2\hbar^2 + p^2}.
\end{aligned}
$$

We then define the FWHM as we did for $\varphi(x)$.

$$
\begin{aligned}
\tilde{\varphi}(p) &= \frac{\tilde{\varphi}_{max}}{2} \\
\sqrt{\frac{\rho}{2\pi\hbar}} \frac{2\hbar^2\rho}{\rho^2\hbar^2 + p^2} &= \sqrt{\frac{\rho}{2\pi\hbar}} \frac{1}{\rho} \\
\frac{2\hbar^2\rho}{\rho^2\hbar^2 + p^2} &= \frac{1}{\rho} \\
2\hbar^2\rho &= \rho\hbar^2 + \frac{p^2}{\rho} \\
p &= \hbar\rho \longrightarrow \Delta p = 2\hbar\rho.
\end{aligned}
$$

The figure of $\tilde{\varphi}(p)$ with Δp is illustrated. Note that the constant $\hbar$ has been set to one only for visualization.

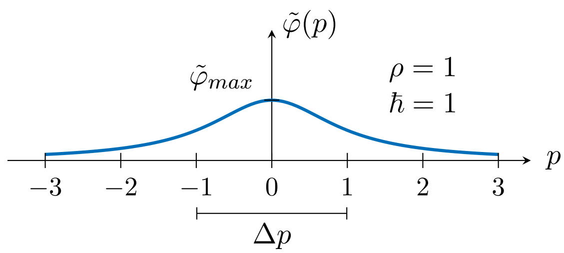

Figure 2: Fourier transform $\tilde{\varphi}(p)$ with a normalized $\hbar = 1$ **only** for visualization.

The product of the widths is then:

$$
\Delta x \Delta p = \frac{2\ln 2}{\rho} 2\hbar\rho = 4\ln 2\ \hbar.
$$

The order of magnitude of Δp and $\Delta x \Delta p$ would be:

$$
\Delta p \sim \hbar\rho, \quad \text{and} \quad \Delta x \Delta p \sim \hbar.
$$

2 Exercise 2

a. Compute the adjoint of the operator $U(m,n)$ is the same that inverting the order (transpose) and conjugate them (complex conjugation). That means that a ket will become a bra and viceversa:

$$U^\dagger(m,n) = (|\varphi_m\rangle\langle\varphi_n|)^\dagger = |\varphi_n\rangle\langle\varphi_m|. \tag{3}$$

b. This is done by algebra of the operation and the definition above. Lets also recall that H is hermitian so that its eigenvalues E_n are real:

$$[H, U(m,n)] = HU(m,n) - U(m,n)H = H|\varphi_m\rangle\langle\varphi_n| - |\varphi_m\rangle\langle\varphi_n|H.$$

The first and last terms corresponds to the eigenvalue problems $H|\varphi_m\rangle = E_m|\varphi_m\rangle$ and $\langle\varphi_n|H^\dagger = \langle\varphi_n|E_n^*$, but $E_n = E_n^*$ and $H = H^\dagger$ as the operator is Hermitian. Replacing them yields

$$[H, U(m,n)] = E_m|\varphi_m\rangle\langle\varphi_n| - |\varphi_m\rangle\langle\varphi_n|E_n = (E_m - E_n)|\varphi_m\rangle\langle\varphi_n| = (E_m - E_n)U(m,n).$$

c. Replacing each projector:

$$U(m,n)U^\dagger(p,q) = |\varphi_m\rangle\langle\varphi_n|\varphi_q\rangle\langle\varphi_p| = \begin{cases} 0, & n \neq q \\ |\varphi_m\rangle\langle\varphi_p|, & n = q \end{cases}$$

When multiplying both operator, there will be created an inner product in the middle: $\langle\varphi_n|\varphi_q\rangle$, which will return a scalar proportion to the "collinearity" of both state vectors. If we assume the basis is composed of linear independent elements $|\varphi_i\rangle$, then all the inner product for which $n \neq q$ will be zero, and only when both index are equal will return 1, if the basis is properly normalized. We have put the cases of these two scenarios, but a compact form would be through the use of the kronecker function δ_{ij}, defined as:

$$\delta_{ij} = \begin{cases} 0, & i \neq j \\ 1, & i = j \end{cases}.$$

In consequence,

$$U(m,n)U^\dagger(p,q) = |\varphi_m\rangle\delta_{nq}\langle\varphi_p| = \delta_{nq}|\varphi_m\rangle\langle\varphi_p| = \delta_{nq}U(m,p).$$

d. The trace over an operator A with the discrete orthonormal basis $\{|\varphi_n\rangle\}$ is the sum of the diagonal element of A:

$$\mathrm{Tr}(A) = \sum_i \langle\varphi_i|A|\varphi_i\rangle.$$

Applying it to $U(m,n) = |\varphi_m\rangle\langle\varphi_n|$ results in

$$\mathrm{Tr}[U(m,n)] = \sum_i \langle\varphi_i|\varphi_m\rangle\langle\varphi_n|\varphi_i\rangle = \sum_i \langle\varphi_n|\varphi_i\rangle\langle\varphi_i|\varphi_m\rangle = \langle\varphi_n|\left(\sum_i |\varphi_i\rangle\langle\varphi_i|\right)|\varphi_m\rangle.$$

The term in parenthesis is a property of closure relation for projectors, which is

$$\sum_i |\varphi_i\rangle\langle\varphi_i| = \mathbb{I}.$$

Therefore, we have

$$\mathrm{Tr}[U(m,n)] = \langle\varphi_n|\mathbb{I}|\varphi_m\rangle = \langle\varphi_n|\varphi_m\rangle = \delta_{nm}.$$

e. If A is an operator with matrix elements $A_{mn} = \langle\varphi_m|A|\varphi_n\rangle$, then

$$\begin{aligned}
A &= \sum_{m,n} A_{mn} U(m,n) \\
&= \sum_{m,n} \langle\varphi_m|A|\varphi_n\rangle |\varphi_m\rangle\langle\varphi_n| \\
&= \sum_{m,n} |\varphi_m\rangle\langle\varphi_m|A|\varphi_n\rangle\langle\varphi_n| \\
&= \left(\sum_m |\varphi_m\rangle\langle\varphi_m|\right) A \left(\sum_n |\varphi_n\rangle\langle\varphi_n|\right) \\
&= \mathbb{I}A\mathbb{I} \\
A &= A.
\end{aligned}$$

Where we have used the closure relation twice

f. Substituting the $U^\dagger(p,q)$ operator obtained in equation (3) with A in the trace operation, and noting that $A_{mn} = \langle\varphi_m|A|\varphi_n\rangle$:

$$\begin{aligned}
A_{pq} &= \mathrm{Tr}\{AU^\dagger(p,q)\} \\
\langle\varphi_p|A|\varphi_q\rangle &= \sum_i \langle\varphi_i|A|\varphi_q\rangle\langle\varphi_p|\varphi_i\rangle \\
&= \sum_i \langle\varphi_p|\varphi_i\rangle\langle\varphi_i|A|\varphi_q\rangle \\
&= \langle\varphi_p| \left(\sum_i |\varphi_i\rangle\langle\varphi_i|\right) A|\varphi_q\rangle \\
&= \langle\varphi_p|\mathbb{I}A|\varphi_q\rangle \\
\langle\varphi_p|A|\varphi_q\rangle &= \langle\varphi_p|A|\varphi_q\rangle \\
A_{pq} &= A_{pq}.
\end{aligned}$$

Using again, the closure relation of projector operator.