Problem Set 9

Physics 442
Quantum Mechanics II

Due on Friday, April 12th, 2024

Problem 1

We discussed a "spherical wave" in class, with

$$\psi(\mathbf{r}) = A\frac{e^{ikr}}{r}. \tag{1}$$

Find the time-dependent form of this time-independent wave function. Make sure your $\Psi(\mathbf{r}, t)$ satisfies Schrödinger's equation for a free particle.

Problem 2

Here, we'll work through the Green's function for the Helmholtz equation in one dimension, solving:

$$\left(\frac{d^2}{dx^2} + k^2\right) G(x, x') = \delta(x - x'). \tag{2}$$

a. Set the source at the origin ($x' = 0$), let $G(x) \equiv G(x, 0)$, and solve the differential equation you get from (2) for points $x \neq 0$. Keep only the "outgoing" term for both $x > 0$ and $x < 0$ (so solve for $G(x)$ in both domains, making sure that your solution is continuous at $x = 0$).

b. We'll normalize to the delta — integrate (2) from $x = -\epsilon \to \epsilon$, and use your solution in the resulting equation to set the lone constant of integration. Finally, move the source from the origin back to x' to get $G(x, x')$.

Problem 3

Using your Green's function from the previous problem, solve

$$\left(\frac{d^2}{dx^2} + k^2\right) P(x) = V(x) \tag{3}$$

with

$$V(x) = \begin{cases} V_0 & -a \leq x \leq a \\ 0 & \text{else} \end{cases} , \tag{4}$$

for $P(x)$ with $x \in (0, a)$. The boundary conditions are built in to the Green's function, so you just need to evaluate the integral form of the solution. Make sure your solution satisfies the differential equation.

Problem 4

Griffiths & Schroeter Problem 10.10 — Soft sphere scattering.

Problem 5

Griffiths & Schroeter Problem 10.11 — Yukawa $f(\theta)$. Compute the integral "by hand" for this one.

Problem 6

Griffiths & Schroeter Problem 10.12 — Yukawa cross section.

Problem 7

Suppose we have a set of (orthonormal) basis functions $\{\psi_j(x)\}_{j=1}^{\infty}$ such that any square-integrable function can be expanded in this set with complex coefficients. In quantum mechanics, the energy eigenfunctions often provide such a basis. Show that the function

$$f(x, x') = \sum_{j=1}^{\infty} \psi_j^*(x)\psi_j(x')$$

"is" (behaves like, under an integral) $\delta(x - x')$.

Presentation Problems

These problems will either be presented in class on Friday (April 12th), or presented in written form, due by Friday. Take a look at them over the weekend, I'll ask for volunteers on Monday. Whether or not you present one of these problems or not, you should solve them and be prepared to discuss them in class.

Problem 1*

Schrödinger's equation in one dimension reads:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x,t)}{dx^2} + U(x)\psi(x,t) = i\hbar\frac{\partial\psi(x,t)}{\partial t}, \tag{5}$$

and we'll use boundary conditions $\psi(0,t) = \psi(a,t) = 0$.

Introducing a grid in position, $x_j = j\Delta x$ with $\Delta x = a/(N+1)$ for $j = 1 \to N$ interior grid points, we can use finite differences to approximate the second derivative of $\psi(x,t)$ at grid location x_j:

$$\left.\frac{\partial^2\psi(x,t)}{\partial x^2}\right|_{x=x_j} \approx \frac{\psi_{j+1} - 2\psi_j + \psi_{j-1}}{\Delta x^2}, \tag{6}$$

for $\psi_j \equiv \psi(x_j,t)$. Using this approximation, and "projecting" the rest of the equation onto the grid (the projection of a function like $U(x,t)$, for example is just $U_j \equiv U(x_j,t)$), show that you can write a "finite difference form" of Schrödinger's equation as

$$\mathbb{H}\begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_N \end{pmatrix} = i\hbar\begin{pmatrix} \dot\psi_1 \\ \dot\psi_2 \\ \vdots \\ \dot\psi_N \end{pmatrix} \tag{7}$$

for a matrix $\mathbb{H}$ (give its entries).

Now discretize in time, as well: let $t^n \equiv n\Delta t$, and let $\psi_j^n \equiv \psi(x_j,t^n)$. We can approximate the temporal derivative using a finite difference in time,

$$\dot\psi_j|_{t=t^n} \approx \frac{\psi_j^{n+1} - \psi_j^n}{\Delta t}. \tag{8}$$

Finally, define

$$\boldsymbol{\psi}^n \dot{\equiv} \begin{pmatrix} \psi_1^n \\ \psi_2^n \\ \vdots \\ \psi_N^n \end{pmatrix}. \tag{9}$$

Schrödinger's equation, in this fully discrete approximation, is

$$i\hbar \left(\frac{\boldsymbol{\psi}^{n+1} - \boldsymbol{\psi}^n}{\Delta t} \right) = \mathbb{H} \left(\frac{\boldsymbol{\psi}^{n+1} + \boldsymbol{\psi}^n}{2} \right), \tag{10}$$

where we have democratically averaged the wavefunction vector on the right.

Viewing this equation as a temporal update algorithm, $\boldsymbol{\psi}^{n+1} = \mathbb{U}\boldsymbol{\psi}^n$, find the matrix $\mathbb{U}$ (not its entries, just its expression in terms of building blocks like $\mathbb{H}$), and show that for this matrix, $\|\boldsymbol{\psi}^{n+1}\| = \|\boldsymbol{\psi}^n\|$, the norm of the wavefunction is the same at every time step — this is a discrete form of probability conservation.

Problem 2*

In classical mechanics, given a one-dimensional Lagrangian, L, the equation of motion is:

$$-\frac{d}{dt}\frac{\partial L}{\partial \dot{x}} + \frac{\partial L}{\partial x} = 0. \tag{11}$$

When dealing with a *field* Lagrangian, $\mathcal{L}$ that depends on $\Psi(t, x, y, z)$ and its derivatives, the structure is similar, but we have to treat all coordinates equally — the "equation of motion" is:

$$-\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \Psi_t} - \frac{d}{dx}\frac{\partial \mathcal{L}}{\partial \Psi_x} - \frac{d}{dy}\frac{\partial \mathcal{L}}{\partial \Psi_y} - \frac{d}{dz}\frac{\partial \mathcal{L}}{\partial \Psi_z} + \frac{\partial \mathcal{L}}{\partial \Psi} = 0, \tag{12}$$

where $\Psi_t \equiv \frac{\partial \Psi}{\partial t}$, $\Psi_x \equiv \frac{\partial \Psi}{\partial x}$, etc. What is the field equation for the Lagrangian:

$$\mathcal{L} = \frac{\hbar^2}{2m}\nabla\Psi^* \cdot \nabla\Psi + U\Psi^*\Psi - \frac{i\hbar}{2}(\Psi^*\Psi_t - \Psi\Psi_t^*)? \tag{13}$$

Note that here there are really two fields, Ψ and Ψ^*, and you are only finding one of the two field equations.

Problem 3*

Make a plot of the classical soft-sphere differential scattering cross section, compare with the quantum mechanical case. Compute the total cross section for the classical case.