Moderne Theoretische Physik I
Grundlagen der Quantenmechanik

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Exercise Sheet 3

Prof. Jörg Schmalian
Grgur Palle, Iksu Jang
Karlsruher Institut für Technologie (KIT)
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The problems whose solutions you need to upload are designated with stars.

⋆ Problem 1 ⋆ Particle in a box

Consider a particle of mass m that lies in the infinitely deep well

$$V(x) = \begin{cases} 0, & \text{for } 0 < x < L, \\ +\infty, & \text{otherwise.} \end{cases} \tag{1}$$

1. If $x(t=0) = x_0 \in \langle 0, L \rangle$ and $p(t=0) = p_0 \neq 0$, what is the solution of the classical equations of motion? By imposing the Sommerfeld quantization condition

$$\oint \mathrm{d}x\, p = \int_0^T \mathrm{d}t\, \dot{x}(t) p(t) = n \cdot 2\pi\hbar, \tag{2}$$

   where the integral goes over one period of motion (T is the time period) and $n \in \mathbb{N}$, find what p_0 must equal. Calculate the corresponding energy.

2. If the wavefunction of the particle at $t = 0$ equals

$$\psi(x) = a_1 \sin(n_1 \pi x/L) + a_2 \sin(n_2 \pi x/L), \tag{3}$$

   where $a_1, a_2 \in \mathbb{C}$ and $n_1, n_2 \in \mathbb{N}$ with $a_1 \neq 0, a_2 \neq 0, n_1 \neq n_2$, then what is the wavefunction at later times?

3. Now using this wavefunction, calculate the corresponding expectation values of $\hat{x}$ and $\hat{p} = -\mathrm{i}\hbar\partial_x$ at later times. For concreteness, set $n_1 = 1$ and $n_2 = 2$.

4. According to Ehrenfest's theorem:

$$\partial_t \langle \hat{x} \rangle = \frac{\langle \hat{p} \rangle}{m}, \qquad \partial_t \langle \hat{p} \rangle = - \langle V'(\hat{x}) \rangle . \tag{4}$$

   Do the results of parts 1 and 3 agree with this? Explain any apparent disagreements.

Solution 1

1. The solution of the classical equations of motion is

$$x(t) = \begin{cases} x_0 + \frac{p_0}{m} t, & \text{for } \frac{m(-x_0)}{p_0} < t < \frac{m(L-x_0)}{p_0} \equiv t_1, \\ L - \frac{p_0}{m}(t - t_1), & \text{for } t_1 < t < t_1 + T/2 \equiv t_2, \\ \frac{p_0}{m}(t - t_2), & \text{for } t_2 < t < t_2 + T/2 \equiv t_3, \\ L - \frac{p_0}{m}(t - t_3), & \text{for } t_3 < t < t_3 + T/2 \equiv t_4, \\ \text{etc.} \end{cases}$$

$$p(t) = \begin{cases} p_0, & \text{for } \frac{m(-x_0)}{p_0} < t < \frac{m(L-x_0)}{p_0} \equiv t_1, \\ -p_0, & \text{for } t_1 < t < t_1 + T/2 \equiv t_2, \\ p_0, & \text{for } t_2 < t < t_2 + T/2 \equiv t_3, \\ -p_0, & \text{for } t_3 < t < t_3 + T/2 \equiv t_4, \\ \text{etc.} \end{cases}$$

when $p_0 > 0$, and analogously for $p_0 < 0$. So the particle moves uniformly, bouncing of the walls every $T/2 = mL/|p_0|$ second, thereby resulting in a "triangle wave" dependence of $x(t)$. The Sommerfeld quantization condition yields

$$\int_0^T \mathrm{d}t \, \frac{p(t)}{m} p(t) = T \cdot \frac{p_0^2}{m} = n \cdot 2\pi\hbar$$
$$\implies p_0 = \hbar \frac{n\pi}{L}.$$

The energy

$$E_n = \frac{p_0^2}{2m} = \frac{\hbar^2}{2m} \left(\frac{n\pi}{L}\right)^2$$

agrees with the quantum result.

2. Since ψ is a superposition of stationary states,

$$\psi(x,t) = a_1 \mathrm{e}^{-\mathrm{i}E_{n_1} t/\hbar} \sin(n_1 \pi x/L) + a_2 \mathrm{e}^{-\mathrm{i}E_{n_2} t/\hbar} \sin(n_2 \pi x/L)$$

where E_n is given above. One may also check this explicitly using $\mathrm{i}\hbar\partial_t \mathrm{e}^{-\mathrm{i}Et/\hbar} = E\mathrm{e}^{-\mathrm{i}Et/\hbar}$ and $\partial_x^2 \sin(kx) = -k^2 \sin(kx)$.

3. We have

$$\begin{aligned} \langle \hat{x} \rangle &= \int_0^L \mathrm{d}x \, \psi^*(x,t) x \psi(x,t) \\ &= |a_1|^2 \int_0^L \mathrm{d}x \sin^2(k_1 x) x + |a_2|^2 \int_0^L \mathrm{d}x \sin^2(k_2 x) x \\ &\quad + 2\,|a_1| \cdot |a_2| \cos\chi(t) \int_0^L \mathrm{d}x \sin(k_1 x) \sin(k_2 x) x \end{aligned}$$

where $k_1 = n_1\pi/L$, $k_2 = n_2\pi/L$, $a_2/a_1 = |a_2/a_1|\,\mathrm{e}^{\mathrm{i}\varphi}$, and $\chi(t) = (E_{n_1} - E_{n_2})t/\hbar + \varphi$. By symmetry, the first two integrals equal $L/2$ so

$$\langle \hat{x} \rangle = \frac{L}{2} + 2\,|a_1| \cdot |a_2| \cos\chi(t) \int_0^L \mathrm{d}x \sin(k_1 x) \sin(k_2 x) x.$$

Similarly

$$\begin{aligned}\langle\hat{p}\rangle &= -\mathrm{i}\hbar\int_0^L \mathrm{d}x\,\psi^*(x,t)\partial_x\psi(x,t)\\ &= -\mathrm{i}\hbar k_1\left|a_1\right|^2\int_0^L \mathrm{d}x\sin(k_1x)\cos(k_1x) - \mathrm{i}\hbar k_2\left|a_2\right|^2\int_0^L \mathrm{d}x\sin(k_2x)\cos(k_2x)\\ &\quad - \mathrm{i}\hbar\left|a_1\right|\cdot\left|a_2\right|\int_0^L \mathrm{d}x\left[k_2\mathrm{e}^{\mathrm{i}\chi(t)}\sin(k_1x)\cos(k_2x) + k_1\mathrm{e}^{-\mathrm{i}\chi(t)}\sin(k_2x)\cos(k_1x)\right].\end{aligned}$$

This time the first two integrals $\propto \int_0^L \mathrm{d}x\,\sin(2kx)$ vanish because $\cos(2kL)=1$, whereas in the third integral the $k_1\cos(k_1x)=\partial_x\sin(k_1x)$ can be partially integrated so as to move the derivative onto the $\sin(k_2x)$. The boundary terms vanish in the process. The result is

$$\langle\hat{p}\rangle = \hbar k_2\cdot 2\left|a_1\right|\cdot\left|a_2\right|\sin\chi(t)\int_0^L \mathrm{d}x\sin(k_1x)\cos(k_2x).$$

Finally, setting $n_1=1$ and $n_2=2$ and evaluating the integrals we get

$$\langle\hat{x}\rangle = \frac{L}{2} + 2\left|a_1\right|\cdot\left|a_2\right|\cos\chi(t)\cdot\frac{-8L^2}{9\pi^2}, \tag{5}$$

$$\langle\hat{p}\rangle = \hbar k_2\cdot 2\left|a_1\right|\cdot\left|a_2\right|\sin\chi(t)\cdot\frac{-2L}{3\pi}. \tag{6}$$

4. The Ehrenfest relation for $\hat{x}$ does indeed hold in an obvious way:

$$\partial_t\langle\hat{x}\rangle = \frac{\langle\hat{p}\rangle}{m} = \frac{-4\hbar}{3m}\cdot 2\left|a_1\right|\cdot\left|a_2\right|\sin\chi(t). \tag{7}$$

Less obvious is the $\hat{p}$ Ehrenfest relation. Naively, $V'(x)=0$ so it's violated. However, this isn't quite correct since $V(x)$ diverges at $x=0,L$ so its derivative diverge there too. More formally, one can consider a finite well

$$V_U(x) = \begin{cases} 0, & \text{for } 0<x<L,\\ +U, & \text{otherwise,}\end{cases}$$

whose

$$V_U'(x) = U\left[\delta(x-L)-\delta(x)\right]$$

and then take the limit $U\to\infty$ to show that $\partial_t\langle\hat{p}\rangle = -\langle V'(\hat{x})\rangle$ indeed holds. To get a grade, one only needs to notice that the resolution of the apparent disagreement between $V'(x)=0$ and $\partial_t\langle\hat{p}\rangle\neq 0$ lies in the boundary.

⋆ Problem 2 ⋆ Delta potential well

Consider the delta potential well

$$V(x) = -V_0\,\delta(x), \tag{8}$$

where $V_0>0$.

1. By integrating the stationary Schrödinger equation from $x=-\epsilon$ to ϵ for small $\epsilon>0$, derive the condition that the wavefunction must obey at $x=0$. You may assume that ψ is continuous at $x=0$.

2. Solve the stationary Schrödinger equation for bounded states, that is, find all eigenfunctions of the Hamiltonian which have a finite norm.

3. What are the corresponding energies? Explicitly calculate them by evaluating the integral arising in the Hamiltonian average $\left\langle\hat{H}\right\rangle$. Evaluate the kinetic energy in two ways: as $\left\langle\psi\middle|\hat{p}^2\psi\right\rangle$ and as $\langle\hat{p}\psi|\hat{p}\psi\rangle$.

Solution 2

1. Starting from

$$\frac{-\hbar^2}{2m}\partial_x^2\psi(x) - V_0\,\delta(x)\psi(x) = E\psi(x)$$

we find that

$$\begin{aligned}\frac{-\hbar^2}{2m}\int_{-\epsilon}^{\epsilon}\mathrm{d}x\,\partial_x^2\psi(x) - V_0\int_{-\epsilon}^{\epsilon}\mathrm{d}x\;\delta(x)\psi(x) = E\int_{-\epsilon}^{\epsilon}\mathrm{d}x\,\psi(x)\\ \implies \frac{-\hbar^2}{2m}\left[\psi'(+\epsilon) - \psi'(-\epsilon)\right] - V_0\psi(0) = 0\end{aligned}$$

for infinitesimal $\epsilon > 0$.

2. For $E > 0$, we get oscillatory solutions which we cannot normalize. The normalizeable eigenfunctions therefore have $E < 0$ and yield exponential solutions for $x \neq 0$. These solutions must decay at infinity, so there is only one option:

$$\psi(x) = A\,\mathrm{e}^{-\kappa|x|}$$

where $\frac{\hbar^2\kappa^2}{2m} = -E$. The $x = 0$ condition gives

$$\begin{aligned}\frac{-\hbar^2}{2m}\left[A(-\kappa) - A\kappa\right] - V_0 A = 0\\ \implies \kappa = \frac{mV_0}{\hbar^2}.\end{aligned}$$

Evidently, there is only one κ that solves this, and therefore only one bounded state associated with a delta potential well. (Later in the course we shall also study unbounded state which arise here.)

3. Setting $A = \sqrt{\kappa}$ normalizes $\psi(x)$ to unity. Moreover

$$\hat{p}\psi(x) = \mathrm{i}\hbar\kappa^{3/2}\,\mathrm{sgn}(x)\mathrm{e}^{-\kappa|x|}$$

and

$$\hat{p}^2\psi(x) = \hbar^2\kappa^{3/2}\left[2\,\delta(x) - \kappa\right]\mathrm{e}^{-\kappa|x|}.$$

Evaluating

$$\begin{aligned}\left\langle\psi\middle|\hat{p}^2\psi\right\rangle &= \int_{-\infty}^{\infty}\mathrm{d}x\hbar^2\kappa^2\left[2\,\delta(x) - \kappa\right]\mathrm{e}^{-2\kappa|x|} = \hbar^2\kappa^2,\\ \langle\hat{p}\psi|\hat{p}\psi\rangle &= \int_{-\infty}^{\infty}\mathrm{d}x\hbar^2\kappa^3\mathrm{e}^{-2\kappa|x|} = \hbar^2\kappa^2\end{aligned}$$

agrees. Likewise evaluating

$$\begin{aligned}\left\langle\hat{H}\right\rangle &= \frac{\left\langle\psi\middle|\hat{p}^2\psi\right\rangle}{2m} + \int_{-\infty}^{\infty}\mathrm{d}x\psi^*(x)\left[-V_0\,\delta(x)\right]\psi(x)\\ &= \frac{\hbar^2\kappa^2}{2m} - V_0\kappa = -\frac{\hbar^2\kappa^2}{2m} = E\end{aligned}$$

agrees with the previous.

Problem 3 Linear differential equations as Schrödinger equations

1. Consider the wave equation describing the vibrations of a string:
$$\partial_t^2 u(x,t) = \partial_x^2 u(x,t), \tag{9}$$
where the speed of sound has been set to unity. Derive the effective Hamiltonian $\hat{H}$ (which is a 2×2 matrix here) arising in
$$\mathrm{i}\sigma_z \partial_t \psi = \hat{H}\psi \tag{10}$$
which describes the evolution of the multicomponent wavefunction
$$\psi = \begin{pmatrix} u + \mathrm{i}\partial_t u \\ u - \mathrm{i}\partial_t u \end{pmatrix}. \tag{11}$$
Here
$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{12}$$

2. Physically, $u^*(x,t) = u(x,t)$ must be real. What is the analogous reality condition on $\psi(x,t)$? Show that Eq. (10) preserves it.

3. Next, consider Maxwell's equations (with $\epsilon_0 = \mu_0 = 1$)
$$\boldsymbol{\nabla}\cdot\boldsymbol{E} = \rho, \qquad \boldsymbol{\nabla}\cdot\boldsymbol{B} = 0, \tag{13}$$
$$\boldsymbol{\nabla}\times\boldsymbol{E} = -\partial_t\boldsymbol{B}, \qquad \boldsymbol{\nabla}\times\boldsymbol{B} = \boldsymbol{j} + \partial_t\boldsymbol{E}. \tag{14}$$
Introduce the complex three-component field
$$\boldsymbol{\psi} = \boldsymbol{B} - \mathrm{i}\boldsymbol{E}. \tag{15}$$
Find the effective Hamiltonian (which is a 3×3 operator matrix) and the right-hand side in
$$(\mathrm{i}\partial_t - \hat{H})\boldsymbol{\psi} = ? \tag{16}$$
Replace all spatial derivatives with the momentum operators $\hat{p}_x = -\mathrm{i}\partial_x$, $\hat{p}_y = -\mathrm{i}\partial_y$, and $\hat{p}_z = -\mathrm{i}\partial_z$ in $\hat{H}$.

4. Confirm that $\hat{H}$ is Hermitian with respect to the scalar product
$$\langle\boldsymbol{\psi}|\boldsymbol{\phi}\rangle = \int \mathrm{d}^3 r\, \boldsymbol{\psi}^*(\boldsymbol{r})\cdot\boldsymbol{\phi}(\boldsymbol{r}). \tag{17}$$
What boundary conditions must $\boldsymbol{\psi}, \boldsymbol{\phi}$ satisfy?

Solution 3

1. Call $v = \partial_t u$; then $\partial_t u = v$ and $\partial_t v = \partial_x^2 u$. Thus
$$\partial_t \psi_{1/2} = v \pm \mathrm{i}\partial_x^2 u = \frac{\psi_1 - \psi_2}{2\mathrm{i}} \pm \mathrm{i}\partial_x^2 \frac{\psi_1 + \psi_2}{2}$$
and we find that
$$\hat{H} = -\frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}\partial_x^2 + \frac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}.$$

2. The analogous reality condition is

$$\psi(x,t) = \sigma_x \psi^*(x,t), \qquad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

To show that the Schrödinger equations preserves it, we must show that if ψ satisfies Eq. (10), that then $\tilde{\psi}(x,t) = \sigma_x \psi^*(x,t)$ also satisfies Eq. (10). To wit

$$\begin{aligned} \mathrm{i}\sigma_z \partial_t \tilde{\psi} &= \mathrm{i}\sigma_z \partial_t \sigma_x \psi^* = -\sigma_x \mathrm{i}\sigma_z \partial_t \psi^* \\ &= \sigma_x \left(\mathrm{i}\sigma_z \partial_t \psi\right)^* = \sigma_x \hat{H}^* \psi^* = \sigma_x \hat{H}^* \sigma_x \tilde{\psi}, \end{aligned}$$

where we used the fact that $\sigma_x \sigma_z = -\sigma_z \sigma_x$ and $\sigma_x \sigma_x = I_{2\times 2}$. Now it's just a matter of multiplying the matrices to show that $\sigma_x \hat{H}^* \sigma_x = \hat{H}$ indeed holds.

3. After a little algebra, one readily finds that

$$\mathrm{i}\partial_t \boldsymbol{\psi} - \boldsymbol{\nabla} \times \boldsymbol{\psi} = \boldsymbol{j},$$

which can also be rewritten as

$$(\mathrm{i}\partial_t - \hat{H})\boldsymbol{\psi} = \boldsymbol{j},$$

where

$$\begin{aligned} \hat{H} &= \boldsymbol{L} \cdot \hat{\boldsymbol{p}} = L_x \hat{p}_x + L_y \hat{p}_y + L_z \hat{p}_z, \\ L_x &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -\mathrm{i} \\ 0 & \mathrm{i} & 0 \end{pmatrix}, \\ L_y &= \begin{pmatrix} 0 & 0 & \mathrm{i} \\ 0 & 0 & 0 \\ -\mathrm{i} & 0 & 0 \end{pmatrix}, \\ L_z &= \begin{pmatrix} 0 & -\mathrm{i} & 0 \\ \mathrm{i} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \end{aligned}$$

4. One immediately sees this from the fact that $\hat{p}_i^\dagger = \hat{p}_i$ and $L_i^\dagger = L_i$ are both Hermitian. In detail:

$$\begin{aligned} \left\langle \boldsymbol{\psi} \middle| \hat{H} \boldsymbol{\phi} \right\rangle &= \sum_i \int \mathrm{d}^3 r \, \boldsymbol{\psi}^\dagger L_i \hat{p}_i \boldsymbol{\phi} \\ &= -\sum_i \int \mathrm{d}^3 r \, \left(\hat{p}_i \boldsymbol{\psi}^\dagger\right) L_i \boldsymbol{\phi} + \sum_i \int \mathrm{d}^3 r \, \hat{p}_i \left(\boldsymbol{\psi}^\dagger L_i \boldsymbol{\phi}\right) \\ &= \sum_i \int \mathrm{d}^3 r \, \left(\hat{p}_i \boldsymbol{\psi}\right)^\dagger L_i \boldsymbol{\phi} + \sum_i \int_{r\to\infty} \mathrm{d}\boldsymbol{S} \cdot \hat{\boldsymbol{e}}_i (-\mathrm{i}\hbar) \boldsymbol{\psi}^\dagger L_i \boldsymbol{\phi} \\ &= \sum_i \int \mathrm{d}^3 r \, \left(L_i \hat{p}_i \boldsymbol{\psi}\right)^\dagger \boldsymbol{\phi} - \mathrm{i}\hbar \int_{r\to\infty} \mathrm{d}\boldsymbol{S} \cdot \boldsymbol{\psi}^\dagger \boldsymbol{L} \boldsymbol{\phi} = \left\langle \hat{H}\boldsymbol{\psi} \middle| \boldsymbol{\phi} \right\rangle + \text{boundary terms} \end{aligned}$$

$\boldsymbol{\psi}, \boldsymbol{\phi}$ have to decay at spatial infinity for the boundary terms to vanish.