Leo Radzihovsky, Fall 2015

PHYS 5250: Quantum Mechanics - I

Homework Set 2

Issued September 4, 2015
Due September 16, 2015

Reading Assignment: Shankar, Ch. 1, 4, 5; Sakurai, Ch. 1, 2.1-2.4; Schiff Ch. 2, 3

1. A wavefunction is generically a complex function and therefore can be written as $\psi(\mathbf{r},t) = |\psi|e^{i\phi}$, where its magnitude and phase are real functions. Using Schrodinger's equation, derive two equations satisfied by $|\psi|$ and $S \equiv \phi\hbar$, showing that one is a continuity equation, and the other reduces to Hamilton-Jacobi equation in $\hbar \to 0$ limit.

2. Consider Feynman's time evolution operator $\hat{U}(t)$, defined by $|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle$.
   (a) Using the formal operator expression for $\hat{U}_t$ show that it satisfies the Schrodinger's equation.
   (b) Using the explicit coordinate representation of $U_0(x, x'; t)$ for a free particle (derived in class), show that it satisfies the free Schrodinger's equation.
   (c) Derive the equation satisfied by the interaction-representation of this evolution operator, $\hat{U}_I(t) \equiv e^{\frac{i}{\hbar}\hat{H}_0 t}e^{-\frac{i}{\hbar}\hat{H}t}$, where $\hat{H} = \hat{H}_0 + \hat{V}$. By formally solving it, show that it is given by
   $$\hat{U}_I(t) = T_t\left[e^{-\frac{i}{\hbar}\int_0^t dt'\hat{V}_I(t')}\right],$$
   where T_t is the time-ordering operator that puts later times to the left of the earlier times and $\hat{V}_I(t) = e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{V}e^{\frac{-i}{\hbar}\hat{H}_0 t}$ is the potential in the interaction representation.

3. (Shankar 4.2.1) Consider the following explicit expressions for components of the angular momentum operator $\hat{\mathbf{L}}$ in the (so called) $L = 1$ representation:
   $$L_x = \frac{1}{2^{1/2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad L_y = \frac{1}{2^{1/2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad L_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \tag{1}$$
   (a) What are the possible values one can obtain if L_z is measured?

(b) Take the state in which $L_z = 1$. In this state, compute $\langle L_x \rangle$, $\langle L_x^2 \rangle$, and variance ΔL_x.

(c) Find the normalized eigenstates and the eigenvalues of L_x in the L_z basis.

(d) If the particle is in the state $L_z = -1$, and L_x is measured, what are the possible outcomes and their probabilities?

(e) Consider the state

$$|\psi\rangle = \frac{1}{2}\begin{pmatrix} 1 \\ 1 \\ 2^{1/2} \end{pmatrix} \tag{2}$$

in the L_z basis. If L_z^2 is measured in this state and a result $+1$ is obtained, what is the state after the measurement? How probable was this result? If L_z is measured immediately afterwards, what are the outcomes and respective probabilities?

(f) A particle is in a state for which the probabilities are $P(L_z = 1) = 1/4$, $P(L_z = 0) = 1/2$, and $P(L_z = -1) = 1/4$. Give an argument that the most general, normalized state with this property is

$$|\psi\rangle = \frac{e^{i\delta_1}}{2}|L_z = 1\rangle + \frac{e^{i\delta_2}}{2^{1/2}}|L_z = 0\rangle + \frac{e^{i\delta_3}}{2}|L_z = -1\rangle. \tag{3}$$

Compute $P(L_x = 0)$ in this state and thereby show that in contrast to an overall phase factor, *relative* phases δ_i are indeed physically observable.

4. Using the well-known expression for the orbital angular momentum, $\mathbf{L} = \mathbf{r} \times \mathbf{p}$ derive:

   (a) the Poisson bracket relation satisfied by its components, and

   (b) the commutation relation satisfied by its components,

   in the classical and quantum case, respectively, in the latter case understood as operators.

   Hint: Take advantage of the canonical Poisson bracket and commutation relations between components of $\mathbf{r}$ and $\mathbf{p}$.

5. Estimate the spectrum and the extent (along z) of the corresponding eigenstates of a bouncing ball using:

   (a) Bohr-Sommerfeld quantization,

   (b) Minimization of the energy, together with the uncertainty principle $p \approx n\hbar/z$

   Hint: Ignore any dissipation or ball's elastic energy.

6. Show that $\langle \psi | \hat{p} | \psi \rangle = 0$ for any state characterized by a *real* (as opposed to complex) wavefunction ψ.

7. Consider a *free* electron whose position at time $t = 0$ was measured to be exactly $x = x_0$.

   (a) (Up to a proportionality constant) what is $\psi(x, 0^+)$ right after ($t = 0^+$) this measurement? Sketch the amplitude of this state.

   (b) What is a measurement of $V(\hat{x})$ in this state, i.e., $\langle\psi(0^+)|V(\hat{x})|\psi(0^+)\rangle$ guaranteed to find?

   (c) Use the coordinate representation of the evolution operator $U(x, x'; t)$ to compute the wavefunction $\psi(x, t)$ at time t later.

   (d) Compute and sketch the corresponding $P(x, t)$ as function of x (for fixed t) and as function of t (for fixed x).

   Comment: Your last answer should perplex you in light of your answer to parts (a,b); What do you think the resolution is?

8. Consider a more physically realistic measurement, where after the measurement at $t = 0$ the *free* electron is localized into a region of size Δ with Gaussian probability, $P(x, 0) = (\pi\Delta^2)^{-\frac{1}{2}} e^{-x^2/\Delta^2}$ and also receives a kick of momentum p_0.

   (a) What is the corresponding wavefunction $\psi(x, 0)$?

   (b) Use the coordinate representation of the evolution operator $U(x, x'; t)$ to compute the wavefunction $\psi(x, t)$ at time t later.

   Comments/hints: (i) To simplify the algebra and to elucidate the physics, it is convenient to introduce a quantum "diffusion" length $a(t) = (\hbar t/m)^{1/2}$, (ii) You will have to take advantage of our Guassian-integral calculus, of which the most important result is: $\int_{-\infty}^{\infty} dx e^{hx - \frac{1}{2}ax^2} = \left(\frac{2\pi}{a}\right)^{\frac{1}{2}} e^{\frac{1}{2}a^{-1}h^2}$, that thankfully can be applied with impunity even for complex a and h (by a deformation of the contour in the complex plane, if you care, but don't need to know this).

   (c) Comment on the structure of this wavefunction, particularly the physical interpretation of the x and t dependence of its phase and amplitude, along the lines of: "I expected this answer because...".

   (d) Compute the corresponding $P(x, t)$.

   Comments/hint: (i) To simplify the algebra, it might be convenient to define a time-dependent length $\Delta(t) \equiv \Delta[1 + (a(t)/\Delta)^4]^{\frac{1}{2}}$. (ii) As complicated as intermediate expressions might appear, please be persistent with your algebra and expressions will simplify into something that makes sense.

   (e) Compute:

      i. $\langle\hat{x}\rangle \equiv \langle\psi(t)|\hat{x}|\psi(t)\rangle$
      ii. $\langle\hat{x}^2\rangle \equiv \langle\psi(t)|\hat{x}^2|\psi(t)\rangle$
      iii. $\langle\hat{p}\rangle \equiv \langle\psi(t)|\hat{p}|\psi(t)\rangle$

iv. $\langle \hat{p}^2 \rangle \equiv \langle \psi(t)|\hat{p}^2|\psi(t)\rangle$

v. Use above results to compute root-mean-squared quantum fluctuations of position $x_{rms}(t) \equiv \sqrt{\langle \hat{x}^2 \rangle - \langle \hat{x} \rangle^2}$ and momentum $p_{rms}(t) \equiv \sqrt{\langle \hat{p}^2 \rangle - \langle \hat{p} \rangle^2}$, and use your result to verify the Heisenberg uncertainty principle.

9. Demonstrate the following list of standard relations:

   (a) $[\hat{A}, \hat{B}\hat{C}] = [\hat{A}, \hat{B}]\hat{C} + \hat{B}[\hat{A}, \hat{C}]$,

   (b) $[\hat{p}, f(\hat{x})] = -i\hbar f'(\hat{x})$, comparing to the analogous Poisson bracket relation $\{p, f(x)\} = -f'(x)$.

   (c) $[e^{i\frac{\hat{p}}{\hbar}a}, \hat{x}] = ae^{i\frac{\hat{p}}{\hbar}a}$

   Use above commutation relation to demonstrate that $\hat{T}_a = e^{i\frac{\hat{p}}{\hbar}a}$ is a spatial translation operator by a, namely that $\hat{T}_a f(\hat{x})\hat{T}_a^\dagger = f(\hat{x} + a)$.

   Hint: You might want to take advantage of Taylor series definition of a function of an operator, and take advantage of coordinate representation of $\hat{p}$ and momentum representation of $\hat{x}$.

10. Show

    (a) using coordinate representation that the momentum, $\hat{p}$ is a Hermitian operator,

    (b) symmetrized product $\frac{1}{2}(\hat{p}\hat{x} + \hat{x}\hat{p})$ are Hermitian operators, while $\hat{p}\hat{x}$ is not.

    Hint: once (a) is demonstrated, (b) can be demonstrated in 1 line in representation-independent way.

11. Density matrix and entanglement entropy

    Consider a system consisting of two qubits ("quantum bit", each realized as any two-level system e.g., a double-well potential or a spin-1/2 or just two atomic levels, a basic element of a quantum computer) A and B, with each taking on two possible values, designated by, say 0 and 1. Take this 2-qubit computer to be in a pure

    (a) *unentangled*, i.e., product state

    $$|\psi_{AB}\rangle = \frac{1}{2}\left(|0\rangle + |1\rangle\right) \otimes \left(|0\rangle + |1\rangle\right).$$

    Construct the two-qubit density matrix $\hat{\rho}_{AB} = |\psi_{AB}\rangle\langle\psi_{AB}|$ for the whole system and extract its corresponding (4×4) matrix representation $\rho_{\sigma\sigma'}$ in this $|\sigma\rangle \otimes |\sigma'\rangle$ $(\sigma = 0, 1)$ basis, namely $\hat{\rho}_{AB} = \sum_{\sigma,\sigma'=0,1} \rho_{\sigma\sigma'} |\sigma\rangle \otimes |\sigma'\rangle\langle\sigma| \otimes \langle\sigma'|$

    i. Verify that this is indeed a density matrix for a pure state by showing $\mathrm{Tr}[\hat{\rho}_{AB}] = \mathrm{Tr}[\hat{\rho}_{AB}^2] = 1$

ii. Show that the von Neumann entropy of this state vanishes, i.e.,

$$S_{vN} = -\langle \ln \hat{\rho}_{AB} \rangle = -\mathrm{Tr}(\hat{\rho}_{AB} \ln \hat{\rho}_{AB}) = 0,$$

as it must for any pure state.
Hint: (i) You can do this by working directly with the matrix $\rho_{\sigma\sigma'}$ or more formally working in a representation-independent way. (ii) One way to define a function of an operator (e.g., $\ln \hat{O}$) is by its eigenvalues by going to its diagonal basis.

iii. Compute the reduced density (2×2) matrix

$$\hat{\rho}_A = \mathrm{Tr}_B \hat{\rho}_{AB} \equiv \sum_{\sigma_B} \langle \sigma_B | \hat{\rho}_{AB} | \sigma_B \rangle,$$

by tracing over the states of the B qubit, that describes the density matrix for the A qubit subsystem.

iv. Show that the *entanglement* entropy (von Neumann entropy of $\hat{\rho}_A$) for subsystem A, described by this reduced density matrix, $\hat{\rho}_A$ still vanishes, i.e.,

$$S_E = -\langle \ln \hat{\rho}_A \rangle_A = -\mathrm{Tr}_A(\hat{\rho}_A \ln \hat{\rho}_A) = 0,$$

demonstrating that the qubits A and B are not entangled, since $\hat{\rho}_{AB}$ was constructed from a *product* state.

(b) *entangled* "cat" state

$$|\psi_{AB}\rangle = \frac{1}{\sqrt{2}} \left(|0\rangle \otimes |0\rangle + |1\rangle \otimes |1\rangle \right).$$

Construct the two-qubit density matrix $\hat{\rho}_{AB} = |\psi_{AB}\rangle\langle\psi_{AB}|$ for the whole system and extract its corresponding (4×4) matrix representation $\rho_{\sigma\sigma'}$ in this $|\sigma\rangle \otimes |\sigma'\rangle$ $(\sigma = 0, 1)$ basis, namely $\hat{\rho}_{AB} = \sum_{\sigma,\sigma'=0,1} \rho_{\sigma\sigma'} |\sigma\rangle \otimes |\sigma'\rangle\langle\sigma| \otimes \langle\sigma'|$

i. Verify that this is indeed a density matrix for a pure state by showing $\mathrm{Tr}[\hat{\rho}_{AB}] = \mathrm{Tr}[\hat{\rho}_{AB}^2] = 1$

ii. Show that the von Neumann entropy of this state vanishes, i.e.,

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Hint: (i) You can do this by working directly with the matrix $\rho_{\sigma\sigma'}$ or more formally working in a representation-independent way. (ii) One way to define a function of an operator (e.g., $\ln \hat{O}$) is by its eigenvalues by going to its diagonal basis.

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$$\hat{\rho}_A = \mathrm{Tr}_B \hat{\rho}_{AB} \equiv \sum_{\sigma_B} \langle \sigma_B | \hat{\rho}_{AB} | \sigma_B \rangle,$$

by tracing over the states of the B qubit, that describes the density matrix for the A qubit subsystem.

iv. Show that the *entanglement* entropy (von Neumann entropy of $\hat{\rho}_A$) for subsystem A, described by this reduced density matrix, $\hat{\rho}_A$ is nonzero, i.e.,

$$S_E = -\langle \ln \hat{\rho}_A \rangle_A = -\mathrm{Tr}_A(\hat{\rho}_A \ln \hat{\rho}_A) = \ln 2,$$

demonstrating that the qubits A and B are *entangled*, since $\hat{\rho}_{AB}$ was constructed from a maximally *entangled* "cat" state.

Now you see how we generate mixed states in quantum mechanics, i.e., by having our system of interest entangle with the rest of the universe.