PHY 6645 Fall 2003 – Homework 6

Due by 5 p.m. on Friday, October 24. No credit will be available for homework submitted after 5 p.m. on Monday, October 27.

Answer questions 1–3. Please write neatly and include your name on the front page of your answers. You must also clearly identify all your collaborators on this assignment. To gain maximum credit you should explain your reasoning and show all working.

1. A quantum-mechanical system is represented by a two-dimensional vector space spanned by an orthonormal basis $|1\rangle$ and $|2\rangle$. The Hamiltonian is $H = \epsilon(-4|1\rangle\langle 1| + 4|2\rangle\langle 2| + 3|1\rangle\langle 2| + 3|2\rangle\langle 1|)$, where $\epsilon > 0$. The energy eigenvalues are denoted E_1 and E_2 $(E_1 < E_2)$, with corresponding eigenkets $|E_1\rangle$ and $|E_2\rangle$. We also consider another Hermitian operator Λ , which can be written $\Lambda = \lambda_0(|1\rangle\langle 2| + |2\rangle\langle 1|)$.

Note: This is the same system as appeared in Mid-Term Exam 1, Question 1. You may quote without proof any (correct) results from Mid-Term Exam 1.

Consider four initial states of this system, each described by its state operator $\rho(t=0)$:

- (a) $\rho(0) = 0.36 |E_1\rangle \langle E_1| + 0.64 |E_2\rangle \langle E_2|.$
- (b) $\rho(0) = 0.36|E_1\rangle\langle E_1| + 0.64|E_2\rangle\langle E_2| 0.48|E_1\rangle\langle E_2| 0.48|E_2\rangle\langle E_1|.$
- (c) $\rho(0) = 0.36|1\rangle\langle 1| + 0.64|2\rangle\langle 2|.$
- (d) $\rho(0) = 0.36|1\rangle\langle 1| + 0.64|E_2\rangle\langle E_2|.$

For each initial state, perform the following:

- i. Determine whether the initial state is pure or mixed. If it is pure, find the corresponding normalized state vector $|\psi\rangle$.
- ii. Find the eigenvalues p_i and eigenkets $|p_i\rangle$ of the initial state operator.
- iii. Calculate the state operator $\rho(t)$ for an arbitrary time $t \ge 0$.
- iv. Use $\rho(t)$ to calculate the expectation values of H and A at time $t \ge 0$.

2. In class, we considered the wave-function decomposition $\psi(\mathbf{r},t) = Ae^{iS/\hbar}$, where A and S are real functions of position \mathbf{r} and time t. The physical interpretation of A and S comes through the relations $\rho = |\psi|^2 = A^2$ and $\mathbf{j} = \rho \nabla S/m$. S for a quantum-mechanical particle moving in a potential $V(\mathbf{r})$ obeys the same equation of motion (the Hamilton-Jacobi equation) as Hamilton's principal function S for a classical particle moving in an effective potential $V_{\text{eff}}(\mathbf{r},t) = V(\mathbf{r}) + V_Q(\mathbf{r},t)$, where $V_Q(\mathbf{r},t) = -\hbar^2 \nabla^2 A/(2mA)$. The classical S is related to the momentum via $\mathbf{p} = \nabla S$. In any situation where V_Q can be neglected (usually, in the limit $\hbar \to 0$), the quantum-mechanical velocity field $\mathbf{v}(\mathbf{r},t) = \mathbf{v}S/m$ for a particle moving in the potential $V(\mathbf{r})$ follows the same equation as the velocity $\mathbf{p}(\mathbf{r},t)/m$ of a classical particle moving in the same potential. This provides an alternative definition of the classical limit from the one based on the equations of motion for expectation values (see Shankar Ch. 6).

Note that the wave-function decomposition is not unique: for a given A at some (\mathbf{r}, t) , S at the same (\mathbf{r}, t) is defined only to within additive integer multiples of Planck's constant $h = 2\pi\hbar$, while a change in the sign of A can be accommodated by an h/2 shift in S. However, the analysis of the Hamilton-Jacobi equation for S implicitly

assumes that A and S are differentiable in both space and time. Accordingly, it is important to choose the sign of A and the shift in S so that each function remains differentiable. This consideration will be come into play in some of the cases below.

- (a) For each of the following one-dimensional stationary-state problems, find A, S, V_Q , and V_{eff} :
 - i. $V(x) = 0, \ \psi(x,t) = C \exp[i(kx Et/\hbar)].$
 - ii. $V(x) = 0, \ \psi(x,t) = C\sin(kx)\exp(-iEt/\hbar).$
 - iii. $V(x) = m\omega^2 x^2/2$, $\psi(x,t) = CH_n(x/b) \exp[-(x^2/2b^2 + iEt/\hbar)]$.

In the above, C is a complex number, while m, k and ω are (as usual) positive, real quantities and E is the energy eigenvalue. In case (iii), $b = \sqrt{\hbar/m\omega}$, and $H_n(y)$ is the n'th Hermite polynomial.

- (b) For each of the cases (i)–(iii) above, re-express V_Q and V_{eff} so that any dependence on \hbar comes implicitly through E.
- (c) If $\psi_E(\mathbf{r}, t)$ is stationary, so is $\psi_E^*(\mathbf{r}, t)$. Therefore, all stationary states can be forced to have real time-independent wave functions, i.e., $\psi_E(\mathbf{r}, t) = \psi_E(\mathbf{r}) \exp(-iEt/\hbar)$, where $\psi_E(\mathbf{r})$ is real. Show that for any such stationary state, $V_{\text{eff}}(\mathbf{r}, t) = E$, implying that the quantum potential does not vanish as $\hbar \to 0$ [unless it happens that V(x) = E for all x].

For unbound cases in one dimension, where the stationary states are doubly degenerate, it is possible to construct traveling-wave solutions for which V_Q vanishes as $\hbar \to 0$. However, bound states are nondegenerate and are always described by a real wave function multiplied by $\exp(-iEt/\hbar)$. In such states, the quantum potential is never negligible, so the states are fundamentally nonclassical in the Hamilton-Jacobi sense.

- (d) Show that for a real, time-independent wave function $\psi(\mathbf{r})$, $\mathbf{j} = \mathbf{0}$ everywhere, and the expectation value of the momentum is $\langle \mathbf{P} \rangle = \mathbf{0}$. These observations cast light on the nonclassical nature of bound states. A classical particle always has a momentum of well-defined magnitude and direction. By contrast, a real, time-independent wave function is a standing wave formed by the superposition of traveling waves having momenta of the same magnitude but opposite direction. Thus, the ensemble described by this wave function has a vanishing velocity field and momentum expectation value. This is true even though any single measurement of \mathbf{v} or \mathbf{p} performed on a member of the quantum-mechanical ensemble would yield a nonzero result, similar to the classical case.
- 3. Consider a one-dimensional harmonic oscillator described by the Hamiltonian $H = P^2/2m + m\omega^2 X^2/2$. Let $|n\rangle$ be the *n*'th eigenket of the number operator (defined with the standard phase convention).
 - (a) Suppose that the oscillator is prepared in the state $|\psi(0)\rangle = (|0\rangle + |1\rangle + |2\rangle)/\sqrt{3}$. Find $|\psi(t)\rangle$, and calculate $\langle X \rangle$, $\langle X^2 \rangle$, $\langle P \rangle$, and $\langle P^2 \rangle$ at time t.
 - (b) Suppose that the oscillator is prepared in the state $\rho(0)\rangle = (|0\rangle\langle 0| + |1\rangle\langle 1| + |2\rangle\langle 2|)/3$. Find $\rho(t)$, and calculate $\langle X \rangle$, $\langle X^2 \rangle$, $\langle P \rangle$, and $\langle P^2 \rangle$ at time t.
 - (c) Working in the Heisenberg picture, calculate $d^n X/dt^n$ and $d^n P/dt^n$. Compare the equations of motion deduced from the n = 1 derivatives with the corresponding classical equations of motion.