PHYS 5250: Quantum Mechanics - I

Homework Set 5

Issued October 12, 2015 Due October 26, 2015

Reading Assignment: Shankar: Chs. 10, 11; Sakurai: Secs. 1.6, 1.7, Chs. 4, 6

1. (Repeated problem from an earlier homework) Using path integral formulation, derive a *free* particle time evolution operator in coordinate representation, $U_0(x, x'; t, 0)$. Rather than following shortcuts we discussed in class, please do this by explicitly evaluating N-1 gaussian integrals that arise in discretizing the path integral for U(x, x'; t, 0).

Hint:

The most direct route is to first demonstrate and then utilize the "closure" property of a propagator, namely to show that $U_0(x, x''; t, t'') = \int_{-\infty}^{\infty} dx' U_0(x, x'; t, t') U_0(x', x''; t', t'')$. To show this you will simply need to do a single gaussian integral, taking advantage of the calculus that we developed in class. There are other, less direct but technically simpler ways of doing it. Can you find one or two other ways of doing it?

- 2. Consider a Hamiltonian of two interacting particles $H = p_1^2/2m_1 + p_2^2/2m_2 + V(\mathbf{r}_1 \mathbf{r}_2)$ moving in 3d.
 - (a) Show that by performing a unitary transformation to the center of mass \mathbf{R}_{cm} , \mathbf{P}_{cm} and relative \mathbf{r}, \mathbf{p} coordinates, the given Hamiltonian decouples into $H = H_{cm} + H_{rel}$, where $H_{cm} = P_{cm}^2/2M$ and $H_{rel} = p^2/2\mu + V(\mathbf{r})$ are the center of mass and relative coordinate Hamiltonians, M and μ are the total and reduced masses, respectively, whose expressions in terms of m_1 and m_2 you should derive.
 - (b) Verify that this transformation is indeed unitary, i.e., that the commutation relations between \mathbf{R}_{cm} and \mathbf{P}_{cm} , and between \mathbf{r} and \mathbf{p} remain canonical. Do this by finding the relations between old and new variables and then computing the commutation relations between all *new* variables ($[R_{cm}^i, p^j], [R_{cm}^i, P_{cm}^j]$, etc.) using commutation relations for the old variables.
 - (c) Take advantage of the above separability of H to find the \mathbf{R}_{cm} dependence of the eigenstates of H, and derive the effective Schrodinger equation satisfied by the part of the wavefunction that only depends on the relative coordinate \mathbf{r} .

(d) Considering a physical case in which $V(\mathbf{r}_1 - \mathbf{r}_2) = V(|\mathbf{r}_1 - \mathbf{r}_2|)$ (i.e., that the interaction is rotationally invariant, depending only on the distance between the two particles), show that the Schrodinger equation for $\psi_{rel}(\mathbf{r})$ can be further separated in a spherical coordinate system by reducing to three independent eigenvalue differential equations for the radial, polar and azimuthal parts, respectively, dependent on r, θ , and ϕ .

Hint: Solutions to the angular components are the spherical harmonics $Y_{\ell m}(\theta, \phi) = \Theta_{\ell}^{m}(\theta)\Phi_{m}(\phi)$. You do not need to find the $\Theta_{\ell}^{m}(\theta)$, only the equation satisfied by it. Please do find the solution $\Phi_{m}(\phi)$.

3. When an energy measurement is made on a system of three spinless *bosons* in a box, the n values for each particle obtained were 3, 3, and 4. Write down a symmetrized, normalized state vector.

Hint: no real calculations are required.

- 4. Imagine a situation in which there are three particles and only three states a, b, and c available to them. What is the total number of allowed, distinct configurations for this system if the particles are:
 - (a) labeled, i.e., distinguishable
 - (b) indistinguishable bosons
 - (c) indistinguishable fermions

Hint: no serious calculations, only counting is required.

5. Bloch theorem and discrete translational invariance

Consider the quantum mechanics of noninteracting electrons in a periodic potential with a period a, or example, physically due to positive ions arranged in a periodic arrangement of a crystalline solid. This problem is at the very heart of much of modern solid-state physics.

- (a) Show explicitly that the corresponding Hamiltonian commutes with a translation operator \hat{T}_{ϵ} only for translations that are a multiple of a, i.e., $\epsilon = na$, $n \in \mathbb{Z}$.
- (b) Use the above result together with the observation that \hat{T}_a is a unitary operator to clearly argue that the eigenstates of H are (the so-called) Bloch states, given by $\psi_{k,n}(x) = e^{ikx}u_{k,n}(x)$, where k is a continuous (for an infinite system) quantum number limited to a finite range (called 1st Brillouin zone) that can be taken to be $0 < k < 2\pi/a$ and $u_{k,n}(x)$ is periodic part of the wavefunction with period a, labeled by k and another discrete quantum number $n \in \mathbb{Z}$).

Hint: Think about what the general form of a unitary operator is and the form of its eigenvalues. Although it is not necessary, it is helpful to recall what the form of the translation operator \hat{T}_a is, expressed in terms of the momentum operator \hat{p} .

- (c) Derive an effective Schrödinger equation satisfied by $u_{k,n}(x)$.
- (d) Show that the energy eigenvalues $E_n(k)$ are periodic in k with period $2\pi/a$.

Note that although the eigenfunctions are *not* periodic with period a, as expected on physical grounds, the probability density $P_{k,n}(x) = |\psi_{k,n}(x)|^2$ of finding a particle at positive x is periodic. This is not different from the special case of constant V(x) (e.g., 0), where the eigenfunctions are plane waves e^{ikx} that are *less* symmetric (i.e., not translationally invariant) than the Hamiltonian.

- 6. Compute the ground state energy of a system of N identical particles confined to a single infinite square-well potential of width L, when the particles are
 - (a) Bosons
 - (b) Fermions

Hint:

For bosons there are nearly no calculation. For fermions, to obtain the final answer you should find it useful to replace a sum by an integral valid for large N and L. Note that the answer for bosons is extensive while for fermions is "super-extensive", i.e., scaling with the number of particles is much faster than the total number of particles in the system.

7. Two identical particles of mass m are in a one-dimensional box of length L (infinite square-well potential). Energy measurement of the system yields the value $E_{sys} = \hbar^2 \pi^2 / (mL^2)$. Write down the eigenstate of the system. Repeat for $E_{sys} = 5\hbar^2 \pi^2 / (mL^2)$ for the case of bosons and fermions. Consider only orbital degrees of freedom, i.e., ignore spin.

Hint: There are nearly no calculations required. In the second case, there are two possible eigenstates.

- 8. Please think about (but do not have to do) Shankar's problems 10.3.5.
- 9. Consider a composite object such as the hydrogen atom. Will it behave as a boson or fermion? Using permutation operator and definition of quantum statistics, argue in general that objects containing an even/odd number of fermions will behave as bosons/fermions.
- 10. Consider a harmonic interaction $V(x_1 x_2) = \frac{1}{2}k(x_1 x_2)^2$ between two particles 1 and 2 in states $|a\rangle$ and $|b\rangle$. Compute the interaction energy $\langle V \rangle = \langle ab|V|ab \rangle$ for
 - (a) distinguishable particles
 - (b) indistinguishable bosons
 - (c) indistinguishable fermions

showing that the interaction energy between two bosons (fermions) is lower (higher) than two distinguishable particles.