Leo Radzihovsky, Fall 2015

PHYS 5250: Quantum Mechanics - I

Homework Set 4

Issued September 28, 2015
Due October 12, 2015

Reading Assignment: Shankar, Chs. 7, 8, 9, 21.1; Sakurai: 1.6, 2.1-2.6

1. Harmonic Oscillator

   (a) Verify explicitly in coordinate representation that 2nd and 0th eigenfunctions of a harmonic oscillator are orthogonal.

   (b) Use creation/annihilation operator algebra $[\hat{a}, \hat{a}^\dagger] = 1$ and the corresponding number eigenstates $|n\rangle$ to demonstrate explicitly the orthonormality of these states, i.e., $\langle n|m\rangle = \delta_{n,m}$.

   (c) Consider a particle in a potential $V(x) = \frac{1}{2}m\omega_0^2 x^2$, for $x > 0$ and $V(x) = \infty$ for $x \leq 0$. Find the spectrum and eigenfunctions.

   Hint: This problem should not require you to do any new computations, just a bit of thinking.

   (d) Find eigenfunctions and spectrum for a particle in a potential $V(x) = \frac{1}{2}m\omega_0^2(x^2 - 2cx)$.

   Hint: This problem should not require you to do too many new computations, just a bit of thinking.

   (e) Using the representation of x and p in terms of the creation and annihilation operators $a^\dagger$ and a, compute the following expectation values:

      i. $\langle n|x|n\rangle$
      ii. $\langle n|p|n\rangle$
      iii. $\langle n|x^2|n\rangle$
      iv. $\langle n|p^2|n\rangle$
      v. $\Delta x_{rms}\Delta p_{rms} = \sqrt{\langle n|(x - \langle x\rangle)^2|n\rangle}\sqrt{\langle n|(p - \langle p\rangle)^2|n\rangle}$, where Δx_{rms} and Δp_{rms} are root-mean-squared (rms) deviations of x and p from their average values.

   (f) Show that $\langle n|x^4|n\rangle = \frac{x_0^4}{4}(3 + 6n(n+1))$, where $x_0 = \sqrt{\hbar/m\omega_0}$ is the quantum oscillator length.

(g) Compute $\langle n|x^2|n\rangle$ directly in coordinate representation using a generating function for Hermite polynomials, similarly to the way we computed normalization factors in class. Compare to your answer with the above one where you used a and $a^\dagger$ representation.

(h) At time $t = 0$ a particle in a harmonic oscillator potential starts out in a state $|\psi(0)\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$. Find:

   i. $|\psi(t)\rangle$,

   ii. $\langle x(0)\rangle = \langle\psi(0)|x|\psi(0)\rangle$, $\langle p(0)\rangle$, $\langle x(t)\rangle$, $\langle p(t)\rangle$,

   iii. $\langle\dot{x}(t)\rangle$ and $\langle\dot{p}(t)\rangle$ using Ehrenfest's theorem and solve for $\langle x(t)\rangle$ and $\langle p(t)\rangle$ and compare with part (ii).

2. Coupled Harmonic Oscillators

Consider two particles characterized by a familiar Hamiltonian $H = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + \frac{1}{2}m\omega_0^2(x_1^2 + x_2^2 + (x_1 - x_2)^2)$.

(a) Find the spectrum and eigenstates of this Hamiltonian by first going to normal modes of vibration, y_1 and y_2 that decouple it into two independent harmonic oscillators (with different frequencies) and then solving each by using two types of annihilation and creation operators, $b_{1,2}$ and $b_{1,2}^\dagger$ that correspond to $y_{1,2}$.

(b) Compute the expectation value of x_1^2 in the ground state of this coupled harmonic oscillator system.

3. Baker-Campbell-Hausdorff Formula

Derive the Baker-Campbell-Hausdorff formula $e^A e^B = e^{A+B+\frac{1}{2}[A,B]}$ for the simplest case where the two operators A and B have a commutator $[A, B]$ that commutes with A and B, i.e., is a c-number.

Do this in two ways:

(a) First (only suggestive), by looking at the Taylor expansion in A and B of the two sides of the equation, verifying the equality at least to quadratic order in A and B.

(b) Second by considering instead operators e^{At}, e^{Bt} and deriving and solving a simple (first order in t) differential equation for $e^{At}e^{Bt}$.

Hint: Consider differentiating this product with respect to t, and then follow your nose.

4. Coherent States

Using the (non-normalized) representation of a coherent state $|z\rangle = e^{za^\dagger}|0\rangle$ show:

(a) $a|z\rangle = z|z\rangle$,

(b) $\langle z_1|z_2\rangle = e^{z_1^* z_2}$,

Hint: You can use Baker-Campbell-Hausdorff formual twice

(c) that the evolution operator for a harmonic oscillator in coherents state basis is given by $U(z, z'; t) = exp[z^* z' e^{-i\omega_0 t}]$,

(d) completeness relation $1 = \int_{-\infty}^{\infty} \frac{dxdy}{\pi} e^{-|z|^2} |z\rangle\langle z|$.

Hint: Since you already know the completeness relation for Fock states $|n\rangle$, you might find it useful for proving above completeness relation by reducing it to that of $|n\rangle$ states.

(e) that the wave function of a coherent state is given by $\psi_z(x) \equiv \langle x|z\rangle = \frac{1}{\pi^{1/4} x_0^{1/2}} e^{-z^2/2 - x^2/2x_0^2 + 2^{1/2} zx/x_0}$.

Hint: (i) Again, you might find the relation between the coherent states $|z\rangle$ and Fock states $|n\rangle$ as well as the generating function for Hermite polynomials useful. (ii) Alternatively, you might want to use the defining equation of a coherent state $a|z\rangle = z|z\rangle$, written in coordinate representation, and solving it in the same way that in class we found the wave function for the ground state $\psi_0(x) = \langle x|0\rangle$ (which is a special coherent state) of harmonic oscillator.

If you can, please solve this last problem using both (i) and (ii) approaches described in the Hint.

(f) Notice that for the normalized coherent state $|z\rangle = e^{-\frac{1}{2}|z|^2} e^{za^\dagger}|0\rangle$ above general coherent wavefunction, $\psi_z(x)$ reduces to a shifted Gaussian wavepacket from homework 3, problem 6, $\psi_z(x) \equiv \psi(x, 0) = \left(\frac{1}{\pi x_0^2}\right)^{\frac{1}{4}} e^{-(x-\sqrt{2}z)^2/2x_0^2}$, where $z = c/\sqrt{2}$ is real. Use this fact and the evolution operator $U(z, z'; t)$ found above to compute $\psi(x, t)$, thereby verifying the result from homework 3.

5. Path Integrals

Compute a time evolution operator $U(x_f, x_i; t_f)$ using its path integral representation for a particle in a potential $V(x)$:

(a) $V(x) = 0$, free particle

i. Using explicit Gaussian form of the evolution operator for a free particle $U_0(x_f, x_i; t_f, t_i)$ first demonstrate the closure relation

$$U(x_3, x_1; t_3, t_1) = \int_{-\infty}^{\infty} dx_2 U(x_3, x_2; t_3, t_2) U(x_2, x_1; t_2, t_1).$$

ii. Apply above (single Gaussian integration) result to the computation of the path integral (N infinitesimal Gaussian integrals) for a free porticle to compute its evolution operator.

Guide: (i) write down the coordinate path integral for a free particle in its explicit discrete form (from class lectures), with the infinitesimal "ϵ" normalization prefactors. (ii) to simplify the algebra, change variables for each x_n

integration to make all $N-1$ integrals dimensionless. (iii) use closure property of Gaussian integrals to evaluate recursively all $N-1$ integrals; in the process you will demonstrate the following identity of Gaussian integrals

$$\int_{-\infty}^{\infty} dy_{N-1}dy_{N-2}\dots dy_1 e^{i\sum_{k=1}^{N}(y_k-y_{k-1})^2} = \left[\frac{(i\pi)^{N-1}}{N}\right]^{1/2} e^{i(y_N-y_0)^2/N}.$$

With all this you have finally explicitly derived both the exponential $e^{iS[x_c]/\hbar}$ and the $A(t)$ prefactor of the free particle evolution operator.

(b) $V(x) = -fx$, corresponding to a particle under a constant force f,

(c) $V(x) = \frac{1}{2}m\omega_0^2 x^2$, corresponding to a particle in a harmonic potential.

Suggestions:

i. Expand the path integration in $y(t)$ about a classical path $x_c(t)$, thereby obtaining most of the answer from the classical action $S[x_c(t)]$, with $x_c(t)$ that satisfies boundary conditions $x_c(0) = x_i$, $x_c(t_f) = x_f$. Note that for the harmonic oscillator you have already solved this latter part of the problem on homework 1, problem 2.

ii. The remaining path integration contribution (which you should find only depends on t_f but not on $x_{i,f}$) is a notoriously tricky problem.
For a particle under force (a) you should not have to do any computation as it should reduce to a path integral that we have already computed in class.
For a particle in the harmonic potential (b), some additional computations are necessary:

A. In the remaining part of the path integral over $y(t)$, make a change of variables (that is linear and therefore does not introduce any complicated Jacobian, J) from $y(t)$ to the Fourier series representation variable $\tilde{y}(\omega_n)$, using $y(t) = \sum_{n=1}^{\infty}\tilde{y}(\omega_n)\sin(\omega_n t)$, where ω_n is a discrete set of frequencies ($n \in \mathcal{Z}$), chosen so that $y(t)$ satisfies appropriate boundary conditions that you should be able to deduce from those on $x(t)$ and $x_c(t)$. This nicely decouples the path integral into N ($\to \infty$) *independent* Gaussian integrals over $\tilde{y}(\omega_n)$ (in contrast to working with $x(t_i)$ where nearest time variables $x(t_i)$ and $x(t_{i\pm1})$ are coupled).

B. Show that this remaining product of independent Gaussian integrals gives $c\prod_{n=1}^{\infty}\left(1-\omega_0^2/\omega_n^2\right)^{-1/2}$, with the final infinite product series computable once you have determined ω_n and using an identity
$\prod_{n=1}^{\infty}\left(1-a^2/n^2\right) = \sin(\pi a)/\pi a$.
The unknown prefactor product of constant c and the Jacobian J (associated with transformation from $y(t)$ to $\tilde{y}(\omega_n)$) that are independent of ω_0, x_f, x_t (and are easiest to not compute until the end) can then be determined by requiring that the final answer for $U(x_f, x_i; t_f)$ reduces to that of a free particle in the limit $\omega_0 \to 0$.

(d) For an initial wavepacket state $\psi(x,0) = \left(\frac{1}{\pi x_0^2}\right)^{\frac{1}{4}} e^{-(x-c)^2/2x_0^2}$ from homework 3, problem 6, derive its form $\psi(x,t)$ at a later time t now using the coordinate representation of the evolution operator for the harmonic oscillator that you derived above.

(e) (Bonus 10 points) Recall that the evolution operator can be expressed in terms of the eigenstates of the Hamiltonian

$$U(x,x';t) = \sum_n \psi_n(x)\psi_n^*(x')e^{-iE_nt/\hbar}.$$

Use it to extract the spectrum and eigenfunctions of the harmonic oscillator.

Hints:

i. Set $x = x' = 0$ inside

$$U(x,x';t) = \left(\frac{m\omega}{2\pi i\hbar \sin\omega t}\right)^{1/2} e^{\frac{im\omega}{2\hbar\sin\omega t}\left[(x^2+x'^2)\cos\omega t - 2xx'\right]},$$

and expand both sides in harmonics in time, $e^{-in\omega t}$. You should find that $E_n = \frac{1}{2}\hbar\omega, \frac{5}{2}\hbar\omega, \frac{9}{2}\hbar\omega, \ldots,$ *etc.* Why are you missing the energy levels in between?

ii. Now extract the eigenfunctions e.g., for $n = 0, 1$ by setting $x = x'$, again expanding in powers of $e^{i\omega t}$ and identifying the coefficients with $|\psi_n(x)|^2$.