943 QUANTUM MECHANICS - Homework #2. Due: Friday, February 20, 2004.

1. First, a warm-up problem. Consider a one-dimensional quantum particle with a gaussian wave function

$$\Psi(x) \;=\; C\;\exp(a\,x^2 + b\,x)\;, \tag{1}$$

where a, b and C are complex numbers. We will limit ourselves to the case $\mathrm{Re}\,a < 0$.

   (a) Calculate the norm $\int dx|\Psi(x)|^2$ of this wave function.

   (b) Calculate the momentum-space wave function $\tilde{\Psi}(p)$ and show that it also has a gaussian form

$$\tilde{\Psi}(p) \;=\; \tilde{C}\;\exp(\tilde{a}\,p^2 + \tilde{b}\,p)\;. \tag{2}$$

   (c) Verify that the momentum-space and the coordinate-space wave functions have the same norm.

   (d) Calculate the expectation values $\langle x\rangle$, $\langle p\rangle$ and the uncertainties Δx and Δp. Show that for any gaussian wave function, $\Delta x \cdot \Delta p \geq \hbar/2$ and that the equality is achieved whenever a is real.

2. This problem is about commutators. The commutator of two linear operators $\hat{A}$ and $\hat{B}$ is the operator $[\hat{A},\hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}$. Two properties of the commutator are obvious: It is antisymmetric, *i.e.* $[\hat{A},\hat{B}] = -[\hat{B},\hat{A}]$, and it is linear with respect to both $\hat{A}$ and $\hat{B}$. Prove the less-obvious properties of the commutator:

   (a) The Leibniz rules: $[\hat{A}\hat{B},\hat{C}] = \hat{A}[\hat{B},\hat{C}]+[\hat{A},\hat{C}]\hat{B}$ and $[\hat{A},\hat{B}\hat{C}] = [\hat{A},\hat{B}]\hat{C}+\hat{B}[\hat{A},\hat{C}]$;

   (b) $[\hat{A}\hat{B},\hat{C}\hat{D}] = \hat{A}[\hat{B},\hat{C}]\hat{D} + \hat{C}[\hat{A},\hat{D}]\hat{B} + \hat{C}\hat{A}[\hat{B},\hat{D}] + [\hat{A},\hat{C}]\hat{B}\hat{D}$
   (Hint: Use Leibniz twice.);

   (c) And the Jacobi identity:
   $[\hat{A},[\hat{B},\hat{C}]] + [\hat{B},[\hat{C},\hat{A}]] + [\hat{C},[\hat{A},\hat{B}]] = 0.$

3. This problem is about classical Poisson brackets. In classical mechanics, the Poisson bracket of two functions $A(q,p)$ and $B(q,p)$ of coordinates (q) and momenta (p) is defined as

$$[\![A,B]\!]_{\mathcal{P}} \;\equiv\; \sum_s \left(\frac{\partial A}{\partial q_s}\frac{\partial B}{\partial p_s} - \frac{\partial B}{\partial q_s}\frac{\partial A}{\partial p_s}\right)\;. \tag{3}$$

The algebra of the classical Poisson brackets is very similar to the algebra of the quantum-mechanical commutator. It is clear from the definition that $[\![A,B]\!]_{\mathcal{P}}$ is linear in both A and B and antisymmetric *i.e.* $[\![A,B]\!]_{\mathcal{P}} = -[\![B,A]\!]_{\mathcal{P}}$, just like the commutator. Prove the less-obvious properties of the Poisson bracket:

   (a) The classical Leibniz rules: $[\![AB,C]\!]_{\mathcal{P}} = A[\![B,C]\!]_{\mathcal{P}} + [\![A,C]\!]_{\mathcal{P}}B$
   and $[\![A,BC]\!]_{\mathcal{P}} = [\![A,B]\!]_{\mathcal{P}}C + B[\![A,C]\!]_{\mathcal{P}}$;

   (b) $[\![AB,CD]\!]_{\mathcal{P}} = A[\![B,C]\!]_{\mathcal{P}}D + C[\![A,D]\!]_{\mathcal{P}}B + CA[\![B,D]\!]_{\mathcal{P}} + [\![A,C]\!]_{\mathcal{P}}BD$;

(c) And the classical Jacobi identity:
$[\![A,[\![B,C]\!]_{\mathcal{P}}]\!]_{\mathcal{P}} + [\![B,[\![C,A]\!]_{\mathcal{P}}]\!]_{\mathcal{P}} + [\![C,[\![A,B]\!]_{\mathcal{P}}]\!]_{\mathcal{P}} = 0.$

4. Now consider extending classical Poisson brackets to quantum mechanics. That is, define a quantum bracket $[\![\hat{A},\hat{B}]\!]$ of operators such that whenever classically $A = [\![B,C]\!]_{\mathcal{P}}$, their quantum counterparts should obey $\hat{A} \approx [\![\hat{B},\hat{C}]\!]$. Quantum brackets should retain as many algebraic properties of the classical Poisson bracket as possible. So we will assume that $[\![\hat{A},\hat{B}]\!]$ is linear in both $\hat{A}$ and $\hat{B}$ and obeys the Leibniz rules: $[\![\hat{A}\hat{B},\hat{C}]\!] = \hat{A}[\![\hat{B},\hat{C}]\!] + [\![\hat{A},\hat{C}]\!]\hat{B}$ and $[\![\hat{A},\hat{B}\hat{C}]\!] = [\![\hat{A},\hat{B}]\!]\hat{C} + \hat{B}[\![\hat{A},\hat{C}]\!]$.

(a) Show that consistency of the two Leibniz rules requires that for any four operators, $\hat{A}$, $\hat{B}$, $\hat{C}$ and $\hat{D}$,

$$\left(\hat{A}\hat{B} - \hat{B}\hat{A}\right)\cdot[\![\hat{C},\hat{D}]\!] \;=\; [\![\hat{A},\hat{B}]\!]\cdot\left(\hat{C}\hat{D} - \hat{D}\hat{C}\right)\,. \tag{4}$$

(Hint: use both Leibniz rules to compute $[\![\hat{A}\hat{C},\hat{B}\hat{D}]\!]$. There are two ways to do this and the two results must be equal.)

(b) Use eq. (4) to show that

$$[\![\hat{A},\hat{B}]\!] \;=\; \frac{1}{i\hbar}[\hat{A},\hat{B}] \tag{5}$$

where $\hbar$ is a universal constant. Put another way, there is only one kind of quantum bracket, the commutator $[\hat{A},\hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}$.

5. The same infinite-dimensional Hilbert space can have both discrete and continuous bases. For example, the Hilbert space of a quantum particle moving in one space dimension has a continuous *position* basis $\{|x\rangle\}$ and an equally continuous *momentum* basis $\{|p\rangle\}$. However, it also may have discrete bases. The purpose of this problem is to explicitly construct a discrete basis $\{|n\rangle\}$ $(n = 0, 1, \ldots)$ for this Hilbert space.

(a) The most common way to construct a basis of a Hilbert space involves eigenstates of some hermitian operator. For example, consider the Hamiltonian operator of a one-dimensional harmonic oscillator:

$$\hat{H} \;=\; \frac{1}{2M}\hat{P}^2 \;+\; \frac{M\omega^2}{2}\hat{X}^2\,. \tag{6}$$

i. Write down the eigenstate equation $\hat{H}\,|\Psi\rangle = E\,|\Psi\rangle$ in the coordinate representation (*i.e.*, in terms of $\Psi(x)$) and show that it has an eigenfunction of a gaussian form $\Psi(x) = \alpha^{1/2}\pi^{-1/4}\exp(-\alpha^2x^2/2)$. Compute the value of α for which this is indeed an eigenfunction and the corresponding eigenvalue E_0.

ii. Prove by induction the following lemma:

$$f^{(n+2)}(\xi) \;+\; 2\xi f^{(n+1)}(\xi) \;=\; -2(n+1)f^{(n)}(\xi)\,, \tag{7}$$

where $f^{(n)}(\xi) \equiv d^n\exp(-\xi^2)/d\xi^n$.

iii. Hermite polynomials $H_n(\xi)$, $n = 0, 1, 2, \ldots$ are defined via the generating function

$$H_n(\xi) \;=\; (-1)^n \exp(\xi^2) \, \frac{d^n \exp(-\xi^2)}{d\xi^n} \;. \tag{8}$$

H_n is a polynomial of order n and can be constructed recursively via $H_0(\xi) = 1$, $H_{n+1}(\xi) \;=\; 2\xi H^n(\xi) \;-\; H_n'(\xi)$.
Show that each of the wave functions $\Psi_n(x) = C_n H_n(\alpha x) \Psi_0(x)$ (C_n is a constant) is an eigenfunction of $\hat{H}$ and compute the corresponding eigenvalue E_n. (Hint: Reexpress Ψ_n in terms of $f^{(n)}$ and use the lemma, eq. (7).)

(b) Eigenstates of any hermitian operator that correspond to different eigenvalues are guaranteed to be orthogonal to each other (this is a theorem we proved in class).

i. Verify that the quantum states $|n\rangle$ described by the wave functions $\Psi_n(x)$ are indeed orthogonal to each other:

$$\langle m|n\rangle \;=\; \int dx \Psi_n^*(x) \Psi_m(x) \;=\; 0 \qquad n \neq m \;. \tag{9}$$

(Hint: Use eq. (8) and the fact that H_n is a polynomial of degree n (and hence $d^m H_n / d\xi^m = 0$ for $m > n$).)

ii. Show that the states $|n\rangle$ are normalized, *i.e.* $\langle n|n\rangle = 1$, provided that we set $C_n = (2^n n!)^{-1/2}$.
In other words, the quantum states $|n\rangle$, $n = 0, 1, \ldots$ form an *orthonormal* set:

$$\langle m|n\rangle \;=\; \int dx \Psi_n^*(x) \Psi_m(x) \;=\; \delta_{n,m} \qquad n, m = 0, 1, 2, 3, \ldots \;. \tag{10}$$

(c) As discussed in class, an infinite orthonormal set of vectors in a Hilbert space $\mathcal{H}$ does not necessarily make a complete basis. The purpose of this problem is to verify that the set $\{|n\rangle\}$ constructed in the first part of this problem is indeed complete, that is, that *any* vector of $\mathcal{H}$ is a linear combination of the $|n\rangle$.

i. Prove another lemma:

$$\Psi_n(x) \;=\; \frac{1}{2\pi^{3/4}\sqrt{\alpha}} \times \frac{\exp(+\frac{1}{2}\alpha^2 x^2)}{\sqrt{2^n n!}(i\alpha)^n} \int_{-\infty}^{+\infty} dk k^n \exp(ixk - \frac{k^2}{4\alpha^2}) \;. \tag{11}$$

ii. Use the lemma, eq. (11), to show that

$$\sum_{n=0}^{\infty} \Psi_n^*(x') \Psi_n(x'') \;=\; \delta(x' - x'') \;. \tag{12}$$

(Hint: Use eq. (11) for both $\Psi_n^*(x')$ and $\Psi_n(x'')$ and sum the series before doing the integrals. Then combine all the exponential factors together and integrate over k'; the remaining integral over k'' should be familiar.

iii. Finally, show that the formula, eq. (12), implies that for *any* wavefunction $\Phi(x)$,

$$\sum_n \langle n|\Phi\rangle \Psi_n(x) \;=\; \Phi(x) \tag{13}$$

and hence for *any* vector $|\Phi\rangle \in \mathcal{H}$,

$$\sum_n |n\rangle \langle n|\Phi\rangle \;=\; |\Phi\rangle \;. \tag{14}$$

In other words, eq. (12) implies that the set $\{|n\rangle\}$ (for $n = 0, 1, \ldots$) is a *complete basis* of the Hilbert space.