FI 001 – Mecânica Quântica I – Lista 2

P.01. P.8.2, P.8.4, and P.8.6, Messiah:

a) Consider a quantum system possessing a classical analogue in one dimension. Derive from the commutation relation $[q, p] = i\hbar$ that the spectrum of p is entirely non-degenerate and continuous, and extends from $-\infty$ to $+\infty$. The suitably normalized eigenvectors of p form a complete orthonormal system in $\mathcal{E}$. Show that with a suitable choice of the phases of the vectors $|p'\rangle$ of this system, the action of the unitary operator $\exp(i\omega q/\hbar)$ (ω an arbitrary constant) on these vectors yields

$$\exp(i\omega q/\hbar)|p'\rangle = |p' + \omega\rangle,$$

and that the operator q has as its matrix element:

$$\langle p'|q|p''\rangle = i\hbar\delta'(p' - p'').$$

Solve the eigenvalue problem of q in this representation.

b) Show that the operator $B(t)$ defined by the expression

$$B(t) = e^{iAt} B_0 e^{-iAt},$$

where A and B_0 are operators independent of t, is a solution of the integral equation

$$B(t) = B_0 + i \left[A, \int_0^t B(\tau) d\tau \right].$$

Solve the equation above by iteration and obtains the expansion of $B(t)$ in a power series of t. From this solution, derive the identity

$$e^{iA} B e^{-iA} = B + i[A, B] + \frac{i^2}{2!}[A, [A, B]] + \dots.$$

c) Show that, if the operator $U(t)$ is unitary, then the operator

$$H(t) = i\hbar \frac{dU}{dt} U^\dagger$$

is necessarily Hermitean. Show that, if the operator $U(t)$ satisfies the equation

$$i\hbar \frac{d}{dt} U(t) = HU,$$

where H is a Hermitean operator possibly depending upon t, then $U^\dagger U$ is independent of t. Show that the operator $UU^\dagger$ is a solution of the equation

$$i\hbar \frac{d}{dt} UU^\dagger = [H, UU^\dagger].$$

From the above equation, show that, if U is unitary at t_0, it remains so for all values of t.

P.02. P.8.7 and P.8.8, Messiah and Ex.15.23, Merzbacher:

a) Let $|1\rangle, |2\rangle, \ldots, |M\rangle$ be a sequence of vectors of norm 1 but not necessarily orthogonal and consider the following density operator

$$\rho = \frac{1}{M} \sum_{i=1}^{M} |i\rangle\langle i|.$$

Show that
(1) if these M vectors are equal to within a phase, then ρ represents a pure state;
(2) if ρ represents a pure state, then these M vectors are equal to within a phase.

b) Show that for the operator ρ, Hermitean definite of trace 1, to represent a pure state, it is necessary and sufficient that $\mathrm{Tr}\rho^2 = 1$.

c) Prove the inequalities (15.120):

$$0 \leq \mathrm{Tr}\rho^2 \leq (\mathrm{Tr}\rho)^2 = 1, \qquad \rho_{ii}\rho_{jj} \geq |\rho_{ij}|^2.$$

Hint: Trace inequalities are most easily proved by using the eigenstates of the density operator as a basis. For the second inequality, maximize the probability of finding the system in a superposition state

$$|\psi\rangle = c_i|\psi_i\rangle + c_j|\psi_j\rangle.$$

P.03. Ex.14.9 and Ex.15.2, Merzbacher:

a) Show that if both A and B are constants of the motion, then they either commute or the commutator $i[A, B]$ is also a constant of the motion.
Prove that if the entire spectrum of H is nondegenerate, then A and B must commute. If the constants of the motion A and B do not commute, there must be degenerate energy eigenvalues.
Illustrate this theorem by constructing an example Hamiltonian for which $A = L_x$ and $B = L_y$ are constants of the motion.

b) Prove that

$$\langle \mathbf{r}|F(\mathbf{r}, \mathbf{p})|\Psi\rangle = F\left(\mathbf{r}', -i\hbar\nabla_{r'}\right)\psi(\mathbf{r}'),$$

$$\langle \mathbf{p}|F(\mathbf{r}, \mathbf{p})|\Psi\rangle = F\left(i\hbar\nabla_{p'}, \mathbf{p}'\right)\psi(\mathbf{p}').$$

P.04. P.3.2, Merzbacher:
For a free particle in one dimension, calculate the variance at time t, $(\Delta x)^2 = \langle x^2 \rangle - \langle x \rangle^2$, without explicit use of the wave function by applying Eq. (3.44) repeatedly. Show that

$$(\Delta x)^2_t = (\Delta x)^2_0 + \frac{2}{m}\left[\frac{1}{2}\langle xp + px\rangle_0 - \langle x\rangle_0\langle p\rangle\right] t + \frac{(\Delta p)^2}{m^2} t^2$$

and

$$(\Delta p)^2_t = (\Delta p)^2_0 = (\Delta p)^2.$$

P.05. P.8.5.5, Le-Bellac:
Thomas-Reiche-Kuhn sum rule: Consider a particle of mass m under the potencial $V(\mathbf{r})$. The Hamiltonian of the system is given by

$$H = \frac{p^2}{2m} + V(\mathbf{r}).$$

Let $|n\rangle$ be the eigenvectors of H with eigenvalues E_n. Show that

$$[[r_i, H], r_j] = \frac{\hbar^2}{m}\delta_{ij}$$

and then

$$\frac{2m}{\hbar^2}\sum_n (E_n - E_0)|\langle n|x|0\rangle|^2 = 1,$$

where $r_1 = x$, $r_2 = y$, and $r_3 = z$.

P.06. P.3.12, Cohen-Tannoudji: Infinite one-dimensional well.

P.07. P.3.13, Cohen-Tannoudji: Infinite two-dimensional well.

P.08. P.3.14, Cohen-Tannoudji: Three-dimensional Hilbert space.

P.09. P.3.16, Cohen-Tannoudji: Two noninteracting particles in one dimension.

Problemas adicionais:

10. P.8.3, Messiah:
The derivative of an operator $A(\xi)$ depending explicitly on a continuous parameter ξ is by definition

$$\frac{dA}{d\xi} = \lim_{\epsilon \to 0} \frac{A(\xi+\epsilon) - A(\xi)}{\epsilon}.$$

if $A(\xi)$ is a function of an observable or of several commuting observables, one shows that its derivative is obtained by means of the ordinary rules of differentiation.

a) If O is an observable, show that

$$\frac{d}{d\xi}\left(e^{i\xi O}\right) = iOe^{i\xi O}.$$

b) If two operators are differentiable, show that

$$\frac{d}{d\xi}(AB) = \frac{dA}{d\xi}B + A\frac{dB}{d\xi}.$$

c) If A is differentiate and possesses an inverse, show that

$$\frac{d}{d\xi}A^{-1} = -A^{-1}\frac{dA}{d\xi}A^{-1}.$$

11. Ex.9.21, Ex.9.22, and Ex.14.5, Merzbacher:

a) Show that, for any function $f(p)$ that can be expressed as a power series of its argument,

$$\langle x''|f(p)|x'\rangle = f\left(-i\hbar\frac{\partial}{\partial x''}\right)\delta(x''-x').$$

b) Change from the coordinate basis to the momentum basis, showing that the transformation coefficients are

$$\langle x'|p'\rangle = \frac{1}{\sqrt{2\pi\hbar}}\exp\left(ip'x'/\hbar\right).$$

c) Show that the operators $x^2p_x^2 + p_x^2x^2$ and $(xp_x + p_xx)^2/2$ differ only by terms of order $\hbar^2$.

12. Ex.14.6, Merzbacher:
Illustrate the validity of Eq. (14.60): Poisson bracket, by letting $G = x^2$ and $F = p_x^2$, and evaluating both the operator expression on the left, in the limit $\hbar \to 0$, and the corresponding Poisson bracket on the right.

13. Ex.15.24 and Ex.15.25, Merzbacher:

a) If the state of a quantum system is given by a density operator

$$\rho = p_1|\psi_1\rangle\langle\psi_1| + p_2|\psi_2\rangle\langle\psi_2|,$$

where $|\psi_{1,2}\rangle$ are two nonorthogonal normalized state vectors, show that the eigenvalues of the density operator are

$$\bar{p}_{1,2} = \frac{1}{2}\left(1 \pm \sqrt{1 - 4p_1p_2(1 - |\langle\psi_1|\psi_2\rangle|^2)}\right).$$

b) If an ensemble $\mathcal{E}$ consists of an equal-probability mixture of two nonorthogonal (but normalized) states $|\psi_1\rangle$ and $|\psi_2\rangle$ with overlap $C = \langle\psi_1|\psi_2\rangle$, evaluate the Shannon mixing entropy $H(\mathcal{E})$ and the von Neumann entropy $S(\rho)$. Compare the latter with the former as $|C|$ varies between 0 and 1. What happens as $C \to 0$?

14. P.9.2, Merzbacher:
Using the momentum representation, calculate the bound-state energy eigenvalue and the corresponding eigenfunction for the potential $V(x) = -g\delta(x)$ (for $g > 0$). Compare with the results in Section 6.4.

15. P.3.10.a, b, Cohen-Tannoudji: Virial theorem.

16. P.3.8 and 3.9, Cohen-Tannoudji: Probability current density.

17. P.3.17, 3.18, and 3.19, Cohen-Tannoudji: Density operator.

18. P 3.1, Weinberg:
Consider a system with a pair of observable quantities A and B, whose commutation relations with the Hamiltonian take the form $[H,A] = i\omega B$, $[H,B] = -i\omega A$, where ω is some real constant. Suppose that the expectation values of A and B are known at time $t = 0$. Give formulas for the expectation values of A and B as a function of time.

19. P 3.2, Weinberg:
Consider a normalized initial state $|\Psi(t=0)\rangle$ with a spread ΔE in energy, defined by

$$\Delta E = \sqrt{\langle (H - \langle H \rangle)^2 \rangle}.$$

Calculate the probability $|\langle \Psi(\delta t)|\Psi(0)\rangle|^2$ that after a very short time δt the system is still in the state $|\Psi(t=0)\rangle$. Express the result in terms of ΔE, $\hbar$ and δt, to second order in δt.

20. P 8.3, Ballentine:
Prove that if for some state of a two-component system one has

$$\langle R(1)R(2)\rangle = \langle R(1)\rangle\langle R(2)\rangle$$

for all Hermitian operators $R(1)$ and $R(2)$, then the density operator must be of the form $\hat{\rho} = \tilde{\rho}(1) \otimes \tilde{\rho}(2)$. (As usual, the superscript 1 or 2 signifies that the operator acts on the factor space of component 1 or 2, respectively.)

21. P 8.6, Ballentine:
Consider a two-component system that evolves under a time development operator of the form

$$U(t) = U(1)(t) \otimes \hat{1}.$$

(This could describe a system with no interaction between the two components, subject to an external perturbation that acts on component 1 but not on component 2.) Let $\hat{\rho}(t)$ be an arbitrary correlated state of the two–component system evolving under the action of $U(t)$. Prove that the partial state of component 2,

$$\tilde{\rho}(2) = \mathrm{Tr}_1 \hat{\rho}(t),$$

is independent of t.

22. P 2.9, Desai:
Consider the operator which corresponds to finite displacement

$$F(d) = e^{-ipd/\hbar}.$$

Show that

$$[x, F(d)] = dF(d).$$

If for a state $|\alpha\rangle$ we define $|\alpha_d\rangle = F(d)|\alpha\rangle$, then show that the expectation values with respect to the two states satisfy

$$\langle x \rangle_d = \langle x \rangle + d.$$

23. P 2.11, Desai:
For a Hamiltonian given by

$$H = \frac{\mathbf{p}^2}{2m} + V(\mathbf{r}),$$

use the properties of the double commutator

$$[[H, \exp(i\mathbf{k}\cdot\mathbf{r})], \exp(-i\mathbf{k}\cdot\mathbf{r})]$$

to obtain

$$\sum_n (E_n - E_s)|\langle n|\exp(i\mathbf{k}\cdot\mathbf{r})|s\rangle|^2.$$

24. P 3.3, Desai:
Express x in the Schrödinger representation as an operator x_H in the Heisenberg representation for the case of a free particle with the Hamiltonian

$$H = \frac{\mathbf{p}^2}{2m}.$$

Carry out the expansion of the exponentials in terms of the corresponding Hamiltonian. Consider also the case where the potential has the form $V(x) = \lambda x^n$, where n is an integer.

25. P 3.7, Desai:
A particle of charge e is subjected to an uniform electric field $\mathbf{E}_0$. Show that the expectation value of the position operator $\langle \mathbf{r} \rangle$ satisfies

$$m\frac{d^2\langle \mathbf{r} \rangle}{dt^2} = e\mathbf{E}_0.$$

26. A free particle of mass m moves in one-dimensional such that its initial state is given by the wave function

$$\psi(x, t=0) = \psi_0(x) = A \exp\left(i\frac{p_0 x}{\hbar} - \frac{x^2}{2a^2} \right),$$

where A, p_0, and a are constants.

a) Determine $\psi(x,t)$ and then calculate $\langle x\rangle(t)$, $\langle p\rangle(t)$, $(\Delta x)^2(t)$, and $(\Delta p)^2(t)$.

b) Determine the position $x_H(t)$ and momentum $p_H(t)$ operators in the Heisenberg picture by (i) using the unitary transformation that relates the operators in the Schrödinger and Heisenberg pictures; (ii) solving the corresponding Heisenberg equations of motion.

c) Repeat item (a), but now using the operators $x_H(t)$ and $p_H(t)$.