Problem Set 1

Note: The problems labeled with a star (\star) are somewhat lengthy or tricky in the derivations. You are encouraged but not obligated to solve them for extra credits.

Lecture 1

Question 1. Let us consider a single particle with mass m moving on a plane around a center (the center is fixed at the origin of the coordinate system, *i.e.*, the translational energy of the system is ignored) under a central potential V(r) = -1/r. The position of the particle is described by the polar coordinates r and φ .

- (1) Write down the classical Hamiltonian of the particle in terms of the generalized coordinates r and φ and the conjugate momenta p_r and p_{φ} .
- (2) Based on the classical Hamilton equations of motion, please derive the expressions for dp_r/dt , dp_{φ}/dt , and $d\varphi/dt$.
- (3) Multiply dr/dt to both sides of the equation of dp_r/dt obtained in (2), and integrate both sides once over t, during which you introduced a constant of integration W. Show that the constant of integration W is the total energy of the particle.
- (4) Substitute $\frac{dr}{dt} = \frac{dr}{d\varphi} \frac{d\varphi}{dt}$ into the expression of W obtained in (3), with $d\varphi/dt$ from (2). With

the aid of a new variable u=1/r, show that the orbit of the particle satisfies the following equation (which actually represents an ellipse):

$$u = \frac{1}{r} = \frac{1 + \lambda \sin(\varphi - \varphi_0)}{a(1 - \lambda^2)}$$
, with $a = -\frac{1}{2W}$ and $\lambda = \sqrt{1 + \frac{2p^2W}{m}}$.

★(5) Apply Sommerfeld quantization condition on p_r and p_{φ} respectively, and show that the quantized total energy of the system W is proportional to $-1/n^2$ (where n is an integer). Note that although the final result for W is equivalent to Bohr's formula for H atom, the current approach (Sommerfeld, 1916) generalizes Bohr's circular orbit (by assumption) to an elliptical orbit. Useful integrals:

(1)
$$\int (-x^2 + c_1 x + c_2)^{-1/2} dx = \arcsin(-\frac{c_1 - 2x}{\sqrt{c_1^2 + 4c_2}}) + \text{const.}$$

(2)
$$\int_{0}^{2\pi} \frac{(\cos\varphi)^{2}}{(1+c\sin\varphi)^{2}} d\varphi = \frac{2\pi}{c^{2}} (\frac{1}{\sqrt{1-c^{2}}} - 1)$$

Question 2. From the definition of the classical Poisson bracket, prove the following simple yet tremendously useful algebraic relations:

(The superscript "c" stands for "classical". You can omit this superscript for the convenience of writing.)

(1)
$$[X, Y]^c = -[Y, X]^c$$

(2)
$$[X, Y+Z]^c = [X, Y]^c + [X, Z]^c$$

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(3) $[X, YZ]^c = Y[X, Z]^c + [X, Y]^cZ$ (4) $[XY, Z]^c = X[Y, Z]^c + [X, Z]^cY$

(4)
$$[XY, Z]^c = X[Y, Z]^c + [X, Z]^c$$

(5)
$$\frac{\partial}{\partial \alpha} [X, Y]^{c} = \left[\frac{\partial X}{\partial \alpha}, Y \right]^{c} + \left[X, \frac{\partial Y}{\partial \alpha} \right]^{c}$$

★(6) Jacobi's identity:
$$[X, [Y, Z]^c]^c + [Y, [Z, X]^c]^c + [Z, [X, Y]^c]^c = 0$$

Hint: Use the relations (1)–(5) comprehensively.

Note: A shortcut to prove this is to use the definition of quantum commutator and argue that it is proportional to the classical Poisson bracket, according to Dirac. However, the purpose here is to explore the general algebraic properties in a purely classical approach, without resorting to the quantum mechanical definition.

(7) Based on Jacobi's identity, show that if X and Y are both constants of motion, then the dynamical variable [X, Y]^c is also a constant of motion.

Question 3. The classical angular momentum L is defined as:

$$L = r \times p = \begin{vmatrix} i & j & k \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix}$$

where r is the position of the particle (with x, y, z being the three components), p is the linear momentum (with p_x , p_y , p_z being the three components). The three unit vectors along the x, y, and z axis are i, j, and k.

- (1) Evaluating the classical Poisson brackets $[L_x, L_y]^c$ and $[L_x, L^2]^c$, in which L_i is the magnitude of the projected L along the *i*-th (*i.e.*, x, y, or z) direction.
- (2) Write down the corresponding quantum commutators via Dirac canonical quantization.
- (3) Write down the condition imposed on the classical Hamiltonian H (time-independent) that ensures the conservation of the angular momentum L.

Lecture 2

Question 4. More on angular momentum:

- (1) Write down the specific forms of the operators \hat{L}_i and \hat{L}^2 in Cartesian coordinates.
- (2) Show that the commutators you wrote down in Question 3 (2) are consistent with the operators.
- (3) Prove the following relation between the total angular momentum \hat{L} and the total linear momentum \hat{p} : $\hat{p} \times \hat{L} + \hat{L} \times \hat{p} = 2i\hbar\hat{p}$
- (4) Based on classical mechanics, what is the conjugate coordinate of L_z ? (You may want to refer to Question 1.) Write down the classical Poisson bracket of L_z and its conjugate coordinate, and based on which, write down the quantum mechanical operator of \hat{L}_z in terms of its conjugate coordinate.
- (5) Prove that \hat{L}_z is a Hermitian operator by evaluating the integral $\langle \chi_m | \hat{L}_z | \chi_n \rangle$ using the operator form presented in (4). Here, the state $|\chi_n\rangle$ is a function of the conjugate coordinate only.

Question 5. Given an orthonormal complete basis set $\{|1\rangle, \dots, |i\rangle, \dots, |N\rangle\}$ in Hilbert space, please prove the resolution of identity (which is also called the closure relation): $\hat{I} = \sum_{i=1}^{N} |i\rangle\langle i|$

Question 6. Given a set of non-orthonormal basis as follows, please use the Gram-Schmidt approach to construct an orthonormalized set:

(1) Real-number space for all $-1 \le x \le 1$: $|a\rangle = 1$, $|b\rangle = x$, $|c\rangle = x^2$, $|d\rangle = x^3$

(2) 3D vector space:
$$\begin{vmatrix} a \\ a \end{vmatrix} = \begin{pmatrix} 3 \\ 0 \\ 0 \end{pmatrix}, \quad \begin{vmatrix} b \\ b \end{vmatrix} = \begin{pmatrix} 0 \\ 1 \\ 2 \end{pmatrix}, \quad \begin{vmatrix} c \\ c \end{vmatrix} = \begin{pmatrix} 0 \\ 2 \\ 5 \end{pmatrix}$$

Question 7. A planewave is $|k\rangle = Ae^{ikx}$ where k is the magnitude of the wavevector, let us consider the orthonormalization between two planewaves $|k\rangle$ and $|k'\rangle$. Dirac defined a function $\delta(x)$ (Dirac delta function) for dealing with planewaves:

$$\delta(x) = \begin{cases} 0 & (x \neq 0) \\ +\infty & (x = 0) \end{cases} \text{ and } \int_{-\infty}^{+\infty} \delta(x) \, dx = 1$$

This definition could be easily extended to three dimensions. We shall only consider the one dimensional case here.

- (1) Evaluate $\int_{-\infty}^{+\infty} f(x)\delta(x-a)dx$
- ★(2) Show that $g(x) = \lim_{n \to +\infty} \frac{\sin(nx)}{\pi x}$ can be used to represent the Dirac delta function. Try to visualize g(x) by plotting it with n=1, 3, and 8.
- (3) With the aid of the function g(x) above, show that $\langle k' | k \rangle = \delta(k k')$, in which the normalized planewave $|k\rangle = \frac{1}{\sqrt{2\pi}} e^{ikx}$.

Question 8. An operator \hat{A} , representing observable A, has two normalized eigenstates $|\alpha_1\rangle$ and $|\alpha_2\rangle$, with eigenvalues a_1 and a_2 , respectively. Operator \hat{B} , representing observable B, has two normalized eigenstates $|\beta_1\rangle$ and $|\beta_2\rangle$, with eigenvalues b_1 and b_2 . The eigenstates are related by:

$$|\alpha_1\rangle = (3|\beta_1\rangle + 4|\beta_2\rangle)/5, \quad |\alpha_2\rangle = (4|\beta_1\rangle - 3|\beta_2\rangle)/5$$

- (1) Observable A is measured, and the value a_1 is obtained. What is the state of the system immediately after this measurement?
- (2) After step (1), if B is now measured, what are the possible results, and what are their probabilities?
- (3) Right after the measurement of B (i.e., step (2)), A is measured again. What is the probability of getting a_1 ?

Lecture 3

Question 9. Calculate the probability flux j given by the following wave functions Ψ :

- (1) $\Psi = c\Phi$, in which c is a constant (real or complex) and Φ is a real function.
- (2) $\Psi = Ae^{ipx/\hbar} + Be^{-ipx/\hbar}$, in which the momentum p is along the positive x direction. A and B are

the normalization constants. (Go ahead and directly use A and B without actually normalizing the wave function.)

Question 10. The potential function used in quantum mechanics, which represents a physical system, is chosen to be a real function in order to keep the Hermicity of the Hamiltonian operator. Nevertheless, for the convenience of describing a process in which a particle is absorbed by a sink, one can artificially write the potential function in a complex form: $V = V_R - iV_I$, where both V_R and V_I are real. V_I is a constant and it is the imaginary part of the potential V.

Please go through the derivation of the continuity equation and show that the total probability given by real wave functions for finding a particle decreases exponentially as $e^{-2V_1t/\hbar}$, which serves as a phenomenological description of the absorption process. (Please note that the probability flux at infinity is zero.)

Question 11. In the Heisenberg picture, we defined the operator \hat{A}^{H} as $\hat{A}^{H} = e^{i\hat{H}t/\hbar}\hat{A}e^{-i\hat{H}t/\hbar}$. To compute this operator, one could use the following formula:

$$e^{\hat{A}}\hat{B}e^{-\hat{A}} = \hat{C}_0 + \hat{C}_1 + \frac{\hat{C}_2}{2!} + \frac{\hat{C}_3}{3!} + \dots = \sum_{n=0}^{+\infty} \frac{\hat{C}_n}{n!}$$

in which,

$$\begin{split} \hat{C}_0 &\equiv \hat{B}\,, \\ \hat{C}_1 &\equiv \left[\hat{A}, \hat{C}_0\right] = \left[\hat{A}, \hat{B}\right], \\ \hat{C}_2 &\equiv \left[\hat{A}, \hat{C}_1\right] = \left[\hat{A}, \left[\hat{A}, \hat{B}\right]\right], \\ \hat{C}_3 &\equiv \left[\hat{A}, \hat{C}_2\right] = \left[\hat{A}, \left[\hat{A}, \left[\hat{A}, \hat{B}\right]\right]\right] \end{split}$$

and so on.

Please prove this formula.

Hint: Consider function $f(\lambda) = e^{\lambda \hat{A}} \hat{B} e^{-\lambda \hat{A}}$ where λ is an arbitrary constant, and evaluate its *n*-th order derivatives $d^n f(\lambda) / d\lambda^n$. Compare these results with the formula to be proven.