

## Problems on Quantum Mechanics (Module 2)

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### Classical Mechanics

1. How many degrees of freedom do the following systems have? (a) One point particle moving on a circle (b) Two point particles moving on a circle (c) Three point particles moving in a lecture hall (d) an irregularly shaped stone moving in the air above the playground.
2. Find Hamilton's equations for a particle in a double well potential with Hamiltonian

$$H = \frac{p^2}{2m} + g(x^2 - a^2)^2, \quad m, g, a > 0. \quad (1)$$

Check that they reduce to Newton's second order equation.

3. Check that the equations of motion  $\dot{f}(x, p) = \{f(x, p), H\}$  reduce to Hamilton's equations for  $f = x$  and  $f = p$  for the above particle.
4. Find all static solutions to Hamilton's equations and classify them as stable/unstable to small perturbations.
5. Draw a phase portrait for the above particle in a double well potential.

### Quantum Mechanics

6. Consider the Pauli matrices in the standard basis. Now  $\sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ . Find  $\sigma_2^\dagger$ . Show that  $\sigma_2$  is hermitian and unitary.
7. What is  $\sigma_2^2$ ? What is the characteristic equation for  $\sigma_2$ ?
8. Find a simple formula (in terms of trigonometric functions) for  $e^{i\theta\sigma_2/2}$  by summing the exponential series.
9. What are the eigenvalues of  $\sigma_2$ ? Find the corresponding eigenvectors  $v_+$  and  $v_-$ .
10. Show that  $v_+$  and  $v_-$  satisfy the completeness relation  $v_+v_+^\dagger + v_-v_-^\dagger = |v_+\rangle\langle v_+| + |v_-\rangle\langle v_-| = I_{2 \times 2}$ .
11. Show that the eigenvalue  $\lambda$  of an operator  $A$  may be interpreted as the expectation value of  $A$  in the corresponding eigenstate.
12. Show that the commutator of two hermitian operators is anti-hermitian.
13. Suppose  $a$  is any operator on a Hilbert space and let  $H_1 = a^\dagger a$  and  $H_2 = aa^\dagger$ . Check that  $H_1$  and  $H_2$  are hermitian. Show that expectation values of  $H_1$  and  $H_2$  in all (non-zero) states are non-negative. We say that  $aa^\dagger$  and  $a^\dagger a$  are positive (more precisely non-negative) operators. Hint: recall the definition of the norm of a vector.
14. Argue that the expectation value of kinetic energy  $T = p^2/2m$  is nonnegative in any state. Also argue that the expectation value of energy  $T + \frac{1}{2}m\omega^2 x^2$  of a simple harmonic oscillator is positive in any state.
15. Consider two finite dimensional matrices  $A, B$ . What is  $\text{tr}[A, B]$ ?

16. Consider the Heisenberg commutation relations  $[x, p] = i\hbar I$ . Comment on the result of calculating the trace of either side.
17. Recall that  $\int_{-\infty}^{\infty} e^{iky} dy = 2\pi\delta(k)$ . Evaluate the integral  $\int_{-\infty}^{\infty} y e^{iky} dy$ .
18. Find the matrix element of the position operator between momentum eigenstates  $\langle k|x|k'\rangle$ . Hint:  $\langle x|k\rangle = e^{ikx}$  and use the completeness relation.
19. Find the matrix element of the momentum operator  $p$  between position eigenstates  $\langle x|p|y\rangle$ .
20. Given two observables (hermitian operators)  $A, B$  with  $[A, B] = iC$  one may show the uncertainty inequality  $(\Delta A)_{\psi}^2 (\Delta B)_{\psi}^2 \geq \frac{1}{4} \langle C \rangle_{\psi}^2$  for any (unit norm) state  $\psi$ . Say how  $(\Delta A)_{\psi}$  is defined. Here  $\langle C \rangle_{\psi}$  is the expectation value of  $C$  in the state  $\psi$ . Consider the angular momentum observables that satisfy  $[L_i, L_j] = i\hbar\epsilon_{ijk}L_k$ . Apply the uncertainty inequality to  $A = L_x$  and  $B = L_y$  and comment on the result. Is there a state where the product of uncertainties can vanish? Contrast this with the case  $A = x, B = p$ .
21. Consider the Schrödinger equation for a particle in a 1d real potential  $V(x)$ :

$$i\hbar \frac{\partial \psi(x, t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x)\psi(x). \quad (2)$$

Find the equation satisfied by the complex conjugate wave function.

22. Derive a local conservation law for probability in 1D:  $\frac{\partial P}{\partial t} + \frac{\partial j}{\partial x} = 0$  where  $P = |\psi(x, t)|^2$ . What is the probability current  $j(x, t)$ ?
23. Show that  $\int_{-\infty}^{\infty} e^{-y^2} dy = \sqrt{\pi}$ .
24. Show that the Gaussian wave packet  $\psi(x) = Ae^{-\frac{x^2}{4a^2}}$  has unit norm if we take  $A = \frac{1}{\sqrt{a(2\pi)^{1/4}}}$ . What is the mean position and mean momentum of a particle in this state?
25. Consider a quantum mechanical particle moving in a potential  $V(x)$  in one dimension. Its state evolves according to the Schrodinger equation. Use the Schrödinger equation to calculate the time evolution of the mean momentum of the particle,  $\frac{d\langle p \rangle}{dt}$  and express the answer in terms of the expectation values of other familiar quantities. Recall that  $\langle 4 \rangle$

$$\langle p \rangle = \int dx \psi^*(x) \left( -i\hbar \frac{\partial}{\partial x} \right) \psi(x). \quad (3)$$

26. Suppose the wave function of a particle in one dimension is bounded and decays like  $\psi(x) \sim \frac{1}{|x|^\alpha}$  as  $|x| \rightarrow \pm\infty$  for some power  $\alpha > 0$ . How small can the power  $\alpha$  be and still ensure that the wave function has a finite norm?  $\langle 3 \rangle$
27. Evaluate the one-dimensional gaussian integral  $I_1$  in closed form.

$$I_1 = \int_{-\infty}^{\infty} dx e^{-x^2} \quad (4)$$

Hint: Consider the Gaussian integral  $I_2$ , and evaluate it by transforming to polar coordinates on the  $x$ - $y$  plane. How is  $I_2$  related to  $I_1$ ?  $\langle 3 \rangle$

$$I_2 = \iint dx dy e^{-x^2-y^2} \quad (5)$$

28. Suppose  $\tilde{f}(k)$  is the Fourier transform of  $f(x)$ ,

$$\tilde{f}(k) = \int_{-\infty}^{\infty} dx e^{-ikx} f(x) \quad (6)$$

Find the Fourier transform  $\tilde{g}(k)$  of the function  $g(x) = xf(x)$ . In other words, express  $\tilde{g}(k)$  in terms of  $\tilde{f}(k)$ .  $\langle 2.5 \rangle$

29. Multiplication by  $x$  in position space is represented by what operation in  $k$ -space?  $\langle 1 \rangle$

30. Let  $u, v$  be vectors and  $A$  an operator on  $\mathcal{H}$ . Simplify (a)  $\langle iAv|u \rangle$ , (b)  $\langle u|iAv \rangle$  and (c)  $\langle iAv|iu \rangle$  for the standard  $L^2$  inner product. In other words, pull out the  $i$ 's properly!  $\langle 2 \rangle$

31. Based on the reality of average experimental measurements of observables, we defined a hermitian operator  $A$  as one with real expectation values in every state  $\psi$ , i.e., ( $\langle \psi|A\psi \rangle \in \mathbb{R}$ ). Say why this is the same as  $\langle 2 \rangle$

$$\langle \psi|A\psi \rangle = \langle A\psi|\psi \rangle. \quad (7)$$

32. A more conventional definition of hermiticity is that the matrix elements of  $A$  satisfy

$$\langle u|Av \rangle = \langle Au|v \rangle \quad (8)$$

for any pair of states  $u, v$ . Say why this is the same as  $A_{uv} = (A_{vu})^*$ .  $\langle 2 \rangle$

33. Now suppose  $A$  satisfies (7). We wish to show that it also satisfies (8). To show this, we put  $\psi = u + v$  and  $\psi = u + iv$  in (7) and add the two resulting equations. Show that this reduces to  $A_{uv} = (A_{vu})^*$ . Thus the reality of expectation values in all states implies that  $A$  is hermitian in the conventional sense. The converse is much simpler.  $\langle 5 \rangle$

34. Consider a particle in a (real) potential  $V(x)$ . Suppose  $\psi(x)$  is a solution of the time-independent Schrödinger equation with (real) energy eigenvalue  $E$ . Find another wave function that has the same eigenvalue  $E$ . When are the two eigenfunctions the same?  $\langle 2 \rangle$

35. Use the result of the previous problem to show that for any energy eigenvalue  $E$ , one can always find a corresponding real eigenfunction of the hamiltonian  $\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$ . This feature is because  $H$  is not just hermitian but also real-symmetric.  $\langle 3 \rangle$

36. If  $P, Q$  are hermitian, what can you say about the commutator  $[P, Q]$ ? Can  $[P, Q]$  be an observable?  $\langle 2 \rangle$

37. It is possible to show (using Cauchy-Schwarz) that for position and momentum  $x$  and  $p$ ,

$$(\Delta x)^2 (\Delta p)^2 \geq -\frac{1}{4} \langle [x, p] \rangle_\psi^2 \quad (9)$$

where  $(\Delta x)^2 = \langle x^2 \rangle_\psi - \langle x \rangle_\psi^2$  is the variance of  $x$  in the state  $\psi$  and similarly for  $\Delta p$ . Show that this reduces to the Heisenberg uncertainty principle.  $\langle 2 \rangle$

38. Consider the momentum operator  $\hat{p} = -i\hbar \frac{\partial}{\partial x}$  of a particle that is constrained to move in the interval  $[-1, 1]$ . Give a convenient choice of boundary condition for  $\psi(\pm 1)$  that ensures that  $\hat{p}$  is hermitian. Give the physical meaning of the boundary condition that you propose.  $\langle 5 \rangle$

39. Consider a free particle that moves in the interval  $0 \leq x \leq L$ . Unlike the square well problem, here we will impose *periodic boundary conditions*: all states must satisfy  $\psi(0) = \psi(L)$  and  $\psi'(0) = \psi'(L)$ <sup>1</sup>.

- (a) Does  $\hat{p} = -i\hbar\frac{\partial}{\partial x}$  have any eigenfunctions satisfying periodic boundary conditions? If so find the orthonormal eigenfunctions and corresponding eigenvalues. ⟨5⟩
- (b) Do you think one could make measurements of  $\hat{p}$  with arbitrary precision (in principle)? If such a measurement is made, what are the possible values of momentum that one might obtain? What is the state of the particle after one such measurement? ⟨3⟩
- (c) For the above particle with hamiltonian  $\hat{H} = \frac{p^2}{2m}$ , find the normalized energy eigenfunctions and eigenvalues. Work with exponentials rather than trigonometric functions here. ⟨5⟩
- (d) Can  $\hat{H}$  and  $\hat{p}$  be simultaneously measured with arbitrary accuracy? Why? ⟨1⟩
- (e) What is the ground state wave function and energy? Plot the absolute square of the ground state wave function in position space. Where along the circle (or the interval  $[0, L]$ ) is the particle most likely to be found in the ground state? ⟨3⟩
- (f) How many linearly independent eigenfunctions are there at each energy level? ⟨2⟩
- (g) The potential here is zero, which is real. So find real energy eigenfunctions (in the position basis) at each energy level. ⟨3⟩
- (h) The potential here is zero, which is an even function of  $x$  about the point  $x = L/2$ . Find the energy eigenfunctions of definite parity (even or odd about  $x = L/2$ ) at each energy level. Is there both an even and an odd state at each energy level? ⟨3⟩

40. Free particle gaussian wave packet and harmonic oscillator.

- (a) Recall that the gaussian wave packet

$$\psi(x, t = 0) = A e^{ik_0 x} e^{-\frac{x^2}{4a^2}}, \quad A^2 = \frac{1}{a\sqrt{2\pi}}. \quad (10)$$

has mean momentum  $\langle p \rangle = \hbar k_0$  at  $t = 0$ . Write down  $\tilde{\psi}(k, t = 0)$  and then obtain  $\tilde{\psi}(k, t)$  in the energy/momentum basis. ⟨3⟩

- (b) Find  $\langle p \rangle$  at  $t > 0$ .  $\langle p \rangle$  is most easily calculated in the momentum basis. ⟨4⟩
- (c) Calculate  $\langle \hat{x} \rangle$  at time  $t$  in the above gaussian wave packet. Since  $\tilde{\psi}(k, t)$  is known, it is good to work in the momentum basis. So you need to know how  $\hat{x}$  acts in  $k$ -space. This was worked out in problem set 6:  $\hat{x} = i\frac{\partial}{\partial k}$ . Hint: In working out the integrals, exploit the fact that integrals of odd functions on even intervals vanish. ⟨9⟩
- (d) Do the obtained mean values satisfy Ehrenfest's principle  $m\frac{\partial \langle x \rangle}{\partial t} = \langle p \rangle$  at all times? ⟨2⟩

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<sup>1</sup>A physical realization is a particle moving on a circle:  $x$  is the coordinate along the circumference (or the polar angle  $\phi$ ), so the coordinates  $x = 0$  and  $x = L$  represent the same physical point (the angles  $\phi = 0, 2\pi$ ). In this physical realization, the momentum we refer to is really the component of angular momentum  $L_\phi$  where  $\phi$  is the polar angle in the plane of the circle.

- (e) Find the probability for a particle in the ground state  $\frac{\sqrt{\beta}}{\pi^{1/4}} e^{-\beta^2 x^2/2}$  of a harmonic oscillator potential  $\frac{1}{2}m\omega^2 x^2$ , to be found outside its classically allowed region. Express this probability as an integral over dimensionless variables. Does it depend on  $m$  or  $\omega$ ? Here  $\beta = \sqrt{\frac{m\omega}{\hbar}}$ .  $\langle 5 \rangle$
- (f) Find the numerical value of this probability. You may use  $\int_1^\infty d\xi e^{-\xi^2} \approx 0.14$ .  $\langle 2 \rangle$