Problems for Quantum Mechanics

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Chapter 1

Problems

1. Estimate De Broglies wavelength of the following object:

    - A tennis ball at its world record speed (232 km/h),
    - A gas molecule at room temperature,
    - A electron in hydrogen atom.

    For which one a quantum mechanical treatment is necessary ? Why ?

Chapter 2

Problems

1. Show that if the wavefunction $\Psi(\mathbf{r}) = c\tilde{\Psi}(\mathbf{r})$, where c is a constant and $\tilde{\Psi}(\mathbf{r})$ is real, then the corresponding current $\mathbf{j}$ vanishes.

2. Consider a one-dimensional wavefunction $\Psi(x,t) = Ae^{ikx-i\omega t} + Be^{-ikx-i\omega t}$, compute the probability density ρ [Eq. (2.17)] and probability current $\mathbf{j}$ [Eq. (2.20)] in the lecture. How do you understand your results ?

3. Consider the case where $V(\mathbf{r}) = V_R(\mathbf{r}) - iV_I$ where the imaginary part of the potential is constant. Is the Hamiltonian Hermitian ? Go through the derivation of the continuity equation an show that the total probability for finding the particle decrease exponentially as $e^{-2V_I t/\hbar}$.

4. Using the Schördinger Equation $H\Psi = i\hbar\frac{\partial\Psi}{\partial t}$ with the Hamiltonian $H = -\frac{\hbar^2}{2\mu}\nabla^2 + V(\mathbf{r})$,

   (a) Show that

   $$\frac{d\mathbf{p}}{dt} = \mathbf{F},$$

   where $\mathbf{p} = -i\hbar\int d\mathbf{r}\Psi^*\nabla\Psi$, and $\mathbf{F} = -\int d\mathbf{r}\Psi^*(\nabla V)\Psi$. What is the physical meaning of this equation ? Does that remind you something familiar from classical mechanics ?

   (b) Show that

   $$\frac{\partial W}{\partial t} + \nabla\cdot\mathbf{S} = 0,$$

   where $W = \frac{\hbar^2}{2\mu}\nabla\Psi^*\cdot\nabla\Psi + \Psi^* V\Psi$, and $\mathbf{S} = -\frac{\hbar^2}{2\mu}(\dot{\Psi}^*\nabla\Psi + \dot{\Psi}\nabla\Psi^*)$. What is the physical meaning of the this equation, and the quantity W and $\mathbf{S}$ respectively ?

5. Suppose $\Psi_1(\mathbf{r},t)$ and $\Psi_2(\mathbf{r},t)$ are two wave functions that satisfy the same Schrödinger equation. Show that their overlap $\int \Psi_1^*\Psi_2 d\mathbf{r}$ is time independent.

6. Show that the velocity field based on the solution of the Schrödinger equation satisfies $\nabla \times \mathbf{v} = 0$, i.e. the field is curl-less.

7. Consider a bound state solution $\Psi(\mathbf{r})$ of the Hamiltonian $H = -\frac{\hbar^2\nabla^2}{2\mu} + V(\mathbf{r})$. Please write down the expression of the expected kinetic energy and potential energy. Show that the kinetic energy is always positive.

Chapter 3

Problems

1. A quantum particle of mass μ and energy E, arriving from left, strikes a potential wall at $x = 0$ given by

$$V(x) = \frac{\hbar^2}{\mu}\Omega\delta(x).$$

   (a) What is the dimensionality of the parameter Ω ?

   (b) Please show the effect of the wall on the particle. Discuss the limiting case of $\Omega \to \infty$, what happens ?

2. A quantum particle of mass μ resides in the following potential

$$V(x) = -\frac{\hbar^2}{\mu}\Omega\left[\delta(x-a) + \delta(x+a)\right]. \tag{3.1}$$

   (a) Please solve the energy level and wavefunction of the quantum particle.

   (b) What happens when $\Omega a \gg 1$, and $\Omega a \ll 1$ respectively ? What are the physical picture of these two cases ?

   (c) In the case of $a = 0$, what is the kinetic energy and potential energy of the quantum particle ?

3. A quantum particle with energy $E = \frac{\hbar^2 k^2}{2\mu}$ hits the potential

$$V(x) = \begin{cases} 0, & x < 0, \\ V_0 & x > 0. \end{cases}$$

   Please calculate the reflection and transmission coefficients.

4. A quantum particle resides in one dimensional space. Show that two bound states $\Psi_m(x)$ and $\Psi_n(x)$ with different eigenenergy $E_m \neq E_n$ are orthogonal, i.e.

$$\int_{-\infty}^{\infty} \Psi_n(x)\Psi_m(x)dx = 0.$$

5. Show that there is no degeneracy in one dimensional bound states. Moreover, show that the bound state wavefunction can always be chosen as to be real.

6. A particle of mass m in one dimension is bound to a fixed center by an attractive δ-function potential

$$V(x) = -\lambda\delta(x), \quad (\lambda > 0).$$

At time $t = 0$, the potential is suddenly switch off. Find the wavefunction for $t > 0$.

7. A particle is in the ground state of a box with hardwalls of length L. The box suddenly expands symmetrically to length λL, leaving the wavefunction undisturbed. What is the probability that the particle resides at the ground state of the new box ?

8. In the study of quark-antiquark bound system (known as *quarkonium*), it is relevant to consider a quantum particle with mass μ bound in the potential

$$V(x) = k|x|.$$

Please solve the energy spectrum of the particle. What is the parity of the ground state ? What is the ground state energy ? What is the excitation energy to the first excited state ? Hint: You may need to refresh your memory about Airy function and its zeros. Comment: This problem is also relevant if you bounce a quantum particle towards the floor under the action of gravity, c.f. Phys. Rev. D **67** 102002, (2003).

Chapter 4

Problems

1. Assuming H is a Hamiltonian which depends on parameter λ, and $|\Psi\rangle$ is its eigenstate, show that

$$\frac{\partial \langle \Psi | H | \Psi \rangle}{\partial \lambda} = \left\langle \Psi \left| \frac{\partial H}{\partial \lambda} \right| \Psi \right\rangle . \tag{4.1}$$

This is the so called *Hellmann-Feynman* Theorem which finds wide applications in quantum physics.

2. Assuming $H = \frac{\mathbf{p}^2}{2\mu} + V(\mathbf{r})$ and $|\Psi\rangle$ is its eigenstate, show that

$$\left\langle \Psi \left| \frac{\mathbf{p}^2}{2\mu} \right| \Psi \right\rangle = \frac{1}{2} \langle \Psi | \mathbf{r} \cdot \nabla V(\mathbf{r}) | \Psi \rangle . \tag{4.2}$$

This is the so called *Virial theorem.* Does this reminds you anything from classical mechanics ? If $V(\mathbf{r})$ is a δ–potential, what can you say about the energy relation from the Virial theorem ? Check this relation for the problem (3.1) you solved in Chapter 3.

3. Suppose the Hamiltonian commutes with the parity operator, i.e. $[H, P] = 0$, and $|\Psi\rangle$ is a nondegenerate eigenstate of H, show that $|\Psi\rangle$ is also a parity eigenstate.

4. Take your solution of (3.1) in the Chapter. 3 and compute $\Delta x \Delta p$. Check that it indeed satisfies the Heisenberg uncertainly principle.

5. Given operator A, B, and

$$\begin{aligned} C_0 &= B, \\ C_1 &= [A, B] = AB - BA, \\ C_2 &= [A, C_1] = [A, [A, B]], \\ &\dots \\ C_n &= [A, C_{n-1}]. \end{aligned} \tag{4.3}$$

Show that $e^A B e^{-A} = C_0 + C_1 + \frac{1}{2!}C_2 + \frac{1}{3!}C_3 + \ldots = \sum_{n=0}^{\infty} \frac{C_n}{n!}$. Apply the formula to the case $A = \mathrm{i}p, B = x$.

6. Consider a quantum particle reside in a symmetric infinite deep potential of the width L, assuming a guess of ground wave-function $\Psi_{\text{guess}}(x) = c_0 + c_1 x + c_2 x^2 + c_3 x^3 + c_4 x^4$.

   (a) What can you say about the coefficients even without calculation ? (Hint: the ground state has even parity.)

   (b) What is the expected energy of $\Psi_{\text{guess}}(x)$?

   (c) Try to vary the coefficient to obtain the lowest possible energy. How does that compared to the exact solution ?

   (d) Could you come up with a good guess of the first excited state ?

7. Show that every attractive potential ($x \to \pm\infty, V(x) \to 0$) in one dimension has at least one bound state. Hint: Evaluate the expected energy on a guessed wavefunction $\Psi_{\text{guess}}(x) \sim e^{-ax^2/2}$. What happens if $a \to 0$?

Chapter 5

Problems

1. The Hamiltonian of certain 2-level system is

$$H = E\left(|1\rangle\langle 1| - |2\rangle\langle 2| + |1\rangle\langle 2| + |2\rangle\langle 1|\right),$$

where $|1\rangle, |2\rangle$ are orthonormal basis and E is a number with the dimension of energy. What is the matrix representation of the Hamiltonian with respect to this basis ? Find its eigenvalues and eigenvectors as linear combination of $|1\rangle, |2\rangle$.

2. The coordinate space basis $|x\rangle$ and momentum space basis $|p\rangle$ satisfy $\langle x|x'\rangle = \delta(x - x')$, $\langle p|p'\rangle = \delta(p - p')$ and $\langle x|p\rangle = e^{ipx/\hbar}/\sqrt{2\pi\hbar}$, please write down the stationary Schrödinger equation for the wavefunction $\Psi(p) = \langle p|\Psi\rangle$ in the momentum space.

3. Solve the problems (3.1) of the Chapter 3 using Schrödinger equation in the momentum space. Hint1: Consider $a = 0$ if you think the full problem is too difficult. Hint2: Make sure you obtain exactly the same result as last time. Sometimes, solving the same problem multiple times using different methods and check consistency is a way to ensure correctness.

4. Consider Hamiltonian $H = \frac{p^2}{2\mu} + V(x)$, please write down the equation of motion for the operators x_H and p_H in the Heisenberg picture.

5. Prove the following sum rules in the energy representation

   (a) Consider a quantum particle with mass μ, and $F(x)$ is a function of the coordinate,

$$\sum_n (E_n - E_k)\,|F_{nk}|^2 = \frac{\hbar^2}{2\mu}\left\langle k\left|\left|\frac{dF}{dx}\right|^2\right|k\right\rangle \tag{5.1}$$

(b) H is the Hamiltonian, and F is an arbitrary Hermitian operator, show that

$$\sum_n (E_n - E_k)^2 \left|F_{nk}\right|^2 = -\left\langle k \left| [H, F]^2 \right| k \right\rangle . \tag{5.2}$$

Chapter 6

Problems

1. Find the expectation value of the potential energy in the nth state of the harmonic oscillator.

2. Evaluate the expected value $\langle n|x^4|n\rangle$ and $\langle n|x^3|n\rangle$.

3. Consider a particle subject to a one-dimensional potential of the following form

$$V(x) = \begin{cases} \frac{1}{2}\mu\omega^2 x^2, & x > 0, \\ \infty & x < 0. \end{cases}$$

   What is the ground state energy ? What is the expectation value $\langle x^2\rangle$ of the ground state ?

4. Consider a particle resides in a three dimensional harmonic potential $V(x, y, z) = \frac{\mu\omega^2}{2}(x^2 + y^2 + z^2)$. What is the energy spectrum of the system ? What is the degeneracy of each energy level ?

5. Suppose at time $t = 0$ the oscillator is in the coherent state $|\Psi(t = 0)\rangle = |\alpha\rangle$, please write down the wavefunction at time t, $|\Psi(t)\rangle$. Show that it is also a coherent state.

6. The magnetic length $\ell = \sqrt{\frac{\hbar c}{eB}}$, and the cyclotron frequency $\omega = \frac{eB}{\mu c}$. Try to estimate them for magnetic field strength $B = 1$ Tesla. What is the corresponding temperature scale of the cyclotron frequency ?

7. Let a and $a^\dagger$ be the annihilation and creation operators for a harmonic oscillator, consider the Hamiltonian

$$H = \epsilon a^\dagger a + \eta \left(aa + a^\dagger a^\dagger\right) ,$$

where ϵ and η are real parameters. Compute the energy spectrum of the Hamiltonian. Hint: try to write the Hamiltonian using the operator $b = a \cosh\theta + a^\dagger \sinh\theta$ and $b^\dagger = a^\dagger \cosh\theta + a \sinh\theta$, where θ is a to be determined parameter. They are called Bogoliubov operator. You will encounter them in the study of superfluids and superconductors in future.

Chapter 7

Problems

1. Given a Hamiltonian $H = \frac{p^2}{2\mu} + V(x)$, does it conserve translation invariance in general ? Under which condition it will be translation invariant ?

2. Let $\Psi(x,t)$ be the wavefunction of a particle, show that $\Psi^*(x,-t)$ is the wavefunction of the particle with the momentum direction reversed.

3. For a given state $|x\rangle$, we have $\langle x'|x\rangle = \delta(x-x')$. Shows that $e^{-ipa}|x\rangle = |x+a\rangle$, where p is the momentum operator and a is a constant.

4. Let momentum state wave function for the state $\langle p|\Psi\rangle = \Psi(p)$. What is the momentum space wavefucntion for the time-reversed state $\langle p|T|\Psi\rangle$?

5. Let Π be a parity operator, prove that if $[\Pi, H] = 0$, a system that starts out in a state of certain parity maintain its parity.

6. Show that magnetic field applied to a system in general breaks the time reversal invariance. How about an electric field ?

Chapter 8

Problems

1. Show that the expected values of L_x and L_y are both zero on the eigenstate of L_z.

2. Show that the Hamiltonian $H = \frac{p^2}{2\mu} + V$ commutes with all three components of the angular momentum $\mathbf{L}$, provided that the potential V only dependents on r. Then show that $d\langle \mathbf{L} \rangle / dt = 0$ for any spherically symmetric potential.

3. A quantum particle is in the common eigenstate, Y_{20}, of the operators $(\mathbf{L}^2, L_z)$, please compute the possible observed values of L_x and their probabilities on the state .

4. Suppose that $\mathbf{J}$ is the angular momentum operator, and $\mathbf{n}_1, \mathbf{n}_2$ commute with $\mathbf{J}$, show that

$$[\mathbf{J} \cdot \mathbf{n}_1, \mathbf{J} \cdot \mathbf{n}_2] = i\mathbf{J} \cdot (\mathbf{n}_1 \times \mathbf{n}_2).$$

.

5. Given an angular momentum operator $\mathbf{J}$, $J_\pm = J_x \pm iJ_y$, show that

   (a) $J_z^n J_\pm = J_\pm (J_z \pm 1)^n$,

   (b) $e^{i\lambda J_z} J_x e^{-i\lambda J_z} = J_x \cos\lambda - J_y \sin\lambda$.

6. Show that $e^{i\lambda \mathbf{n} \cdot \boldsymbol{\sigma}} = \cos\lambda + i\mathbf{n} \cdot \boldsymbol{\sigma} \sin\lambda$, where λ is a constant and $\mathbf{n}$ is a unit vector.

7. Given two $S = 1/2$ spins with the Hamiltonian $H = J\mathbf{S}_1 \cdot \mathbf{S}_2$, what is the ground state of the system for $J > 0$ and $J < 0$ respectively ?

Chapter 9

Problems

1. The radial part of a quantum particle in central potential is

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + V(r) + \frac{l(l+1)\hbar^2}{2\mu r^2}\right] u_{nl}(r) = E u_{nl}(r),$$

   show that the bound state energy is larger for larger angular quantum number l, given the same radial quantum number n.

2. Show that for a bound state in a central potential, one has

$$\left\langle \frac{dV}{dr} \right\rangle - \frac{l(l+1)\hbar^2}{\mu} \left\langle \frac{1}{r^3} \right\rangle = \frac{2\pi\hbar^2}{\mu} |\Psi(0)|^2 ,$$

   where $\Psi = R(r)Y_{lm}(\theta, \phi)$ is the eigenstate of $(H, \mathbf{L}^2, L_z)$

3. Try to relate the radial equation of the isotropic Harmonic oscillator $V(r) = \alpha r^2$ and the Coulomb potential $V(r) = \beta/r$. In this way, you can deduce the eigenenergy with the knowledge of one to another.

4. Show that the kinetic energy and potential energy of the electron in hydrogen atom satisfy $\langle T \rangle = -\langle V \rangle/2$. Based on that, compute the expected value $\left\langle \frac{1}{r} \right\rangle$.

5. Let μ be the mass of electron, and c be the speed of light.

   (a) Convince yourself that $\mu c^2 \simeq 0.511 \times 10^6 eV$, and $\alpha = \frac{1}{4\pi\epsilon_0}\frac{e^2}{\hbar c} \simeq \frac{1}{137.04}$ is a dimensionless number (fine-structure constant),

   (b) Use these results to estimate the Bohr radius $a_0 = \frac{4\pi\epsilon_0\hbar^2}{\mu e^2}$ and Rydberg energy $\mathrm{Ry} = \frac{\hbar^2}{2\mu a_0^2} = \frac{\mu}{2}c^2\alpha^2 = \frac{\mu}{2}\left(\frac{e^2}{4\pi\epsilon_0\hbar}\right)^2$.

6. A single valence electron feel the following effective potential of the nuclei,

$$V(r) = \frac{-e^2}{r} - \lambda \frac{e^2 a_0}{r^2},$$

where a_0 is the Bohr radius, and $0 < \lambda \ll 1$. Please solve the energy spectrum and compare with the one of Hydrogen atom.

Chapter 10

Problems

1. Compute the ground state energy of anharmonic oscillator $V(x) = \frac{\mu\omega^2 x^2}{2} + \lambda x^4$ to the second order of the perturbation λ.

2. The relativistic correction to the Hamiltonian

$$H = \frac{\mathbf{p}^2}{2\mu} - \frac{\mathbf{p}^4}{8\mu^3 c^2} + V(r).$$

   Please compute the relativistic correction to the energy levels of the hydrogen atom $V(r) = -e^2/r$.

3. The spin-orbit correction to the Hamiltonian of the hydrogen atom is

$$H = \frac{\mathbf{p}^2}{2\mu} - e^2/r + \frac{e^2}{2\mu^2 c^2 r^3}\mathbf{L}\cdot\mathbf{S},$$

   Please compute its spin-orbit correction to the energy levels using first order Perturbation Theory.

4. A particle resides in a two dimensional infinite deep potential

$$V = \begin{cases} 0, & 0 < x < a,\ 0 < y < a, \\ \infty, & \text{otherwise} \end{cases},$$

   Please compute the effect of perturbation $H' = \lambda xy$ to the lowest two energy levels.

5. Consider certain ligand environment that gives the following perturbation $H' = \lambda(x^4 + y^4 + z^4 - \frac{3}{5}r^4)$ to the 3d orbitals in the central symmetric potential

$$
\begin{aligned}
\psi_1 &= \frac{1}{2}(y^2 - z^2) f(r), \\
\psi_2 &= \frac{1}{2\sqrt{3}}\left(2x^2 - y^2 - z^2\right) f(r), \\
\psi_3 &= yz f(r), \\
\psi_4 &= xz f(r), \\
\psi_5 &= xy f(r),
\end{aligned}
$$

try to analyze the splitting of each energy levels.

6. A system has two energy levels in the absence of perturbation, and its unperturbed Hamiltonian H_0 can be written as

$$
H_0 = \begin{bmatrix} E_1^{(0)} & 0 & 0 \\ 0 & E_1^{(0)} & 0 \\ 0 & 0 & E_2^{(0)} \end{bmatrix}, \qquad E_2^{(0)} > E_1^{(0)}
$$

After considering the perturbation, the Hamiltonian is represented as

$$
H = \begin{bmatrix} E_1^{(0)} & 0 & a \\ 0 & E_1^{(0)} & b \\ a^\star & b^\star & E_2^{(0)} \end{bmatrix},
$$

(a) Please calculate the eigenvalues of H by perturbation theory, up to the second order correction.

(b) Compute the exact eigenvalues by directly diagonalizing the H, and then compare the result with that in (a).