Solutions to Problems in Quantum Mechanics

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Most of the problems presented here are taken from the book
Sakurai, J. J., *Modern Quantum Mechanics*, Reading, MA: Addison-Wesley, 1985.

Contents

Part I

Problems

1 Fundamental Concepts

1.1 Consider a ket space spanned by the eigenkets $\{|a'\rangle\}$ of a Hermitian operator A. There is no degeneracy.
(a) Prove that

$$\prod_{a'}(A - a')$$

is a null operator.
(b) What is the significance of

$$\prod_{a''\neq a'} \frac{(A - a'')}{a' - a''}?$$

(c) Illustrate (a) and (b) using A set equal to S_z of a spin $\frac{1}{2}$ system.

1.2 A spin $\frac{1}{2}$ system is known to be in an eigenstate of $\vec{S}\cdot\hat{n}$ with eigenvalue $\hbar/2$, where $\hat{n}$ is a unit vector lying in the xz-plane that makes an angle γ with the positive z-axis.
(a) Suppose S_x is measured. What is the probability of getting $+\hbar/2$?
(b) Evaluate the dispersion in S_x, that is,

$$\langle (S_x - \langle S_x\rangle)^2\rangle.$$

(For your own peace of mind check your answers for the special cases $\gamma = 0$, $\pi/2$, and π.)

1.3 (a) The simplest way to derive the Schwarz inequality goes as follows. First observe

$$(\langle\alpha| + \lambda^*\langle\beta|)\cdot(|\alpha\rangle + \lambda|\beta\rangle) \geq 0$$

for any complex number λ; then choose λ in such a way that the preceding inequality reduces to the Schwarz inequility.

(b) Show that the equility sign in the generalized uncertainty relation holds if the state in question satisfies

$$\Delta A|\alpha\rangle = \lambda \Delta B|\alpha\rangle$$

with λ purely *imaginary.*

(c) Explicit calculations using the usual rules of wave mechanics show that the wave function for a Gaussian wave packet given by

$$\langle x'|\alpha\rangle = (2\pi d^2)^{-1/4} \exp\left[\frac{i\langle p\rangle x'}{\hbar} - \frac{(x' - \langle x\rangle)^2}{4d^2}\right]$$

satisfies the uncertainty relation

$$\sqrt{\langle(\Delta x)^2\rangle}\sqrt{\langle(\Delta p)^2\rangle} = \frac{\hbar}{2}.$$

Prove that the requirement

$$\langle x'|\Delta x|\alpha\rangle = (\textbf{imaginary number})\langle x'|\Delta p|\alpha\rangle$$

is indeed satisfied for such a Gaussian wave packet, in agreement with (b).

1.4 (a) Let x and p_x be the coordinate and linear momentum in one dimension. Evaluate the classical Poisson bracket

$$[x, F(p_x)]_{classical}\,.$$

(b) Let x and p_x be the corresponding quantum-mechanical operators this time. Evaluate the commutator

$$\left[x, \exp\left(\frac{ip_x a}{\hbar}\right)\right].$$

(c) Using the result obtained in (b), prove that

$$\exp\left(\frac{ip_x a}{\hbar}\right)|x'\rangle, \quad (x|x'\rangle = x'|x'\rangle)$$

is an eigenstate of the coordinate operator x. What is the corresponding eigenvalue?

1.5 (a) Prove the following:

$$\begin{aligned} (i) \quad \langle p'|x|\alpha\rangle &= i\hbar\frac{\partial}{\partial p'}\langle p'|\alpha\rangle, \\ (ii) \quad \langle\beta|x|\alpha\rangle &= \int dp'\phi_\beta^*(p')i\hbar\frac{\partial}{\partial p'}\phi_\alpha(p'), \end{aligned}$$

where $\phi_\alpha(p') = \langle p'|\alpha\rangle$ and $\phi_\beta(p') = \langle p'|\beta\rangle$ are momentum-space wave functions.
(b) What is the physical significance of

$$\exp\left(\frac{ix\Xi}{\hbar}\right),$$

where x is the position operator and Ξ is some number with the dimension of momentum? Justify your answer.

2 Quantum Dynamics

2.1 Consider the spin-procession problem discussed in section 2.1 in Jackson. It can also be solved in the Heisenberg picture. Using the Hamiltonian

$$H = -\left(\frac{eB}{mc}\right)S_z = \omega S_z,$$

write the Heisenberg equations of motion for the time-dependent operators $S_x(t)$, $S_y(t)$, and $S_z(t)$. Solve them to obtain $S_{x,y,z}$ as functions of time.

2.2 Let $x(t)$ be the coordinate operator for a free particle in one dimension in the Heisenberg picture. Evaluate

$$[x(t), x(0)].$$

2.3 Consider a particle in three dimensions whose Hamiltonian is given by

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

By calculating $[\vec{x} \cdot \vec{p}, H]$ obtain

$$\frac{d}{dt}\langle \vec{x} \cdot \vec{p} \rangle = \left\langle \frac{p^2}{m} \right\rangle - \langle \vec{x} \cdot \vec{\nabla} V \rangle.$$

To identify the preceding relation with the quantum-mechanical analogue of the virial theorem it is essential that the left-hand side vanish. Under what condition would this happen?

2.4 (a) Write down the wave function (in coordinate space) for the state

$$\exp\left(\frac{-ipa}{\hbar}\right)|0\rangle.$$

You may use

$$\langle x'|0\rangle = \pi^{-1/4} x_0^{-1/2} \exp\left[-\tfrac{1}{2}\left(\frac{x'}{x_0}\right)^2\right], \quad \left(x_0 \equiv \left(\frac{\hbar}{m\omega}\right)^{1/2}\right).$$

(b) Obtain a simple expression that the probability that the state is found in the ground state at $t = 0$. Does this probability change for $t > 0$?

2.5 Consider a function, known as the *correlation function*, defined by

$$C(t) = \langle x(t) x(0) \rangle,$$

where $x(t)$ is the position operator in the Heisenberg picture. Evaluate the correlation function explicitly for the ground state of a one-dimensional simple harmonic oscillator.

2.6 Consider again a one-dimensional simple harmonic oscillator. Do the following algebraically, that is, without using wave functions.

(a) Construct a linear combination of $|0\rangle$ and $|1\rangle$ such that $\langle x\rangle$ is as large as possible.

(b) Suppose the oscillator is in the state constructed in (a) at $t = 0$. What is the state vector for $t > 0$ in the Schrödinger picture? Evaluate the expectation value $\langle x\rangle$ as a function of time for $t > 0$ using (i) the Schrödinger picture and (ii) the Heisenberg picture.

(c) Evaluate $\langle (\Delta x)^2\rangle$ as a function of time using either picture.

2.7 A *coherent state* of a one-dimensional simple harmonic oscillator is defined to be an eigenstate of the (non-Hermitian) annihilation operator a:

$$a|\lambda\rangle = \lambda|\lambda\rangle,$$

where λ is, in general, a complex number.

(a) Prove that

$$|\lambda\rangle = e^{-|\lambda|^2/2} e^{\lambda a^\dagger}|0\rangle$$

is a normalized coherent state.

(b) Prove the minimum uncertainty relation for such a state.

(c) Write $|\lambda\rangle$ as

$$|\lambda\rangle = \sum_{n=0}^{\infty} f(n)|n\rangle.$$

Show that the distribution of $|f(n)|^2$ with respect to n is of the Poisson form. Find the most probable value of n, hence of E.

(d) Show that a coherent state can also be obtained by applying the translation (finite-displacement) operator $e^{-ipl/\hbar}$ (where p is the momentum operator, and l is the displacement distance) to the ground state.

(e) Show that the coherent state $|\lambda\rangle$ remains coherent under time-evolution and calculate the time-evolved state $|\lambda(t)\rangle$. (Hint: directly apply the time-evolution operator.)

2.8 The quntum mechanical propagator, for a particle with mass m, moving in a potential is given by:

$$K(x,y;E) = \int_0^\infty dt e^{iEt/\hbar} K(x,y;t,0) = A\sum_n \frac{\sin(nrx)\sin(nry)}{E - \frac{\hbar^2 r^2}{2m} n^2}$$

where A is a constant.
(a) What is the potential?

(b) Determine the constant A in terms of the parameters describing the system (such as m, r etc.).

2.9 Prove the relation

$$\frac{d\theta(x)}{dx} = \delta(x)$$

where $\theta(x)$ is the (unit) step function, and $\delta(x)$ the Dirac delta function. (Hint: study the effect on testfunctions.)

2.10 Derive the following expression

$$S_{cl} = \frac{m\omega}{2\sin(\omega T)}\left[(x_0^2 + 2x_T^2)\cos(\omega T) - x_0 x_T\right]$$

for the classical action for a harmonic oscillator moving from the point x_0 at $t = 0$ to the point x_T at $t = T$.

2.11 The Lagrangian of the single harmonic oscillator is

$$\mathcal{L} = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}m\omega^2 x^2$$

(a) Show that

$$\langle x_b t_b | x_a t_a \rangle = exp\left[\frac{iS_{cl}}{\hbar}\right] G(0, t_b; 0, t_a)$$

where S_{cl} **is the action along the classical path** x_{cl} **from** (x_a, t_a) **to** (x_b, t_b) **and** G **is**

$$G(0, t_b; 0, t_a) =$$
$$\lim_{N\to\infty} \int dy_1 \dots dy_N \left(\frac{m}{2\pi i\hbar\varepsilon}\right)^{\frac{(N+1)}{2}} exp\left\{\frac{i}{\hbar}\sum_{j=0}^{N}\left[\frac{m}{2\varepsilon}(y_{j+1}-y_j)^2 - \frac{1}{2}\varepsilon m\omega^2 y_j^2\right]\right\}$$

where $\varepsilon = \frac{t_b - t_a}{(N+1)}$.

(Hint: Let $y(t) = x(t) - x_{cl}(t)$ **be the new integration variable,** $x_{cl}(t)$ **being the solution of the Euler-Lagrange equation.)**

(b) Show that G **can be written as**

$$G = \lim_{N\to\infty}\left(\frac{m}{2\pi i\hbar\varepsilon}\right)^{\frac{(N+1)}{2}} \int dy_1 \dots dy_N exp(-n^T \sigma n)$$

where $n = \begin{bmatrix} y_1 \\ \vdots \\ y_N \end{bmatrix}$ **and** n^T **is its transpose. Write the *symmetric* matrix** σ**.**

(c) Show that

$$\int dy_1 \dots dy_N exp(-n^T\sigma n) \equiv \int d^N y e^{-n^T\sigma n} = \frac{\pi^{N/2}}{\sqrt{det\sigma}}$$

[Hint: Diagonalize σ **by an orhogonal matrix.]**

(d) Let $\left(\frac{2i\hbar\varepsilon}{m}\right)^N det\sigma \equiv det\sigma'_N \equiv p_N$**. Define** $j \times j$ **matrices** σ'_j **that consist of the first** j **rows and** j **columns of** σ'_N **and whose determinants are** p_j**. By expanding** σ'_{j+1} **in minors show the following recursion formula for the** p_j**:**

$$p_{j+1} = (2 - \varepsilon^2\omega^2)p_j - p_{j-1} \qquad j = 1, \dots, N \qquad (2.1)$$

(e) Let $\phi(t) = \varepsilon p_j$ for $t = t_a + j\varepsilon$ and show that (2.1) implies that in the limit $\varepsilon \to 0, \phi(t)$ satisfies the equation

$$\frac{d^2\phi}{dt^2} = -\omega^2\phi(t)$$

with initial conditions $\phi(t = t_a) = 0, \frac{d\phi(t=t_a)}{dt} = 1$.

(f) Show that

$$\langle x_b t_b | x_a t_a \rangle = \sqrt{\frac{m\omega}{2\pi i\hbar \sin(\omega T)}} exp\left\{\frac{im\omega}{2\hbar \sin(\omega T)}[(x_b^2 + x_a^2)\cos(\omega T) - 2x_a x_b]\right\}$$

where $T = t_b - t_a$.

2.12 Show the composition property

$$\int dx_1 K_f(x_2, t_2; x_1, t_1) K_f(x_1, t_1; x_0, t_0) = K_f(x_2, t_2; x_0, t_0)$$

where $K_f(x_1, t_1; x_0, t_0)$ is the free propagator (Sakurai 2.5.16), by explicitly performing the integral (*i.e.* do *not* use completeness).

2.13 (a) Verify the relation

$$[\Pi_i, \Pi_j] = \left(\frac{i\hbar e}{c}\right)\varepsilon_{ijk}B_k$$

where $\vec{\Pi} \equiv m\frac{\vec{x}}{dt} = \vec{p} - \frac{e\vec{A}}{c}$ and the relation

$$m\frac{d^2\vec{x}}{dt^2} = \frac{d\vec{\Pi}}{dt} = e\left[\vec{E} + \frac{1}{2c}\left(\frac{d\vec{x}}{dt} \times \vec{B} - \vec{B} \times \frac{d\vec{x}}{dt}\right)\right].$$

(b) Verify the continuity equation

$$\frac{\partial\rho}{\partial t} + \vec{\nabla}' \cdot \vec{j} = 0$$

with $\vec{j}$ given by

$$\vec{j} = \left(\frac{\hbar}{m}\right) \Im(\psi^* \vec{\nabla}' \psi) - \left(\frac{e}{mc}\right) \vec{A}|\psi|^2.$$

2.14 An electron moves in the presence of a uniform magnetic field in the z-direction ($\vec{B} = B\hat{z}$).

(a) Evaluate

$$[\Pi_x, \Pi_y],$$

where

$$\Pi_x \equiv p_x - \frac{eA_x}{c}, \qquad \Pi_y \equiv p_y - \frac{eA_y}{c}.$$

(b) By comparing the Hamiltonian and the commutation relation obtained in (a) with those of the one-dimensional oscillator problem show how we can immediately write the energy eigenvalues as

$$E_{k,n} = \frac{\hbar^2 k^2}{2m} + \left(\frac{|eB|\hbar}{mc}\right)\left(n + \frac{1}{2}\right),$$

where $\hbar k$ is the continuous eigenvalue of the p_z operator and n is a nonnegative integer including zero.

2.15 Consider a particle of mass m and charge q in an impenetrable cylinder with radius R and height a. Along the axis of the cylinder runs a thin, impenetrable solenoid carrying a magnetic flux Φ. Calculate the ground state energy and wavefunction.

2.16 A particle in one dimension ($-\infty < x < \infty$) is subjected to a constant force derivable from

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

(a) Is the energy spectrum continuous or discrete? Write down an approximate expression for the energy eigenfunction specified by E.

(b) Discuss briefly what changes are needed if V is replaced be

$$V = \lambda |x|.$$

3 Theory of Angular Momentum

3.1 Consider a sequence of Euler rotations represented by

$$\begin{aligned}
\mathcal{D}^{(1/2)}(\alpha, \beta, \gamma) &= \exp\left(\frac{-i\sigma_3\alpha}{2}\right)\exp\left(\frac{-i\sigma_2\beta}{2}\right)\exp\left(\frac{-i\sigma_3\gamma}{2}\right) \\
&= \begin{pmatrix} e^{-i(\alpha+\gamma)/2}\cos\frac{\beta}{2} & -e^{-i(\alpha-\gamma)/2}\sin\frac{\beta}{2} \\ e^{i(\alpha-\gamma)/2}\sin\frac{\beta}{2} & e^{i(\alpha+\gamma)/2}\cos\frac{\beta}{2} \end{pmatrix}.
\end{aligned}$$

Because of the group properties of rotations, we expect that this sequence of operations is equivalent to a *single* rotation about some axis by an angle ϕ. Find ϕ.

3.2 An angular-momentum eigenstate $|j, m = m_{\max} = j\rangle$ is rotated by an infinitesimal angle ε about the y-axis. Without using the explicit form of the $d^{(j)}_{m'm}$ function, obtain an expression for the probability for the new rotated state to be found in the original state up to terms of order ε^2.

3.3 The wave function of a patricle subjected to a spherically symmetrical potential $V(r)$ is given by

$$\psi(\vec{x}) = (x + y + 3z)f(r).$$

(a) Is ψ an eigenfunction of $\vec{L}$? If so, what is the l-value? If not, what are the possible values of l we may obtain when $\vec{L}^2$ is measured?

(b) What are the probabilities for the particle to be found in various m_l states?

(c) Suppose it is known somehow that $\psi(\vec{x})$ is an energy eigenfunction with eigenvalue E. Indicate how we may find $V(r)$.

3.4 Consider a particle with an ***intrinsic*** angular momentum (or spin) of one unit of $\hbar$. (One example of such a particle is the ϱ-meson). Quantum-mechanically, such a particle is described by a ketvector $|\varrho\rangle$ or in $\vec{x}$ representation a wave function

$$\varrho^i(\vec{x}) = \langle \vec{x}; i|\varrho\rangle$$

where $|\vec{x}, i\rangle$ correspond to a particle at $\vec{x}$ with spin in the i:th direction.

(a) Show explicitly that infinitesimal rotations of $\varrho^i(\vec{x})$ are obtained by acting with the operator

$$u_{\vec{\varepsilon}} = 1 - i\frac{\vec{\varepsilon}}{\hbar} \cdot (\vec{L} + \vec{\mathcal{S}}) \tag{3.1}$$

where $\vec{L} = \frac{\hbar}{i}\hat{r} \times \vec{\nabla}$. Determine $\vec{\mathcal{S}}$!

(b) Show that $\vec{L}$ and $\vec{\mathcal{S}}$ commute.

(c) Show that $\vec{\mathcal{S}}$ is a vector operator.

(d) Show that $\vec{\nabla} \times \vec{\varrho}(\vec{x}) = \frac{1}{\hbar^2}(\vec{\mathcal{S}} \cdot \vec{p})\vec{\varrho}$ where $\vec{p}$ is the momentum operator.

3.5 We are to add angular momenta $j_1 = 1$ and $j_2 = 1$ to form $j = 2, 1$, and 0 states. Using the ladder operator method express all

(nine) j, m eigenkets in terms of $|j_1 j_2; m_1 m_2\rangle$. Write your answer as

$$|j=1, m=1\rangle = \frac{1}{\sqrt{2}}|+,0\rangle - \frac{1}{\sqrt{2}}|0,+\rangle, \ldots, \tag{3.2}$$

where $+$ and 0 stand for $m_{1,2} = 1, 0$, respectively.

3.6 (a) Construct a spherical tensor of rank 1 out of two different vectors $\vec{U} = (U_x, U_y, U_z)$ and $\vec{V} = (V_x, V_y, V_z)$. Explicitly write $T^{(1)}_{\pm 1,0}$ in terms of $U_{x,y,z}$ and $V_{x,y,z}$.

(b) Construct a spherical tensor of rank 2 out of two different vectors $\vec{U}$ and $\vec{V}$. Write down explicitly $T^{(2)}_{\pm 2, \pm 1, 0}$ in terms of $U_{x,y,z}$ and $V_{x,y,z}$.

3.7 (a) Evaluate

$$\sum_{m=-j}^{j} |d^{(j)}_{mm'}(\beta)|^2 m$$

for any j (integer or half-integer); then check your answer for $j = \frac{1}{2}$.

(b) Prove, for any j,

$$\sum_{m=-j}^{j} m^2 |d^{(j)}_{m'm}(\beta)|^2 = \tfrac{1}{2} j(j+1) \sin\beta + m'^2 + \tfrac{1}{2}(3\cos^2\beta - 1).$$

[*Hint*: This can be proved in many ways. You may, for instance, examine the rotational properties of J_z^2 using the spherical (irreducible) tensor language.]

3.8 (a) Write xy, xz, and $(x^2 - y^2)$ as components of a spherical (irreducible) tensor of rank 2.

(b) The expectation value

$$Q \equiv e\langle \alpha, j, m=j|(3z^2 - r^2)|\alpha, j, m=j\rangle$$

is known as the *quadrupole moment.* Evaluate

$$e\langle \alpha, j, m'|(x^2 - y^2)|\alpha, j, m=j\rangle,$$

(where $m' = j, j-1, j-2, \dots$)in terms of Q and appropriate Clebsch-Gordan coefficients.

4 Symmetry in Quantum Mechanics

4.1 (a) Assuming that the Hamiltonian is invariant under time reversal, prove that the wave function for a spinless nondegenerate system at any given instant of time can always be chosen to be real.

(b) The wave function for a plane-wave state at $t = 0$ is given by a complex function $e^{i\vec{p}\cdot\vec{x}/\hbar}$. Why does this not violate time-reversal invariance?

4.2 Let $\phi(\vec{p}')$ be the momentum-space wave function for state $|\alpha\rangle$, that is, $\phi(\vec{p}') = \langle\vec{p}'|\alpha\rangle$.Is the momentum-space wave function for the time-reversed state $\Theta|\alpha\rangle$ given by $\phi(\vec{p}'$, $\phi(-\vec{p}')$, $\phi^*(\vec{p}')$, or $\phi^*(-\vec{p}')$? Justify your answer.

4.3 Read section 4.3 in Sakurai to refresh your knowledge of the quantum mechanics of periodic potentials. You know that the energybands in solids are described by the so called Bloch functions $\psi_{n,k}$ fullfilling,

$$\psi_{n,k}(x+a) = e^{ika}\psi_{n,k}(x)$$

where a is the lattice constant, n labels the band, and the lattice momentum k is restricted to the Brillouin zone $[-\pi/a, \pi/a]$.

Prove that any Bloch function can be written as,

$$\psi_{n,k}(x) = \sum_{R_i} \phi_n(x - R_i) e^{ikR_i}$$

where the sum is over all lattice vectors R_i. (In this simble one dimensional problem $R_i = ia$, but the construction generalizes easily to three dimensions.).

The functions ϕ_n are called Wannier functions, and are important in the tight-binding description of solids. Show that the Wannier functions are corresponding to different sites and/or different bands are orthogonal, *i.e.* prove

$$\int dx \phi_m^\star(x - R_i) \phi_n(x - R_j) \sim \delta_{ij} \delta_{mn}$$

Hint: Expand the ϕ_ns in Bloch functions and use their orthonormality properties.

4.4 Suppose a spinless particle is bound to a fixed center by a potential $V(\vec{x})$ so assymetrical that no energy level is degenerate. Using the time-reversal invariance prove

$$\langle \vec{L} \rangle = 0$$

for any energy eigenstate. (This is known as *quenching* of orbital angular momemtum.) If the wave function of such a nondegenerate eigenstate is expanded as

$$\sum_l \sum_m F_{lm}(r) Y_l^m(\theta, \phi),$$

what kind of phase restrictions do we obtain on $F_{lm}(r)$?

4.5 The Hamiltonian for a spin 1 system is given by

$$H = AS_z^2 + B(S_x^2 - S_y^2).$$