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.

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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:

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

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**:**

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

(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 $m' = j, j-1, j-2, \ldots$)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

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

Solve this problem *exactly* to find the normalized energy eigenstates and eigenvalues. (A spin-dependent Hamiltonian of this kind actually appears in crystal physics.) Is this Hamiltonian invariant under time reversal? How do the normalized eigenstates you obtained transform under time reversal?

5 Approximation Methods

5.1 Consider an isotropic harmonic oscillator in *two* dimensions. The Hamiltonian is given by

$$H_0 = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{m\omega^2}{2}(x^2 + y^2)$$

(a) What are the energies of the three lowest-lying states? Is there any degeneracy?

(b) We now apply a perturbation

$$V = \delta m\omega^2 xy$$

where δ is a dimensionless real number much smaller than unity. Find the zeroth-order energy eigenket and the corresponding energy to first order [that is the unperturbed energy obtained in (a) plus the first-order energy shift] for each of the three lowest-lying states.

(c) Solve the $H_0 + V$ problem *exactly.* Compare with the perturbation results obtained in (b).
[You may use $\langle n'|x|n\rangle = \sqrt{\hbar/2m\omega}(\sqrt{n+1}\delta_{n',n+1} + \sqrt{n}\delta_{n',n-1})$.]

5.2 A system that has three unperturbed states can be represented by the perturbed Hamiltonian matrix

$$\begin{pmatrix} E_1 & 0 & a \\ 0 & E_1 & b \\ a^* & b^* & E_2 \end{pmatrix}$$

where $E_2 > E_1$. The quantities a and b are to be regarded as perturbations that are of the same order and are small compared with $E_2 - E_1$. Use the second-order nondegenerate perturbation theory to calculate the perturbed eigenvalues. (Is this procedure correct?) Then diagonalize the matrix to find the exact eigenvalues. Finally, use the second-order degenerate perturbation theory. Compare the three results obtained.

5.3 A one-dimensional harmonic oscillator is in its ground state for $t < 0$. For $t \geq 0$ it is subjected to a time-dependent but spatially uniform *force* (not potential!) in the x-direction,

$$F(t) = F_0 e^{-t/\tau}$$

(a) Using time-dependent perturbation theory to first order, obtain the probability of finding the oscillator in its first excited state for $t > 0$). Show that the $t \to \infty$ (τ finite) limit of your expression is independent of time. Is this reasonable or surprising?

(b) Can we find higher excited states?
[You may use $\langle n'|x|n\rangle = \sqrt{\hbar/2m\omega}(\sqrt{n+1}\delta_{n',n+1} + \sqrt{n}\delta_{n',n-1})$.]

5.4 Consider a composite system made up of two spin $\frac{1}{2}$ objects. for $t < 0$, the Hamiltonian does not depend on spin and can be taken to be zero by suitably adjusting the energy scale. For $t > 0$, the Hamiltonian is given by

$$H = \left(\frac{4\Delta}{\hbar^2}\right) \vec{S}_1 \cdot \vec{S}_2.$$

Suppose the system is in $|+-\rangle$ for $t \leq 0$. Find, as a function of time, the probability for being found in each of the following states $|++\rangle$, $|+-\rangle$, $|-+\rangle$, $|--\rangle$:

(a) By solving the problem exactly.

(b) By solving the problem assuming the validity of first-order time-dependent perturbation theory with H as a perturbation switched on at $t = 0$. Under what condition does (b) give the correct results?

5.5 The ground state of a hydrogen atom ($n = 1, l = 0$) is subjected to a time-dependent potential as follows:

$$V(\vec{x}, t) = V_0 \cos(kz - \omega t).$$

Using time-dependent perturbation theory, obtain an expression for the transition rate at which the electron is emitted with momentum $\vec{p}$. Show, in particular, how you may compute the angular distribution of the ejected electron (in terms of θ and ϕ defined with respect to the z-axis). Discuss ***briefly*** the similarities and the differences between this problem and the (more realistic) photoelectric effect. (***note:*** For the initial wave function use

$$\Psi_{n=1,l=0}(\vec{x}) = \frac{1}{\sqrt{\pi}} \left(\frac{Z}{a_0} \right)^{\frac{3}{2}} e^{-Zr/a_0}.$$

If you have a normalization problem, the final wave function may be taken to be

$$\Psi_f(\vec{x}) = \left(\frac{1}{L^{\frac{3}{2}}} \right) e^{i\vec{p}\cdot\vec{x}/\hbar}$$

with L very large, but you should be able to show that the observable effects are independent of L.)

Part II

Solutions

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.

(a) Assume that $|\alpha\rangle$ is an arbitrary state ket. Then

$$\begin{aligned}\prod_{a'}(A-a')|\alpha\rangle &= \prod_{a'}(A-a')\sum_{a''}|a''\rangle\underbrace{\langle a''|\alpha\rangle}_{c_{a''}} = \sum_{a''}c_{a''}\prod_{a'}(A-a')|a''\rangle \\ &= \sum_{a''}c_{a''}\prod_{a'}(a''-a')|a''\rangle \overset{a''\in\{a'\}}{=} 0. \qquad (1.1)\end{aligned}$$

(b) Again for an arbitrary state $|\alpha\rangle$ we will have

$$\begin{aligned}\left[\prod_{a''\neq a'}\frac{(A-a'')}{a'-a''}\right]|\alpha\rangle &= \left[\prod_{a''\neq a'}\frac{(A-a'')}{a'-a''}\right]\overbrace{\sum_{a'''}|a'''\rangle\langle a'''|}^{1}|\alpha\rangle \\ &= \sum_{a'''}\langle a'''|\alpha\rangle\prod_{a''\neq a'}\frac{(a'''-a'')}{a'-a''}|a'''\rangle = \\ &= \sum_{a'''}\langle a'''|\alpha\rangle\delta_{a'''a'}|a'''\rangle = \langle a'|\alpha\rangle|a'\rangle \Rightarrow \\ \left[\prod_{a''\neq a'}\frac{(A-a'')}{a'-a''}\right] &= |a'\rangle\langle a'| \equiv \Lambda_{a'}. \qquad (1.2)\end{aligned}$$

So it projects to the eigenket $|a'\rangle$.

(c) It is $S_z \equiv \hbar/2(|+\rangle\langle+| - |-\rangle\langle-|)$. This operator has eigenkets $|+\rangle$ and $|-\rangle$ with eigenvalues $\hbar/2$ and -$\hbar/2$ respectively. So

$$\begin{aligned}
\prod_{a'}(S_z - a') &= \prod_{a'}(S_z - a'1) \\
&= \left[\frac{\hbar}{2}(|+\rangle\langle+| - |-\rangle\langle-|) - \frac{\hbar}{2}(|+\rangle\langle+| + |-\rangle\langle-|)\right] \\
&\quad \times \left[\frac{\hbar}{2}(|+\rangle\langle+| - |-\rangle\langle-|) + \frac{\hbar}{2}(|+\rangle\langle+| + |-\rangle\langle-|)\right] \\
&= [-\hbar|-\rangle\langle-|][\hbar|+\rangle\langle+|] = -\hbar^2|-\rangle\overbrace{\langle-|+\rangle}^{0}\langle+| = 0, \qquad (1.3)
\end{aligned}$$

where we have used that $|+\rangle\langle+| + |-\rangle\langle-| = 1$.

For $a' = \hbar/2$ we have

$$\begin{aligned}
\prod_{a''\neq a'}\frac{(S_z - a'')}{a' - a''} &= \prod_{a''\neq\hbar/2}\frac{(S_z - a''1)}{\hbar/2 - a''} = \frac{S_z + \frac{\hbar}{2}1}{\hbar/2 + \hbar/2} \\
&= \frac{1}{\hbar}\left[\frac{\hbar}{2}(|+\rangle\langle+| - |-\rangle\langle-|) + \frac{\hbar}{2}(|+\rangle\langle+| + |-\rangle\langle-|)\right] \\
&= \frac{1}{\hbar}\hbar|+\rangle\langle+| = |+\rangle\langle+|. \qquad (1.4)
\end{aligned}$$

Similarly for $a' = -\hbar/2$ we have

$$\begin{aligned}
\prod_{a''\neq a'}\frac{(S_z - a'')}{a' - a''} &= \prod_{a''\neq-\hbar/2}\frac{(S_z - a''1)}{-\hbar/2 - a''} = \frac{S_z - \frac{\hbar}{2}1}{-\hbar/2 - \hbar/2} \\
&= -\frac{1}{\hbar}\left[\frac{\hbar}{2}(|+\rangle\langle+| - |-\rangle\langle-|) - \frac{\hbar}{2}(|+\rangle\langle+| + |-\rangle\langle-|)\right] \\
&= -\frac{1}{\hbar}(-\hbar|-\rangle\langle-|) = |-\rangle\langle-|. \qquad (1.5)
\end{aligned}$$

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.)

Since the unit vector $\hat{n}$ makes an angle γ with the positive z-axis and is lying in the xz-plane, it can be written in the following way

$$\hat{n} = \hat{e}_z \cos\gamma + \hat{e}_x \sin\gamma \tag{1.6}$$

So

$$\begin{aligned} \vec{S}\cdot\hat{n} &= S_z \cos\gamma + S_x \sin\gamma = \quad \text{[(S-1.3.36),(S-1.4.18)]} \\ &= \left[\frac{\hbar}{2}\left(|+\rangle\langle+| - |-\rangle\langle-|\right)\right]\cos\gamma + \left[\frac{\hbar}{2}\left(|+\rangle\langle-| + |-\rangle\langle+|\right)\right]\sin\gamma \end{aligned} \tag{1.7}$$

Since the system is in an eigenstate of $\vec{S}\cdot\hat{n}$ with eigenvalue $\hbar/2$ it has to satisfay the following equation

$$\vec{S}\cdot\hat{n}|\vec{S}\cdot\hat{n};+\rangle = \hbar/2|\vec{S}\cdot\hat{n};+\rangle. \tag{1.8}$$

From (1.7) we have that

$$\vec{S}\cdot\hat{n} \doteq \frac{\hbar}{2}\begin{pmatrix} \cos\gamma & \sin\gamma \\ \sin\gamma & -\cos\gamma \end{pmatrix}. \tag{1.9}$$

The eigenvalues and eigenfuncions of this operator can be found if one solves the secular equation

$$\det(\vec{S}\cdot\hat{n} - \lambda I) = 0 \Rightarrow \det\begin{pmatrix} \hbar/2\cos\gamma - \lambda & \hbar/2\sin\gamma \\ \hbar/2\sin\gamma & -\hbar/2\cos\gamma - \lambda \end{pmatrix} = 0 \Rightarrow$$

$$-\frac{\hbar^2}{4}\cos^2\gamma + \lambda^2 - \frac{\hbar^2}{4}\sin^2\gamma = 0 \Rightarrow \lambda^2 - \frac{\hbar^2}{4} = 0 \Rightarrow \lambda = \pm\frac{\hbar}{2}. \tag{1.10}$$

Since the system is in the eigenstate $|\vec{S}\cdot\hat{n};+\rangle \equiv \begin{pmatrix} a \\ b \end{pmatrix}$ we will have that

$$\frac{\hbar}{2}\begin{pmatrix} \cos\gamma & \sin\gamma \\ \sin\gamma & -\cos\gamma \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} a \\ b \end{pmatrix} \Rightarrow \left\{\begin{array}{c} a\cos\gamma + b\sin\gamma = a \\ a\sin\gamma - b\cos\gamma = b \end{array}\right\} \Rightarrow$$

$$b = a\frac{1-\cos\gamma}{\sin\gamma} = a\frac{2\sin^2\frac{\gamma}{2}}{2\sin\frac{\gamma}{2}\cos\frac{\gamma}{2}} = a\tan\frac{\gamma}{2}. \tag{1.11}$$

But we want also the eigenstate $|\vec{S}\cdot\hat{n};+\rangle$ to be normalized, that is

$$\begin{aligned} a^2+b^2=1 \quad &\Rightarrow \quad a^2+a^2\tan^2\frac{\gamma}{2}=1 \Rightarrow a^2\cos^2\frac{\gamma}{2}a^2\sin^2\frac{\gamma}{2}=\cos^2\frac{\gamma}{2} \\ &\Rightarrow \quad a^2=\cos^2\frac{\gamma}{2} \Rightarrow a=\pm\sqrt{\cos^2\frac{\gamma}{2}}=\cos\frac{\gamma}{2}, \end{aligned} \tag{1.12}$$

where the real positive convention has been used in the last step. This means that the state in which the system is in, is given in terms of the eigenstates of the S_z operator by

$$|\vec{S}\cdot\hat{n};+\rangle=\cos\frac{\gamma}{2}|+\rangle+\sin\frac{\gamma}{2}|-\rangle. \tag{1.13}$$

(a) From (S-1.4.17) we know that

$$|S_x;+\rangle=\frac{1}{\sqrt{2}}|+\rangle+\frac{1}{\sqrt{2}}|-\rangle. \tag{1.14}$$

So the propability of getting $+\hbar/2$ when S_x is measured is given by

$$\begin{aligned} \left|\langle S_x;+|\vec{S}\cdot\hat{n};+\rangle\right|^2 &= \left|\left(\frac{1}{\sqrt{2}}\langle+|+\frac{1}{\sqrt{2}}\langle-|\right)\left(\cos\frac{\gamma}{2}|+\rangle+\sin\frac{\gamma}{2}|-\rangle\right)\right|^2 \\ &= \left|\frac{1}{\sqrt{2}}\cos\frac{\gamma}{2}+\frac{1}{\sqrt{2}}\sin\frac{\gamma}{2}\right|^2 \\ &= \frac{1}{2}\cos^2\frac{\gamma}{2}+\frac{1}{2}\sin^2\frac{\gamma}{2}+\cos\frac{\gamma}{2}\sin\frac{\gamma}{2} \\ &= \tfrac{1}{2}+\tfrac{1}{2}\sin\gamma=\tfrac{1}{2}(1+\sin\gamma). \end{aligned} \tag{1.15}$$

For $\gamma=0$ which means that the system is in the $|S_z;+\rangle$ eigenstate we have

$$|\langle S_x;+|S_z;+\rangle|^2=\tfrac{1}{2}(1)=\tfrac{1}{2}. \tag{1.16}$$

For $\gamma=\pi/2$ which means that the system is in the $|S_x;+\rangle$ eigenstate we have

$$|\langle S_x;+|S_x;+\rangle|^2=1. \tag{1.17}$$

For $\gamma=\pi$ which means that the system is in the $|S_z;-\rangle$ eigenstate we have

$$|\langle S_x;+|S_z;-\rangle|^2=\tfrac{1}{2}(1)=\tfrac{1}{2}. \tag{1.18}$$

(b) We have that

$$\langle (S_x - \langle S_x \rangle)^2 \rangle = \langle S_x^2 \rangle - (\langle S_x \rangle)^2. \tag{1.19}$$

As we know

$$\begin{aligned} S_x &= \frac{\hbar}{2}\left(|+\rangle\langle -| + |-\rangle\langle +|\right) \Rightarrow \\ S_x^2 &= \frac{\hbar^2}{4}\left(|+\rangle\langle -| + |-\rangle\langle +|\right)\left(|+\rangle\langle -| + |-\rangle\langle +|\right) \Rightarrow \\ S_x^2 &= \frac{\hbar^2}{4}\underbrace{\left(|+\rangle\langle +| + |-\rangle\langle -|\right)}_{1} = \frac{\hbar^2}{4}. \end{aligned} \tag{1.20}$$

So

$$\begin{aligned} \langle S_x \rangle &= \left[\cos\frac{\gamma}{2}\langle +| + \sin\frac{\gamma}{2}\langle -|\right]\frac{\hbar}{2}\left(|+\rangle\langle -| + |-\rangle\langle +|\right)\left[\cos\frac{\gamma}{2}|+\rangle + \sin\frac{\gamma}{2}|-\rangle\right] \\ &= \frac{\hbar}{2}\cos\frac{\gamma}{2}\sin\frac{\gamma}{2} + \frac{\hbar}{2}\sin\frac{\gamma}{2}\cos\frac{\gamma}{2} = \frac{\hbar}{2}\sin\gamma \Rightarrow \\ (\langle S_x \rangle)^2 &= \frac{\hbar^2}{4}\sin^2\gamma \text{ and} \\ \langle S_x^2 \rangle &= \left[\cos\frac{\gamma}{2}\langle +| + \sin\frac{\gamma}{2}\langle -|\right]\frac{\hbar^2}{4}\left[\cos\frac{\gamma}{2}|+\rangle + \sin\frac{\gamma}{2}|-\rangle\right] \\ &= \frac{\hbar^2}{4}[\cos^2\frac{\gamma}{2} + \sin^2\frac{\gamma}{2}] = \frac{\hbar^2}{4}. \end{aligned} \tag{1.21}$$

So substituting in (1.19) we will have

$$\langle (S_x - \langle S_x \rangle)^2 \rangle = \frac{\hbar^2}{4}(1 - \sin^2\gamma) = \frac{\hbar^2}{4}\cos^2\gamma. \tag{1.22}$$

and finally

$$\langle (\Delta S_x)^2 \rangle_{\gamma=0;|S_z;+\rangle} = \frac{\hbar^2}{4}, \tag{1.23}$$

$$\langle (\Delta S_x)^2 \rangle_{\gamma=\pi/2;|S_x;+\rangle} = 0, \tag{1.24}$$

$$\langle (\Delta S_x)^2 \rangle_{\gamma=0;|S_z;-\rangle} = \frac{\hbar^2}{4}. \tag{1.25}$$

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).

(a) We know that for an arbitrary state $|c\rangle$ the following relation holds

$$\langle c|c\rangle \geq 0. \tag{1.26}$$

This means that if we choose $|c\rangle = |\alpha\rangle + \lambda|\beta\rangle$ where λ is a complex number, we will have

$$(\langle\alpha| + \lambda^*\langle\beta|)\cdot(|\alpha\rangle + \lambda|\beta\rangle) \geq 0 \Rightarrow \tag{1.27}$$

$$\langle\alpha|\alpha\rangle + \lambda\langle\alpha|\beta\rangle + \lambda^*\langle\beta|\alpha\rangle + |\lambda|^2\langle\beta|\beta\rangle \geq 0. \tag{1.28}$$

If we now choose $\lambda = -\langle\beta|\alpha\rangle/\langle\beta|\beta\rangle$ the previous relation will be

$$\langle\alpha|\alpha\rangle - \frac{\langle\beta|\alpha\rangle\langle\alpha|\beta\rangle}{\langle\beta|\beta\rangle} - \frac{\langle\beta|\alpha\rangle\langle\alpha|\beta\rangle}{\langle\beta|\beta\rangle} + \frac{|\langle\beta|\alpha\rangle|^2}{\langle\beta|\beta\rangle} \geq 0 \quad \Rightarrow$$
$$\langle\alpha|\alpha\rangle\langle\beta|\beta\rangle \geq |\langle\beta|\alpha\rangle|^2. \tag{1.29}$$

Notice that the equality sign in the last relation holds when

$$|c\rangle = |\alpha\rangle + \lambda|\beta\rangle = 0 \Rightarrow |\alpha\rangle = -\lambda|\beta\rangle \tag{1.30}$$

that is if $|\alpha\rangle$ and $|\beta\rangle$ are colinear.

(b) The uncertainty relation is

$$\langle(\Delta A)^2\rangle\langle(\Delta B)^2\rangle \geq \frac{1}{4}\left|\langle[A,B]\rangle\right|^2. \tag{1.31}$$

To prove this relation we use the Schwarz inequality (1.29) for the vectors $|\alpha\rangle = \Delta A|a\rangle$ and $|\beta\rangle = \Delta B|a\rangle$ which gives

$$\langle(\Delta A)^2\rangle\langle(\Delta B)^2\rangle \geq |\langle\Delta A\Delta B\rangle|^2. \tag{1.32}$$

The equality sign in this relation holds according to (1.30) when

$$\Delta A|a\rangle = \lambda\Delta B|a\rangle. \tag{1.33}$$

On the other hand the right-hand side of (1.32) is

$$|\langle\Delta A\Delta B\rangle|^2 = \frac{1}{4}\left|\langle[A,B]\rangle\right|^2 + \frac{1}{4}\left|\langle\{\Delta A,\Delta B\}\rangle\right|^2 \tag{1.34}$$

which means that the equality sign in the uncertainty relation (1.31) holds if

$$\begin{aligned} &\frac{1}{4}\left|\langle\{\Delta A,\Delta B\}\rangle\right|^2 = 0 \Rightarrow \langle\{\Delta A,\Delta B\}\rangle = 0 \\ \Rightarrow\ &\langle a|\Delta A\Delta B + \Delta B\Delta A|a\rangle = 0 \overset{(1.33)}{\Rightarrow} \lambda^*\langle a|(\Delta B)^2|a\rangle + \lambda\langle a|(\Delta B)^2|a\rangle = 0 \\ \Rightarrow\ &(\lambda + \lambda^*)\langle a|(\Delta B)^2|a\rangle = 0. \end{aligned} \tag{1.35}$$

Thus the equality sign in the uncertainty relation holds when

$$\Delta A|a\rangle = \lambda\Delta B|a\rangle \tag{1.36}$$

with λ purely imaginary.

(c) We have

$$\begin{aligned}\langle x'|\Delta x|\alpha\rangle &\equiv \langle x'|(x-\langle x\rangle)|\alpha\rangle = x'\langle x'|\alpha\rangle - \langle x\rangle\langle x'|\alpha\rangle \\ &= (x'-\langle x\rangle)\langle x'|\alpha\rangle. \end{aligned} \tag{1.37}$$

On the other hand

$$\begin{aligned}\langle x'|\Delta p|\alpha\rangle &\equiv \langle x'|(p-\langle p\rangle)|\alpha\rangle \\ &= -i\hbar\frac{\partial}{\partial x'}\langle x'|\alpha\rangle - \langle p\rangle\langle x'|\alpha\rangle \end{aligned} \tag{1.38}$$

But

$$\begin{aligned}\frac{\partial}{\partial x'}\langle x'|\alpha\rangle &= \langle x'|\alpha\rangle\frac{\partial}{\partial x'}\left[\frac{i\langle p\rangle x'}{\hbar} - \frac{(x'-\langle x\rangle)^2}{4d^2}\right] \\ &= \langle x'|\alpha\rangle\left[\frac{i\langle p\rangle}{\hbar} - \frac{1}{2d^2}(x'-\langle x\rangle)\right] \end{aligned} \tag{1.39}$$

So substituting in (1.38) we have

$$\begin{aligned}\langle x'|\Delta p|\alpha\rangle &= \langle p\rangle\langle x'|\alpha\rangle + \frac{i\hbar}{2d^2}(x'-\langle x\rangle)\langle x'|\alpha\rangle - \langle p\rangle\langle x'|\alpha\rangle \\ &= \frac{i\hbar}{2d^2}(x'-\langle x\rangle)\langle x'|\alpha\rangle = \frac{i\hbar}{2d^2}\langle x'|\Delta x|\alpha\rangle \Rightarrow \\ \langle x'|\Delta x|\alpha\rangle &= \frac{-i2d^2}{\hbar}\langle x'|\Delta p|\alpha\rangle. \end{aligned} \tag{1.40}$$

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?

(a) We have

$$\begin{aligned}[x, F(p_x)]_{classical} &\equiv \frac{\partial x}{\partial x}\frac{\partial F(p_x)}{\partial p_x} - \frac{\partial x}{\partial p_x}\frac{\partial F(p_x)}{\partial x} \\ &= \frac{\partial F(p_x)}{\partial p_x}. \end{aligned} \tag{1.41}$$

(b) When x and p_x are treated as quantum-mechanical operators we have

$$\begin{aligned}\left[x, \exp\left(\frac{ip_x a}{\hbar}\right)\right] &= \left[x, \sum_{n=0}^{\infty}\frac{(ia)^n}{\hbar^n}\frac{p_x^n}{n!}\right] = \sum_{n=0}^{\infty}\frac{1}{n!}\frac{(ia)^n}{\hbar^n}\left[x, p_x^n\right] \\ &= \sum_{n=0}^{\infty}\frac{1}{n!}\frac{(ia)^n}{\hbar^n}\sum_{k=0}^{n-1}p_x^k\left[x, p_x\right]p_x^{n-k-1} \\ &= \sum_{n=1}^{\infty}\frac{1}{n!}\frac{(ia)^n}{\hbar^n}(i\hbar)\sum_{k=0}^{n-1}p_x^k p_x^{n-k-1} = \sum_{n=1}^{\infty}\frac{n}{n!}\frac{(ia)^{n-1}}{\hbar^{n-1}}p_x^{n-1}(-a) \\ &= -a\sum_{n=1}^{\infty}\frac{1}{(n-1)!}\left(\frac{ia}{\hbar}p_x\right)^{n-1} = -a\exp\left(\frac{ip_x a}{\hbar}\right). \end{aligned} \tag{1.42}$$

(c) We have now

$$\begin{aligned} x\left[\exp\left(\frac{ip_x a}{\hbar}\right)\right]|x'\rangle &\stackrel{(b)}{=} \exp\left(\frac{ip_x a}{\hbar}\right)x|x'\rangle - a\exp\left(\frac{ip_x a}{\hbar}\right)|x'\rangle \\ &= x'\exp\left(\frac{ip_x a}{\hbar}\right)|x'\rangle - a\exp\left(\frac{ip_x a}{\hbar}\right)|x'\rangle \\ &= (x'-a)\exp\left(\frac{ip_x a}{\hbar}\right)|x'\rangle. \end{aligned} \tag{1.43}$$

So $\exp\left(\frac{ip_x a}{\hbar}\right)|x'\rangle$ is an eigenstate of the operator x with eigenvalue $x'-a$. So we can write

$$|x'-a\rangle = C\exp\left(\frac{ip_x a}{\hbar}\right)|x'\rangle, \tag{1.44}$$

where C is a constant which due to normalization can be taken to be 1.

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.

(a) We have
(i)

$$
\begin{aligned}
\langle p'|x|\alpha\rangle &= \langle p'|x\overbrace{\int dx'|x'\rangle\langle x'|}^{1}\alpha\rangle = \int dx'\langle p'|x|x'\rangle\langle x'|\alpha\rangle \\
&= \int dx' x'\langle p'|x'\rangle\langle x'|\alpha\rangle \overset{(S-1.7.32)}{=} \int dx' x' A e^{-\frac{ip'x'}{\hbar}}\langle x'|\alpha\rangle \\
&= A\int dx' \frac{\partial}{\partial p'}\left(e^{-\frac{ip'x'}{\hbar}}\right)(i\hbar)\langle x'|\alpha\rangle = i\hbar\frac{\partial}{\partial p'}\left[\int dx' A e^{-\frac{ip'x'}{\hbar}}\langle x'|\alpha\rangle\right] \\
&= i\hbar\frac{\partial}{\partial p'}\left[\int dx'\langle p'|x'\rangle\langle x'|\alpha\rangle\right] = i\hbar\frac{\partial}{\partial p'}\langle p'|\alpha\rangle \Rightarrow \\
\langle p'|x|\alpha\rangle &= i\hbar\frac{\partial}{\partial p'}\langle p'|\alpha\rangle. \qquad (1.45)
\end{aligned}
$$

(ii)

$$
\langle\beta|x|\alpha\rangle = \int dp'\langle\beta|p'\rangle\langle p'|x|\alpha\rangle = \int dp'\phi^*_\beta(p') i\hbar\frac{\partial}{\partial p'}\phi_\alpha(p'), \qquad (1.46)
$$

where we have used (1.45) and that $\langle\beta|p'\rangle = \phi^*_\beta(p')$ and $\langle p'|\alpha\rangle = \phi_\alpha(p')$.

(b) The operator $\exp\left(\frac{ix\Xi}{\hbar}\right)$ gives translation in momentum space. This can be justified by calculating the following operator

$$\begin{aligned}
\left[p, \exp\left(\frac{ix\Xi}{\hbar}\right)\right] &= \left[p, \sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{ix\Xi}{\hbar}\right)^n\right] = \sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{i\Xi}{\hbar}\right)^n [p, x^n] \\
&= \sum_{n=1}^{\infty}\frac{1}{n!}\left(\frac{i\Xi}{\hbar}\right)^n \sum_{k=1}^{n} x^{n-k}[p,x]x^{k-1} \\
&= \sum_{n=1}^{\infty}\frac{1}{n!}\left(\frac{i\Xi}{\hbar}\right)^n \sum_{k=1}^{n}(-i\hbar)x^{n-1} = \sum_{n=1}^{\infty}\frac{1}{n!}\left(\frac{i\Xi}{\hbar}\right)^n n(-i\hbar)x^{n-1} \\
&= \sum_{n=1}^{\infty}\frac{1}{(n-1)!}\left(\frac{i\Xi}{\hbar}\right)^{n-1} x^{n-1}(-i\hbar)\left(\frac{i\Xi}{\hbar}\right) = \Xi\sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{ix\Xi}{\hbar}\right)^n \\
&= \Xi \exp\left(\frac{ix\Xi}{\hbar}\right). \qquad (1.47)
\end{aligned}$$

So when this commutator acts on an eigenstate $|p'\rangle$ of the momentum operator we will have

$$\begin{aligned}
\left[p, \exp\left(\frac{ix\Xi}{\hbar}\right)\right]|p'\rangle &= p\left[\exp\left(\frac{ix\Xi}{\hbar}\right)|p'\rangle\right] - \left[\exp\left(\frac{ix\Xi}{\hbar}\right)\right]p'|p'\rangle \Rightarrow \\
\Xi \exp\left(\frac{ix\Xi}{\hbar}\right) &= p\left[\exp\left(\frac{ix\Xi}{\hbar}\right)|p'\rangle\right] - p'\left[\exp\left(\frac{ix\Xi}{\hbar}\right)\right]|p'\rangle \Rightarrow \\
p\left[\exp\left(\frac{ix\Xi}{\hbar}\right)|p'\rangle\right] &= (p'+\Xi)\left[\exp\left(\frac{ix\Xi}{\hbar}\right)|p'\rangle\right]. \qquad (1.48)
\end{aligned}$$

Thus we have that

$$\exp\left(\frac{ix\Xi}{\hbar}\right)|p'\rangle \equiv A|p'+\Xi\rangle, \qquad (1.49)$$

where A is a constant which due to normalization can be taken to be 1.

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.

Let us first prove the following

$$[A_S, B_S] = C_S \Rightarrow [A_H, B_H] = C_H. \tag{2.1}$$

Indeed we have

$$\begin{aligned} [A_H, B_H] &= \left[\mathcal{U}^\dagger A_S \mathcal{U}, \mathcal{U}^\dagger B_S \mathcal{U}\right] = \mathcal{U}^\dagger A_S B_S \mathcal{U} - \mathcal{U}^\dagger B_S A_S \mathcal{U} \\ &= \mathcal{U}^\dagger \left[A_S, B_S\right] \mathcal{U} = \mathcal{U}^\dagger C_S \mathcal{U} = C_H. \end{aligned} \tag{2.2}$$

The Heisenberg equation of motion gives

$$\frac{dS_x}{dt} = \frac{1}{i\hbar}\left[S_x, H\right] = \frac{1}{i\hbar}\left[S_x, \omega S_z\right] \overset{(S-1.4.20)}{=} \frac{\omega}{i\hbar}(-i\hbar S_y) = -\omega S_y, \tag{2.3}$$

$$\frac{dS_y}{dt} = \frac{1}{i\hbar}\left[S_y, H\right] = \frac{1}{i\hbar}\left[S_y, \omega S_z\right] \overset{(S-1.4.20)}{=} \frac{\omega}{i\hbar}(i\hbar S_x) = \omega S_x, \tag{2.4}$$

$$\frac{dS_z}{dt} = \frac{1}{i\hbar}\left[S_z, H\right] = \frac{1}{i\hbar}\left[S_z, \omega S_z\right] \overset{(S-1.4.20)}{=} 0 \Rightarrow S_z = \text{constant}. \tag{2.5}$$

Differentiating once more eqs. (2.3) and (2.4) we get

$$\begin{aligned} \frac{d^2 S_x}{dt^2} &= -\omega \frac{dS_y}{dt} \overset{(2.4)}{=} -\omega^2 S_x \Rightarrow S_x(t) = A\cos\omega t + B\sin\omega t \Rightarrow S_x(0) = A \\ \frac{d^2 S_y}{dt^2} &= \omega \frac{dS_x}{dt} \overset{(2.3)}{=} -\omega^2 S_y \Rightarrow S_y(t) = C\cos\omega t + D\sin\omega t \Rightarrow S_y(0) = C. \end{aligned}$$

But on the other hand

$$\begin{aligned} \frac{dS_x}{dt} &= -\omega S_y \Rightarrow \\ -A\omega\sin\omega t + B\omega\cos\omega t &= -C\omega\cos\omega t - D\omega\sin\omega t \Rightarrow \\ A = D \qquad & C = -B. \end{aligned} \tag{2.6}$$

So, finally

$$\begin{aligned} S_x(t) &= S_x(0)\cos\omega t - S_y(0)\sin\omega t && (2.7)\\ S_y(t) &= S_y(0)\cos\omega t + S_x(0)\sin\omega t && (2.8)\\ S_z(t) &= S_z(0). && (2.9) \end{aligned}$$

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

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

The Hamiltonian for a free particle in one dimension is given by

$$H = \frac{p^2}{2m}. \qquad (2.10)$$

This means that the Heisenberg equations of motion for the operators x and p will be

$$\begin{aligned} \frac{\partial p(t)}{\partial t} &= \frac{1}{i\hbar}[p(t), H(t)] = \frac{1}{i\hbar}\left[p(t), \frac{p^2(t)}{2m}\right] = 0 \Rightarrow \\ p(t) &= p(0) && (2.11)\\ \frac{\partial x(t)}{\partial t} &= \frac{1}{i\hbar}[x, H] = \frac{1}{i\hbar}\left[x(t), \frac{p^2(t)}{2m}\right] = \frac{1}{2mi\hbar}2p(t)i\hbar = \frac{p(t)}{m} \overset{(2.11)}{=} \frac{p(0)}{m} \Rightarrow \\ x(t) &= \frac{t}{m}p(0) + x(0). && (2.12) \end{aligned}$$

Thus finally

$$[x(t), x(0)] = \left[\frac{t}{m}p(0) + x(0), x(0)\right] = \frac{t}{m}[p(0), x(0)] = -\frac{i\hbar t}{m}. \qquad (2.13)$$

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?

Let us first calculate the commutator $[\vec{x}\cdot\vec{p}, H]$

$$\begin{aligned}
[\vec{x}\cdot\vec{p}, H] &= \left[\vec{x}\cdot\vec{p}, \frac{\vec{p}^2}{2m} + V(\vec{x})\right] = \left[\sum_{i=1}^{3} x_i p_i, \sum_{j=1}^{3}\frac{p_j^2}{2m} + V(\vec{x})\right] \\
&= \sum_{ij}\left[x_i, \frac{p_j^2}{2m}\right] p_i + \sum_i x_i\,[p_i, V(\vec{x})]\,. \qquad (2.14)
\end{aligned}$$

The first commutator in (2.14) will give

$$\begin{aligned}
\left[x_i, \frac{p_j^2}{2m}\right] &= \frac{1}{2m}[x_i, p_j^2] = \frac{1}{2m}(p_j[x_i, p_j] + [x_i, p_j]p_j) = \frac{1}{2m}(p_j i\hbar\delta_{ij} + i\hbar\delta_{ij}p_j) \\
&= \frac{1}{2m}2i\hbar\delta_{ij}p_j = \frac{i\hbar}{m}\delta_{ij}p_j. \qquad (2.15)
\end{aligned}$$

The second commutator can be calculated if we Taylor expand the function $V(\vec{x})$ in terms of x_i which means that we take $V(\vec{x}) = \sum_n a_n x_i^n$ with a_n independent of x_i. So

$$\begin{aligned}
[p_i, V(\vec{x})] &= \left[p_i, \sum_{n=0}^{\infty} a_n x_i^n\right] = \sum_n a_n\,[p_i, x_i^n] = \sum_n a_n \sum_{k=0}^{n-1} x_i^k\,[p_i, x_i]\,x_i^{n-k-1} \\
&= \sum_n a_n \sum_{k=0}^{n-1}(-i\hbar)x_i^{n-1} = -i\hbar\sum_n a_n n x_i^{n-1} = -i\hbar\frac{\partial}{\partial x_i}\sum_n a_n x_i^n \\
&= -i\hbar\frac{\partial}{\partial x_i}V(\vec{x}). \qquad (2.16)
\end{aligned}$$

The right-hand side of (2.14) now becomes

$$\begin{aligned}
[\vec{x}\cdot\vec{p}, H] &= \sum_{ij}\frac{i\hbar}{m}\delta_{ij}p_j p_i + \sum_i(-i\hbar)x_i\frac{\partial}{\partial x_i}V(\vec{x}) \\
&= \frac{i\hbar}{m}\vec{p}^2 - i\hbar\vec{x}\cdot\vec{\nabla}V(\vec{x}). \qquad (2.17)
\end{aligned}$$

The Heisenberg equation of motion gives

$$\begin{aligned} \frac{d}{dt}\vec{x}\cdot\vec{p} &= \frac{1}{i\hbar}\left[\vec{x}\cdot\vec{p}, H\right] \overset{(2.17)}{=} \frac{\vec{p}^2}{m} - \vec{x}\cdot\vec{\nabla}V(\vec{x}) \Rightarrow \\ \frac{d}{dt}\langle\vec{x}\cdot\vec{p}\rangle &= \left\langle\frac{p^2}{m}\right\rangle - \langle\vec{x}\cdot\vec{\nabla}V\rangle, \end{aligned} \tag{2.18}$$

where in the last step we used the fact that the state kets in the Heisenberg picture are independent of time.

The left-hand side of the last equation vanishes for a stationary state. Indeed we have

$$\frac{d}{dt}\langle n|\vec{x}\cdot\vec{p}|n\rangle = \frac{1}{i\hbar}\langle n|\left[\vec{x}\cdot\vec{p}, H\right]|n\rangle = \frac{1}{i\hbar}\left(E_n\langle n|\vec{x}\cdot\vec{p}|n\rangle - E_n\langle n|\vec{x}\cdot\vec{p}|n\rangle\right) = 0.$$

So to have the quantum-mechanical analogue of the virial theorem we can take the expectation values with respect to a stationaru state.

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 $t > 0$?

(a) We have

$$\begin{aligned} |\alpha, t=0\rangle &= \exp\left(\frac{-ipa}{\hbar}\right)|0\rangle \Rightarrow \\ \langle x'|\alpha, t=0\rangle &= \langle x'\exp\left(\frac{-ipa}{\hbar}\right)|0\rangle \overset{(Pr.1.4.c)}{=} \langle x'-a|0\rangle \\ &= \pi^{-1/4}x_0^{-1/2}\exp\left[-\tfrac{1}{2}\left(\frac{x'-a}{x_0}\right)^2\right]. \end{aligned} \tag{2.19}$$

(b) This probability is given by the expression

$$|\langle 0|\alpha, t=0\rangle|^2 = |\langle \exp\left(\frac{-ipa}{\hbar}\right)|0\rangle|^2. \tag{2.20}$$

It is

$$\begin{aligned}
\langle \exp\left(\frac{-ipa}{\hbar}\right)|0\rangle &= \int dx' \langle 0|x'\rangle\langle x'|\exp\left(\frac{-ipa}{\hbar}\right)|0\rangle \\
&= \int dx' \pi^{-1/4} x_0^{-1/2} \exp\left[-\tfrac{1}{2}\left(\frac{x'}{x_0}\right)^2\right] \pi^{-1/4} x_0^{-1/2} \\
&\quad \times \exp\left[-\tfrac{1}{2}\left(\frac{x'-a}{x_0}\right)^2\right] \\
&= \int dx' \pi^{-1/2} x_0^{-1} \exp\left[-\frac{1}{2x_0^2}\left(x'^2 + x'^2 + a^2 - 2ax'\right)\right] \\
&= \frac{1}{\sqrt{\pi}x_0}\int dx' \exp\left[-\frac{2}{2x_0^2}\left(x'^2 - 2x'\frac{a}{2} + \frac{a^2}{4} + \frac{a^2}{4}\right)\right] \\
&= \exp\left(-\frac{a^2}{4x_0^2}\right)\frac{1}{\sqrt{\pi}x_0}\sqrt{\pi}x_0 = \exp\left(-\frac{a^2}{4x_0^2}\right).
\end{aligned} \tag{2.21}$$

So

$$|\langle 0|\alpha, t=0\rangle|^2 = \exp\left(-\frac{a^2}{2x_0^2}\right). \tag{2.22}$$

For $t > 0$

$$\begin{aligned}
|\langle 0|\alpha, t\rangle|^2 &= |\langle 0|\mathcal{U}(t)|\alpha, t=0\rangle|^2 = |\langle 0|\exp\left(-\frac{iHt}{\hbar}\right)|\alpha, t=0\rangle|^2 \\
&= \left|e^{-iE_0 t/\hbar}\langle 0|\alpha, t=0\rangle\right|^2 = |\langle 0|\alpha, t=0\rangle|^2.
\end{aligned} \tag{2.23}$$

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

$$C(t) = \langle x(t)x(0)\rangle, \tag{2.24}$$

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.

The Hamiltonian for a one-dimensional harmonic oscillator is given by

$$H = \frac{p^2(t)}{2m} + \tfrac{1}{2}m\omega^2 x^2(t). \tag{2.25}$$

So the Heisenberg equations of motion will give

$$\begin{aligned}
\frac{dx(t)}{dt} &= \frac{1}{i\hbar}[x(t), H] = \frac{1}{i\hbar}\left[x(t), \frac{p^2(t)}{2m} + \tfrac{1}{2}m\omega^2 x^2(t)\right] \\
&= \frac{1}{2mi\hbar}\left[x(t), p^2(t)\right] + \tfrac{1}{2}m\omega^2\frac{1}{i\hbar}\left[x(t), x^2(t)\right] \\
&= \frac{2i\hbar}{2i\hbar m}p(t) = \frac{p(t)}{m} \qquad (2.26) \\
\frac{dp(t)}{dt} &= \frac{1}{i\hbar}[p(t), H] = \frac{1}{i\hbar}\left[p(t), \frac{p^2(t)}{2m} + \tfrac{1}{2}m\omega^2 x^2(t)\right] \\
&= \frac{m\omega^2}{2i\hbar}\left[p(t), x^2(t)\right] = \frac{m\omega^2}{2i\hbar}[-2i\hbar x(t)] = -m\omega^2 x(t). \qquad (2.27)
\end{aligned}$$

Differentiating once more the equations (2.26) and (2.27) we get

$$\begin{aligned}
\frac{d^2x(t)}{dt^2} &= \frac{1}{m}\frac{dp(t)}{dt} \overset{(2.27)}{=} -\omega^2 x(t) \Rightarrow x(t) = A\cos\omega t + B\sin\omega t \Rightarrow x(0) = A \\
\frac{d^2p(t)}{dt^2} &= \frac{1}{m}\frac{dx(t)}{dt} \overset{(2.26)}{=} -\omega^2 p(t) \Rightarrow p(t) = C\cos\omega t + D\sin\omega t \Rightarrow p(0) = C.
\end{aligned}$$

But on the other hand from (2.26) we have

$$\begin{aligned}
\frac{dx(t)}{dt} &= \frac{p(t)}{m} \Rightarrow \\
-\omega x(0)\sin\omega t + B\omega\cos\omega t &= \frac{p(0)}{m}\cos\omega t + \frac{D}{m}\sin\omega t \Rightarrow \\
B = \frac{p(0)}{m\omega} & \qquad D = -m\omega x(0). \qquad (2.28)
\end{aligned}$$

So

$$x(t) = x(0)\cos\omega t + \frac{p(0)}{m\omega}\sin\omega t \tag{2.29}$$

and the correlation function will be

$$C(t) = \langle x(t)x(0)\rangle \overset{(2.29)}{=} \langle x^2(0)\rangle\cos\omega t + \langle p(0)x(0)\rangle\frac{1}{m\omega}\sin\omega t. \tag{2.30}$$

Since we are interested in the ground state the expectation values appearing in the last relation will be

$$\begin{aligned}\langle x^2(0)\rangle &= \langle 0|\frac{\hbar}{2m\omega}(a+a^\dagger)(a+a^\dagger)|0\rangle = \frac{\hbar}{2m\omega}\langle 0|aa^\dagger|0\rangle = \frac{\hbar}{2m\omega} \quad (2.31)\\ \langle p(0)x(0)\rangle &= i\sqrt{\frac{m\hbar\omega}{2}}\sqrt{\frac{\hbar}{2m\omega}}\langle 0|(a^\dagger - a)(a+a^\dagger)|0\rangle \\ &= -i\frac{\hbar}{2}\langle 0|aa^\dagger|0\rangle = -i\frac{\hbar}{2}. \quad (2.32)\end{aligned}$$

Thus

$$C(t) = \frac{\hbar}{2m\omega}\cos\omega t - i\frac{\hbar}{2m\omega}\sin\omega t = \frac{\hbar}{2m\omega}e^{-i\omega t}. \quad (2.33)$$

2.6 Consider 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.

(a) We want to find a state $|\alpha\rangle = c_0|0\rangle + c_1|1\rangle$ such that $\langle x\rangle$ is as large as possible. The state $|\alpha\rangle$ should be normalized. This means

$$|c_0|^2 + |c_1|^2 = 1 \Rightarrow |c_1| = \sqrt{1-|c_0|^2}. \quad (2.34)$$

We can write the constands c_0 and c_1 in the following form

$$\begin{aligned} c_0 &= |c_0|e^{i\delta_0} \\ c_1 &= |c_1|e^{i\delta_1} \stackrel{(2.34)}{=} e^{i\delta_1}\sqrt{1-|c_0|^2}. \quad (2.35)\end{aligned}$$

The average $\langle x\rangle$ in a one-dimensional simple harmonic oscillator is given by

$$\begin{aligned}
\langle x\rangle &= \langle\alpha|x|\alpha\rangle = (c_0^*\langle 0| + c_1^*\langle 1|)\, x\, (c_0|0\rangle + c_1|1\rangle) \\
&= |c_0|^2\langle 0|x|0\rangle + c_0^*c_1\langle 0|x|1\rangle + c_1^*c_0\langle 1|x|0\rangle + |c_1|^2\langle 1|x|1\rangle \\
&= |c_0|^2\sqrt{\frac{\hbar}{2m\omega}}\langle 0|a+a^\dagger|0\rangle + c_0^*c_1\sqrt{\frac{\hbar}{2m\omega}}\langle 0|a+a^\dagger|1\rangle \\
&\quad + c_1^*c_0\sqrt{\frac{\hbar}{2m\omega}}\langle 1|a+a^\dagger|0\rangle + |c_1|^2\sqrt{\frac{\hbar}{2m\omega}}\langle 1|a+a^\dagger|1\rangle \\
&= \sqrt{\frac{\hbar}{2m\omega}}(c_0^*c_1 + c_1^*c_0) = 2\sqrt{\frac{\hbar}{2m\omega}}\Re(c_0^*c_1) \\
&= 2\sqrt{\frac{\hbar}{2m\omega}}\cos(\delta_1-\delta_0)|c_0|\sqrt{1-|c_0|^2}, \qquad (2.36)
\end{aligned}$$

where we have used that $x = \sqrt{\frac{\hbar}{2m\omega}}(a+a^\dagger)$.

What we need is to find the values of $|c_0|$ and $\delta_1 - \delta_0$ that make the average $\langle x\rangle$ as large as possible.

$$\frac{\partial\langle x\rangle}{\partial|c_0|} = 0 \qquad \Rightarrow \sqrt{1-|c_0|^2} - \frac{|c_0|^2}{\sqrt{1-|c_0|^2}} \overset{|c_0|\neq 1}{\Rightarrow} 1 - |c_0|^2 - |c_0|^2 = 0$$

$$\Rightarrow |c_0| = \frac{1}{\sqrt{2}} \qquad (2.37)$$

$$\frac{\partial\langle x\rangle}{\partial\delta_1} = 0 \qquad \Rightarrow -\sin(\delta_1-\delta_0) = 0 \Rightarrow \delta_1 = \delta_0 + n\pi, \quad n\in\mathcal{Z}. \qquad (2.38)$$

But for $\langle x\rangle$ maximum we want also

$$\left.\frac{\partial^2\langle x\rangle}{\partial\delta_1^2}\right|_{\delta_1=\delta_{1max}} < 0 \Rightarrow n = 2k, \quad k\in\mathcal{Z}. \qquad (2.39)$$

So we can write that

$$|\alpha\rangle = e^{i\delta_0}\frac{1}{\sqrt{2}}|0\rangle + e^{i(\delta_0+2k\pi)}\frac{1}{\sqrt{2}}|1\rangle = e^{i\delta_0}\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle). \qquad (2.40)$$

We can always take $\delta_0 = 0$. Thus

$$|\alpha\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle). \qquad (2.41)$$

(b) We have $|\alpha, t_0\rangle = |\alpha\rangle$. So

$$\begin{aligned} |\alpha, t_0; t\rangle &= \mathcal{U}(t, t_0 = 0)|\alpha, t_0\rangle = e^{-iHt/\hbar}|\alpha\rangle = \frac{1}{\sqrt{2}}e^{-iE_0 t/\hbar}|0\rangle + \frac{1}{\sqrt{2}}e^{-iE_1 t/\hbar}|1\rangle \\ &= \frac{1}{\sqrt{2}}\left(e^{-i\omega t/2}|0\rangle + e^{-i\omega 3t/2}|1\rangle\right) = \frac{1}{\sqrt{2}}e^{-i\omega t/2}\left(|0\rangle + e^{-i\omega t}|1\rangle\right). \end{aligned} \tag{2.42}$$

(i) In the Schrödinger picture

$$\begin{aligned} \langle x\rangle_S &= \langle \alpha, t_0; t|x_S|\alpha, t_0; t\rangle_S \\ &= \left[\frac{1}{\sqrt{2}}\left(e^{i\omega t/2}\langle 0| + e^{i\omega 3t/2}\langle 1|\right)\right] x \left[\frac{1}{\sqrt{2}}\left(e^{-i\omega t/2}|0\rangle + e^{-i\omega 3t/2}|1\rangle\right)\right] \\ &= \tfrac{1}{2}e^{i(\omega t/2 - \omega 3t/2)}\langle 0|x|1\rangle + \tfrac{1}{2}e^{i(\omega 3t/2 - \omega t/2)}\langle 1|x|0\rangle \\ &= \tfrac{1}{2}e^{-i\omega t}\sqrt{\frac{\hbar}{2m\omega}} + \tfrac{1}{2}e^{i\omega t}\sqrt{\frac{\hbar}{2m\omega}} = \sqrt{\frac{\hbar}{2m\omega}}\cos\omega t. \end{aligned} \tag{2.43}$$

(ii) In the Heisenberg picture we have from (2.29) that

$$x_H(t) = x(0)\cos\omega t + \frac{p(0)}{m\omega}\sin\omega t.$$

So

$$\begin{aligned} \langle x\rangle_H &= \langle \alpha|x_H|\alpha\rangle \\ &= \left[\frac{1}{\sqrt{2}}\langle 0| + \frac{1}{\sqrt{2}}\langle 1|\right]\left(x(0)\cos\omega t + \frac{p(0)}{m\omega}\sin\omega t\right)\left[\frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle\right] \\ &= \tfrac{1}{2}\cos\omega t\langle 0|x|1\rangle + \tfrac{1}{2}\cos\omega t\langle 1|x|0\rangle + \tfrac{1}{2}\frac{1}{m\omega}\sin\omega t\langle 0|p|1\rangle \\ &\quad + \tfrac{1}{2}\frac{1}{m\omega}\sin\omega t\langle 1|p|0\rangle \\ &= \tfrac{1}{2}\sqrt{\frac{\hbar}{2m\omega}}\cos\omega t + \tfrac{1}{2}\sqrt{\frac{\hbar}{2m\omega}}\cos\omega t + \frac{1}{2m\omega}\sin\omega t(-i)\sqrt{\frac{m\hbar\omega}{2}} \\ &\quad + \frac{1}{2m\omega}\sin\omega t\, i\sqrt{\frac{m\hbar\omega}{2}} \\ &= \sqrt{\frac{\hbar}{2m\omega}}\cos\omega t. \end{aligned} \tag{2.44}$$

(c) It is known that

$$\langle(\Delta x)^2\rangle = \langle x^2\rangle - \langle x\rangle^2 \tag{2.45}$$

In the Schödinger picture we have

$$x^2 = \left[\sqrt{\frac{\hbar}{2m\omega}}(a+a^\dagger)\right]^2 = \frac{\hbar}{2m\omega}(a^2+a^{\dagger 2}+aa^\dagger+a^\dagger a), \qquad (2.46)$$

which means that

$$\begin{aligned}
\langle x\rangle_S^2 &= \langle\alpha,t_0;t|x^2|\alpha,t_0;t\rangle_S \\
&= \left[\frac{1}{\sqrt{2}}\left(e^{i\omega t/2}\langle 0| + e^{i\omega 3t/2}\langle 1|\right)\right] x^2 \left[\frac{1}{\sqrt{2}}\left(e^{-i\omega t/2}|0\rangle + e^{-i\omega 3t/2}|1\rangle\right)\right] \\
&= \left[\tfrac{1}{2}e^{i(\omega t/2-\omega t/2)}\langle 0|aa^\dagger|0\rangle + \tfrac{1}{2}e^{i(\omega 3t/2-\omega 3t/2)}\langle 1|aa^\dagger|1\rangle + \tfrac{1}{2}\langle 1|a^\dagger a|1\rangle\right]\frac{\hbar}{2m\omega} \\
&= \left[\tfrac{1}{2}+2\tfrac{1}{2}+\tfrac{1}{2}\right]\frac{\hbar}{2m\omega} = \frac{\hbar}{2m\omega}. \qquad (2.47)
\end{aligned}$$

So

$$\langle(\Delta x)^2\rangle_S \overset{(2.43)}{=} \frac{\hbar}{2m\omega} - \frac{\hbar}{2m\omega}\cos^2\omega t = \frac{\hbar}{2m\omega}\sin^2\omega t. \qquad (2.48)$$

In the Heisenberg picture

$$\begin{aligned}
x_H^2(t) &= \left[x(0)\cos\omega t + \frac{p(0)}{m\omega}\sin\omega t\right]^2 \\
&= x^2(0)\cos^2\omega t + \frac{p^2(0)}{m^2\omega^2}\sin^2\omega t \\
&\quad + \frac{x(0)p(0)}{m\omega}\cos\omega t\sin\omega t + \frac{p(0)x(0)}{m\omega}\cos\omega t\sin\omega t \\
&= \frac{\hbar}{2m\omega}(a^2+a^{\dagger 2}+aa^\dagger+a^\dagger a)\cos^2\omega t \\
&\quad - \frac{m\hbar\omega}{2m^2\omega^2}(a^2+a^{\dagger 2}-aa^\dagger-a^\dagger a)\sin^2\omega t \\
&\quad + \frac{i}{m\omega}\sqrt{\frac{\hbar m\hbar\omega}{4m\omega}}(a+a^\dagger)(a^\dagger-a)\frac{\sin 2\omega t}{2} \\
&\quad + \frac{i}{m\omega}\sqrt{\frac{\hbar m\hbar\omega}{4m\omega}}(a^\dagger-a)(a+a^\dagger)\frac{\sin 2\omega t}{2} \\
&= \frac{\hbar}{2m\omega}(a^2+a^{\dagger 2}+aa^\dagger+a^\dagger a)\cos^2\omega t
\end{aligned}$$

$$
\begin{aligned}
& -\frac{\hbar}{2m\omega}(a^2 + a^{\dagger 2} - aa^\dagger - a^\dagger a)\sin^2\omega t + \frac{i\hbar}{2m\omega}(a^{\dagger 2} - a^2)\sin 2\omega t \\
= \; & \frac{\hbar}{2m\omega}(aa^\dagger + a^\dagger a) + \frac{\hbar}{2m\omega}a^2\cos 2\omega t + \frac{\hbar}{2m\omega}a^{\dagger 2}\cos 2\omega t \\
& + \frac{i\hbar}{2m\omega}(a^{\dagger 2} - a^2)\sin 2\omega t, \qquad (2.49)
\end{aligned}
$$

which means that

$$
\begin{aligned}
\langle x_H^2 \rangle_H &= \langle \alpha | x_H^2 | \alpha \rangle_H \\
&= \frac{\hbar}{2m\omega}\left[\frac{1}{\sqrt{2}}\langle 0| + \frac{1}{\sqrt{2}}\langle 1|\right] \\
& \quad \times \left[aa^\dagger + a^\dagger a + a^2\cos 2\omega t + a^{\dagger 2}\cos 2\omega t + i(a^{\dagger 2} - a^2)\sin 2\omega t\right] \\
& \quad \times \left[\frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle\right] \\
&= \frac{\hbar}{4m\omega}\left[\langle 0|aa^\dagger|0\rangle + \langle 1|aa^\dagger|1\rangle + \langle 1|a^\dagger a|1\rangle\right] \\
&= \frac{\hbar}{4m\omega}[1 + 2 + 1] = \frac{\hbar}{m\omega}. \qquad (2.50)
\end{aligned}
$$

So

$$
\langle (\Delta x)^2 \rangle_H \overset{(2.44)}{=} \frac{\hbar}{2m\omega} - \frac{\hbar}{2m\omega}\cos^2\omega t = \frac{\hbar}{2m\omega}\sin^2\omega t. \qquad (2.51)
$$

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.)

(a) We have

$$a|\lambda\rangle = e^{-|\lambda|^2/2} a e^{\lambda a^\dagger}|0\rangle = e^{-|\lambda|^2/2}\left[a, e^{\lambda a^\dagger}\right]|0\rangle, \tag{2.52}$$

since $a|0\rangle = 0$. The commutator is

$$\begin{aligned}
\left[a, e^{\lambda a^\dagger}\right] &= \left[a, \sum_{n=0}^{\infty}\frac{1}{n!}(\lambda a^\dagger)^n\right] = \sum_{n=0}^{\infty}\frac{1}{n!}\lambda^n\left[a, (a^\dagger)^n\right] \\
&= \sum_{n=1}^{\infty}\frac{1}{n!}\lambda^n\sum_{k=1}^{n}(a^\dagger)^{k-1}\left[a, a^\dagger\right](a^\dagger)^{n-k} = \sum_{n=1}^{\infty}\frac{1}{n!}\lambda^n\sum_{k=1}^{n}(a^\dagger)^{n-1} \\
&= \sum_{n=1}^{\infty}\frac{1}{(n-1)!}\lambda^n(a^\dagger)^{n-1} = \lambda\sum_{n=0}^{\infty}\frac{1}{n!}(\lambda a^\dagger)^n = \lambda e^{\lambda a^\dagger}.
\end{aligned} \tag{2.53}$$

So from (2.52)

$$a|\lambda\rangle = e^{-|\lambda|^2/2}\lambda e^{\lambda a^\dagger}|0\rangle = \lambda|\lambda\rangle, \tag{2.54}$$

which means that $|\lambda\rangle$ is a coherent state. If it is normalized, it should satisfy also $\langle\lambda|\lambda\rangle = 1$. Indeed

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

$$
\begin{aligned}
&= e^{-|\lambda|^2}\sum_{n,m}\frac{1}{n!m!}(\lambda^*)^n\lambda^m\langle 0|a^n|(a^\dagger)^m|0\rangle \quad [(a^\dagger)^m|0\rangle = \sqrt{m!}|m\rangle] \\
&= e^{-|\lambda|^2}\sum_{n,m}\frac{\sqrt{n!}}{n!}\frac{\sqrt{m!}}{m!}(\lambda^*)^n\lambda^m\langle n|m\rangle = e^{-|\lambda|^2}\sum_n\frac{1}{n!}(|\lambda|^2)^n \\
&= e^{-|\lambda|^2}e^{|\lambda|^2} = 1. \qquad (2.55)
\end{aligned}
$$

(b) According to problem (1.3) the state should satisfy the following relation

$$
\Delta x|\lambda\rangle = c\Delta p|\lambda\rangle, \qquad (2.56)
$$

where $\Delta x \equiv x - \langle\lambda|x|\lambda\rangle$, $\Delta p \equiv p - \langle\lambda|p|\lambda\rangle$ and c is a purely imaginary number.

Since $|\lambda\rangle$ is a coherent state we have

$$
a|\lambda\rangle = \lambda|\lambda\rangle \Rightarrow \langle\lambda|a^\dagger = \langle\lambda|\lambda^*. \qquad (2.57)
$$

Using this relation we can write

$$
x|\lambda\rangle = \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger)|\lambda\rangle = \sqrt{\frac{\hbar}{2m\omega}}(\lambda + a^\dagger)|\lambda\rangle \qquad (2.58)
$$

and

$$
\begin{aligned}
\langle x\rangle &= \langle\lambda|x|\lambda\rangle = \sqrt{\frac{\hbar}{2m\omega}}\langle\lambda|(a + a^\dagger)|\lambda\rangle = \sqrt{\frac{\hbar}{2m\omega}}(\langle\lambda|a|\lambda\rangle + \langle\lambda|a^\dagger|\lambda\rangle) \\
&= \sqrt{\frac{\hbar}{2m\omega}}(\lambda + \lambda^*) \qquad (2.59)
\end{aligned}
$$

and so

$$
\Delta x|\lambda\rangle = (x - \langle x\rangle)|\lambda\rangle = \sqrt{\frac{\hbar}{2m\omega}}(a^\dagger - \lambda^*)|\lambda\rangle. \qquad (2.60)
$$

Similarly for the momentum $p = i\sqrt{\frac{m\hbar\omega}{2}}(a^\dagger - a)$ we have

$$
p|\lambda\rangle = \sqrt{i}\sqrt{\frac{m\hbar\omega}{2}}(a^\dagger - a)|\lambda\rangle = i\sqrt{\frac{m\hbar\omega}{2}}(a^\dagger - \lambda)|\lambda\rangle \qquad (2.61)
$$

and

$$\begin{aligned}\langle p\rangle &= \langle\lambda|p|\lambda\rangle = i\sqrt{\frac{m\hbar\omega}{2}}\langle\lambda|(a^\dagger - a)|\lambda\rangle = i\sqrt{\frac{m\hbar\omega}{2}}(\langle\lambda|a^\dagger|\lambda\rangle - \langle\lambda|a|\lambda\rangle)\\ &= i\sqrt{\frac{m\hbar\omega}{2}}(\lambda^* - \lambda) \qquad (2.62)\end{aligned}$$

and so

$$\begin{aligned}\Delta p|\lambda\rangle &= (p - \langle p\rangle)|\lambda\rangle = i\sqrt{\frac{m\hbar\omega}{2}}(a^\dagger - \lambda^*)|\lambda\rangle \Rightarrow\\ (a^\dagger - \lambda^*)|\lambda\rangle &= -i\sqrt{\frac{2}{m\hbar\omega}}\Delta p|\lambda\rangle. \qquad (2.63)\end{aligned}$$

So using the last relation in (2.60)

$$\Delta x|\lambda\rangle = \sqrt{\frac{\hbar}{2m\omega}}(-i)\sqrt{\frac{2}{m\hbar\omega}}\Delta p|\lambda\rangle = \underbrace{-\frac{i}{m\omega}}_{\text{purely imaginary}}\Delta p|\lambda\rangle \qquad (2.64)$$

and thus the minimum uncertainty condition is satisfied.

(c) The coherent state can be expressed as a superposition of energy eigenstates

$$|\lambda\rangle = \sum_{n=0}^{\infty}|n\rangle\langle n|\lambda\rangle = \sum_{n=0}^{\infty}f(n)|n\rangle. \qquad (2.65)$$

for the expansion coefficients $f(n)$ we have

$$\begin{aligned}f(n) &= \langle n|\lambda\rangle = \langle n|e^{-|\lambda|^2/2}e^{\lambda a^\dagger}|0\rangle = e^{-|\lambda|^2/2}\langle n|e^{\lambda a^\dagger}|0\rangle\\ &= e^{-|\lambda|^2/2}\langle n|\sum_{m=0}^{\infty}\frac{1}{m!}(\lambda a^\dagger)^m|0\rangle = e^{-|\lambda|^2/2}\sum_{m=0}^{\infty}\frac{1}{m!}\lambda^m\langle n|(a^\dagger)^m|0\rangle\\ &= e^{-|\lambda|^2/2}\sum_{m=0}^{\infty}\frac{1}{m!}\lambda^m\sqrt{m!}\langle n|m\rangle = e^{-|\lambda|^2/2}\frac{1}{\sqrt{n!}}\lambda^n \Rightarrow \qquad (2.66)\\ |f(n)|^2 &= \frac{(|\lambda|^2)^n}{n!}\exp(-|\lambda|^2) \qquad (2.67)\end{aligned}$$

which means that the distribution of $|f(n)|^2$ with respect to n is of the Poisson type about some mean value $\overline{n} = |\lambda|^2$.

The most probable value of n is given by the maximum of the distribution $|f(n)|^2$ which can be found in the following way

$$\frac{|f(n+1)|^2}{|f(n)|^2} = \frac{\frac{(|\lambda|^2)^{n+1}}{(n+1)!}\exp(-|\lambda|^2)}{\frac{(|\lambda|^2)^n}{n!}\exp(-|\lambda|^2)} = \frac{|\lambda|^2}{n+1} \geq 1 \tag{2.68}$$

which means that the most probable value of n is $|\lambda|^2$.

(d) We should check if the state $\exp\left(-ipl/\hbar\right)|0\rangle$ is an eigenstate of the annihilation operator a. We have

$$a\exp\left(-ipl/\hbar\right)|0\rangle = \left[a, e^{(-ipl/\hbar)}\right]|0\rangle \tag{2.69}$$

since $a|0\rangle = 0$. For the commutator in the last relation we have

$$\begin{aligned}\left[a, e^{(-ipl/\hbar)}\right] &= \sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{-il}{\hbar}\right)^n [a, p^n] = \sum_{n=1}^{\infty}\frac{1}{n!}\left(\frac{-il}{\hbar}\right)^n \sum_{k=1}^{n} p^{k-1}[a,p]p^{n-k} \\ &= \sum_{n=1}^{\infty}\frac{1}{n!}\left(\frac{-il}{\hbar}\right)^n \sum_{k=1}^{n} p^{n-1} i\sqrt{\frac{m\hbar\omega}{2}} \\ &= i\sqrt{\frac{m\hbar\omega}{2}}\left(\frac{-il}{\hbar}\right)\sum_{n=1}^{\infty}\frac{1}{(n-1)!}\left(\frac{-ilp}{\hbar}\right)^{n-1} \\ &= l\sqrt{\frac{m\omega}{2\hbar}}e^{(-ipl/\hbar)},\end{aligned} \tag{2.70}$$

where we have used that

$$[a, p] = i\sqrt{\frac{m\hbar\omega}{2}}[a, a^\dagger - a] = i\sqrt{\frac{m\hbar\omega}{2}}. \tag{2.71}$$

So substituting (2.70) in (2.69) we get

$$a\left[\exp\left(-ipl/\hbar\right)|0\rangle\right] = l\sqrt{\frac{m\omega}{2\hbar}}\left[\exp\left(-ipl/\hbar\right)|0\rangle\right] \tag{2.72}$$

which means that the state $\exp\left(-ipl/\hbar\right)|0\rangle$ is a coherent state with eigenvalue $l\sqrt{\frac{m\omega}{2\hbar}}$.

(e) Using the hint we have

$$|\lambda(t)\rangle = \mathcal{U}(t)|\lambda\rangle = e^{-iHt/\hbar}|\lambda\rangle \overset{(2.66)}{=} e^{-iHt/\hbar}\sum_{n=0}^{\infty} e^{-|\lambda|^2/2}\frac{1}{\sqrt{n!}}\lambda^n|n\rangle$$

$$\begin{aligned}
&= \sum_{n=0}^{\infty} e^{-iE_nt/\hbar} e^{-|\lambda|^2/2} \frac{1}{\sqrt{n!}} \lambda^n |n\rangle \overset{(2.3.9)}{=} \sum_{n=0}^{\infty} e^{\frac{-it}{\hbar}\hbar\omega(n+\frac{1}{2})} e^{-|\lambda|^2/2} \frac{1}{\sqrt{n!}} \lambda^n |n\rangle \\
&= \sum_{n=0}^{\infty} \left(e^{-i\omega t}\right)^n e^{-i\omega t/2} e^{-|\lambda|^2/2} \frac{1}{\sqrt{n!}} \lambda^n |n\rangle \\
&= e^{-i\omega t/2} \sum_{n=0}^{\infty} e^{-|\lambda e^{-i\omega t}|^2/2} \frac{\left(\lambda e^{-i\omega t}\right)^n}{\sqrt{n!}} |n\rangle \overset{(2.66)}{=} e^{-i\omega t/2} |\lambda e^{-i\omega t}\rangle \qquad (2.73)
\end{aligned}$$

Thus

$$\begin{aligned}
a|\lambda(t)\rangle &= e^{-i\omega t/2} a|\lambda e^{-i\omega t}\rangle = \lambda e^{-i\omega t} e^{-i\omega t/2} |\lambda e^{-i\omega t}\rangle \\
&= \lambda e^{-i\omega t} |\lambda(t)\rangle. \qquad (2.74)
\end{aligned}$$

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.).

We have

$$\begin{aligned}
K(x,y;E) &\equiv \int_0^{\infty} dt e^{iEt/\hbar} K(x,y;t,0) \equiv \int_0^{\infty} dt e^{iEt/\hbar} \langle x,t|y,0\rangle \\
&= \int_0^{\infty} dt e^{iEt/\hbar} \langle x|e^{-iHt/\hbar}|y\rangle \\
&= \int_0^{\infty} dt e^{iEt/\hbar} \sum_n \langle x|e^{-iHt/\hbar}|n\rangle\langle n|y\rangle \\
&= \int_0^{\infty} dt e^{iEt/\hbar} \sum_n e^{-iE_nt/\hbar} \langle x|n\rangle\langle n|y\rangle \\
&= \sum_n \phi_n(x)\phi_n^*(y) \int_0^{\infty} e^{i(E-E_n)t/\hbar} dt
\end{aligned}$$

$$
\begin{aligned}
&= \sum_n \phi_n(x)\phi_n^*(y) \lim_{\varepsilon\to 0}\left[\frac{-i\hbar}{E-E_n+i\varepsilon}e^{i(E-E_n+i\varepsilon)t/\hbar}\right]_0^\infty \\
&= \sum_n \phi_n(x)\phi_n^*(y)\frac{i\hbar}{E-E_n}. \qquad (2.75)
\end{aligned}
$$

So

$$
\sum_n \phi_n(x)\phi_n^*(y)\frac{i\hbar}{E-E_n} = A\sum_n \frac{\sin(nrx)\sin(nry)}{E-\frac{\hbar^2r^2}{2m}n^2} \Rightarrow
$$

$$
\phi_n(x) = \sqrt{\frac{A}{i\hbar}}\sin(nrx), \quad E_n = \frac{\hbar^2r^2}{2m}n^2. \qquad (2.76)
$$

For a one dimensional infinite square well potential with size L the energy eigenvalue E_n and eigenfunctions $\phi_n(x)$ are given by

$$
\phi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right), \quad E_n = \frac{\hbar^2}{2m}\left(\frac{\pi}{L}\right)^2 n^2. \qquad (2.77)
$$

Comparing with (2.76) we get $\frac{\pi}{L} = r \Rightarrow L = \frac{\pi}{r}$ and

$$
V = \begin{cases} 0 & \text{for } 0 < x < \frac{\pi}{r} \\ \infty & \text{otherwise} \end{cases} \qquad (2.78)
$$

while

$$
\frac{A}{i\hbar} = \frac{2r}{\pi} \Rightarrow A = i\frac{2\hbar r}{\pi}. \qquad (2.79)
$$

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.)

For an arbitrary test function $f(x)$ we have

$$
\int_{-\infty}^{+\infty}\frac{d\theta(x)}{dx}f(x)dx = \int_{-\infty}^{+\infty}\frac{d}{dx}\left[\theta(x)f(x)\right]dx - \int_{-\infty}^{+\infty}\theta(x)\frac{df(x)}{dx}dx
$$

$$
\begin{aligned}
&= \theta(x)f(x)\Big|_{-\infty}^{+\infty} - \int_0^{+\infty} \frac{df(x)}{dx}dx \\
&= \lim_{x\to+\infty} f(x) - f(x)\Big|_0^{+\infty} = f(0) \\
&= \int_{-\infty}^{+\infty} \delta(x)f(x)dx \Rightarrow \\
\frac{d\theta(x)}{dx} &= \delta(x). \qquad (2.80)
\end{aligned}
$$

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 $t = T$.

The Lagrangian for the one dimensional harmonic oscillator is given by

$$
\mathcal{L}(x, \dot{x}) = \tfrac{1}{2}m\dot{x}^2 - \tfrac{1}{2}m\omega^2 x^2. \qquad (2.81)
$$

From the Lagrange equation we have

$$
\begin{aligned}
&\frac{\partial\mathcal{L}}{\partial x} - \frac{d}{dt}\frac{\partial\mathcal{L}}{\partial\dot{x}} = 0 \overset{(2.81)}{\Rightarrow} -m\omega^2 x - \frac{d}{dt}(m\dot{x}) = 0 \Rightarrow \\
&\ddot{x} + \omega^2 x = 0. \qquad (2.82)
\end{aligned}
$$

which is the equation of motion for the system. This can be solved to give

$$
x(t) = A\cos\omega t + B\sin\omega t \qquad (2.83)
$$

with boundary conditions

$$
\begin{aligned}
x(t=0) &= x_0 = A \qquad (2.84) \\
x(t=T) &= x_T = x_0\cos\omega T + B\sin\omega T \Rightarrow B\sin\omega T = x_T - x_0\cos\omega T \Rightarrow \\
& B = \frac{x_T - x_0\cos\omega T}{\sin\omega T}. \qquad (2.85)
\end{aligned}
$$

So

$$
\begin{aligned}
x(t) &= x_0 \cos \omega t + \frac{x_T - x_0 \cos \omega T}{\sin \omega T} \sin \omega t \\
&= \frac{x_0 \cos \omega t \sin \omega T + x_T \sin \omega t - x_0 \cos \omega T \sin \omega t}{\sin \omega T} \\
&= \frac{x_T \sin \omega t + x_0 \sin \omega (T-t)}{\sin \omega T} \Rightarrow \qquad (2.86) \\
\dot{x}(t) &= \frac{x_T \omega \cos \omega t - x_0 \omega \cos \omega (T-t)}{\sin \omega T}. \qquad (2.87)
\end{aligned}
$$

With these at hand we have

$$
\begin{aligned}
S &= \int_0^T dt \mathcal{L}(x, \dot{x}) = \int_0^T dt \left(\tfrac{1}{2} m \dot{x}^2 - \tfrac{1}{2} m \omega^2 x^2 \right) \\
&= \int_0^T dt \left[\tfrac{1}{2} m \frac{d}{dt} (x \dot{x}) - \tfrac{1}{2} m x \ddot{x} - \tfrac{1}{2} m \omega^2 x^2 \right] \\
&= -\tfrac{1}{2} m \int_0^T dt x [\ddot{x} + \omega^2 x] + \frac{m}{2} x \dot{x} \Big|_0^T \\
&\overset{(2.82)}{=} \frac{m}{2} [x(T) \dot{x}(T) - x(0) \dot{x}(0)] \\
&= \frac{m}{2} \left[\frac{x_T \omega}{\sin \omega T} (x_T \cos \omega T - x_0) - \frac{x_0 \omega}{\sin \omega T} (x_T - x_0 \cos \omega T) \right] \\
&= \frac{m \omega}{2 \sin \omega T} \left[x_T^2 \cos \omega T - x_0 x_T - x_0 x_T + x_0^2 \cos \omega T \right] \\
&= \frac{m \omega}{2 \sin \omega T} \left[(x_T^2 + x_0^2) \cos \omega T - 2 x_0 x_T \right]. \qquad (2.88)
\end{aligned}
$$

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

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

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

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

[Hint: Diagonalize σ **by an orthogonal 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:

$$p_{j+1} = (2-\varepsilon^2\omega^2)p_j - p_{j-1} \qquad j=1,\dots,N \tag{2.89}$$

(e) Let $\phi(t) = \varepsilon p_j$ **for** $t = t_a + j\varepsilon$ **and show that (2.89) 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 $T = t_b - t_a$**.**

(a) Because at any given point the position kets in the Heisenberg picture form a complete set, it is legitimate to insert the identity operator written as

$$\int dx |xt\rangle\langle xt| = 1 \tag{2.90}$$

So

$$\begin{aligned} \langle x_b t_b | x_a t_a \rangle &= \lim_{N\to\infty} \int dx_1 dx_2 \ldots dx_N \langle x_b t_b | x_N t_N \rangle \langle x_N t_N | x_{N-1} t_{N-1} \rangle \ldots \times \\ & \langle x_{i+1} t_{i+1} | x_i t_i \rangle \ldots \langle x_1 t_1 | x_a t_a \rangle. \end{aligned} \tag{2.91}$$

It is

$$\begin{aligned} \langle x_{i+1} t_{i+1} | x_i t_i \rangle &= \langle x_{i+1} | e^{-iH(t_{i+1}-t_i)/\hbar} | x_i \rangle = \langle x_{i+1} | e^{-iH\varepsilon/\hbar} | x_i \rangle \\ &= \langle x_{i+1} | e^{-i\frac{\varepsilon}{\hbar}(\frac{1}{2}mp^2 + \frac{1}{2}m\omega^2 x^2)} | x_i \rangle \quad \text{(since } \varepsilon \text{ is very small)} \\ &= \langle x_{i+1} | e^{-i\frac{\varepsilon}{\hbar}\frac{p^2}{2m}} e^{-i\frac{\varepsilon}{\hbar}\frac{1}{2}m\omega^2 x^2} | x_i \rangle \\ &= e^{-i\frac{\varepsilon}{\hbar}\frac{1}{2}m\omega^2 x_i^2} \langle x_{i+1} | e^{-i\frac{\varepsilon}{\hbar}\frac{p^2}{2m}} | x_i \rangle. \end{aligned} \tag{2.92}$$

For the second term in this last equation we have

$$\begin{aligned} \langle x_{i+1} | e^{-i\frac{\varepsilon}{\hbar}\frac{p^2}{2m}} | x_i \rangle &= \int dp_i \langle x_{i+1} | e^{-i\frac{\varepsilon}{\hbar}\frac{p^2}{2m}} | p_i \rangle \langle p_i | x_i \rangle \\ &= \int dp_i e^{-i\frac{\varepsilon}{\hbar}\frac{p_i^2}{2m}} \langle x_{i+1} | p_i \rangle \langle p_i | x_i \rangle \\ &= \frac{1}{2\pi\hbar} \int dp_i e^{-i\frac{\varepsilon}{\hbar}\frac{{p_i}^2}{2m}} e^{ip_i(x_{i+1}-x_i)/\hbar} \\ &= \frac{1}{2\pi\hbar} \int dp_i e^{-i\frac{\varepsilon}{2m\hbar}\left[p_i^2 - 2p_i\frac{m}{\varepsilon}(x_{i+1}-x_i) + \frac{m^2}{\varepsilon^2}(x_{i+1}-x_i)^2 - \frac{m^2}{\varepsilon^2}(x_{i+1}-x_i)^2\right]} \\ &= \frac{1}{2\pi\hbar} e^{\frac{i\varepsilon}{2m\hbar}\frac{m^2}{\varepsilon^2}(x_{i+1}-x_i)^2} \int dp_i e^{-i\frac{\varepsilon}{2m\hbar}\left[p_i - p_i\frac{m}{\varepsilon}(x_{i+1}-x_i)\right]^2} \end{aligned}$$

$$
\begin{aligned}
&= \frac{1}{2\pi\hbar} e^{\frac{i\varepsilon}{2m\hbar}\frac{m^2}{\varepsilon^2}(x_{i+1}-x_i)^2} \sqrt{\frac{\pi 2\hbar m}{i\varepsilon}} \\
&= \sqrt{\frac{m}{2\pi\hbar i\varepsilon}} e^{\frac{im}{2\hbar\varepsilon}(x_{i+1}-x_i)^2}.
\end{aligned} \tag{2.93}
$$

Substituting this in (2.92) we get

$$
\langle x_{i+1}t_{i+1}|x_i t_i\rangle = \left(\frac{m}{2\pi i\hbar\varepsilon}\right)^{\frac{1}{2}} e^{\frac{i}{\hbar}\left[\frac{m}{2\varepsilon}(x_{i+1}-x_i)^2 - \frac{1}{2}\varepsilon m\omega^2 x_i\right]} \tag{2.94}
$$

and this into (2.91):

$$
\begin{aligned}
&\langle x_b t_b|x_a t_a\rangle \equiv \int \mathcal{D}x \exp\left\{\frac{i}{\hbar}S[x]\right\} = \\
&\lim_{N\to\infty} \int dx_1 \dots dx_N \left(\frac{m}{2\pi i\hbar\varepsilon}\right)^{\frac{(N+1)}{2}} exp\left\{\frac{i}{\hbar}\sum_{j=0}^{N}\left[\frac{m}{2\varepsilon}(x_{j+1}-x_j)^2 - \frac{1}{2}\varepsilon m\omega^2 x_j^2\right]\right\}.
\end{aligned}
$$

Let $y(t) = x(t) - x_{cl}(t) \Rightarrow x(t) = y(t) + x_{cl}(t) \Rightarrow \dot{x}(t) = \dot{y}(t) + \dot{x}_{cl}(t)$ with boundary conditions $y(t_a) = y(t_b) = 0$. For this new integration variable we have $\mathcal{D}x = \mathcal{D}y$ and

$$
\begin{aligned}
S[x] &= S[y + x_{cl}] = \int_{t_a}^{t_b} \mathcal{L}(y + x_{cl}, \dot{y} + \dot{x}_{cl})dt \\
&= \int_{t_a}^{t_b} \left[\mathcal{L}(x_{cl}, \dot{x}_{cl}) + \left.\frac{\partial\mathcal{L}}{\partial x}\right|_{x_{cl}} y + \left.\frac{\partial\mathcal{L}}{\partial\dot{x}}\right|_{x_{cl}} \dot{y} + \tfrac{1}{2}\left.\frac{\partial^2\mathcal{L}}{\partial^2 x}\right|_{x_{cl}} y^2 + \tfrac{1}{2}\left.\frac{\partial^2\mathcal{L}}{\partial\dot{x}^2}\right|_{x_{cl}} \dot{y}^2\right] \\
&= S_{cl} + \left.\frac{\partial\mathcal{L}}{\partial\dot{x}}y\right|_{t_a}^{t_b} + \int_{t_a}^{t_b}\left.\left[\frac{\partial\mathcal{L}}{\partial x} - \frac{d}{dt}\left(\frac{\partial\mathcal{L}}{\partial\dot{x}}\right)\right]\right|_{x_{cl}} y + \int_{t_a}^{t_b}\left[\tfrac{1}{2}m\dot{y}^2 - \tfrac{1}{2}m\omega^2 y^2\right]dt.
\end{aligned}
$$

So

$$
\begin{aligned}
\langle x_b t_b|x_a t_a\rangle &= \int \mathcal{D}y \exp\left\{\frac{i}{\hbar}S_{cl} + \frac{i}{\hbar}\int_{t_a}^{t_b}\left[\tfrac{1}{2}m\dot{y}^2 - \tfrac{1}{2}m\omega^2 y^2\right]dt\right\} \\
&= exp\left[\frac{iS_{cl}}{\hbar}\right] G(0, t_b; 0, t_a)
\end{aligned} \tag{2.95}
$$

with

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

(b) For the argument of the exponential in the last relation we have

$$\frac{i}{\hbar}\sum_{j=0}^{N}\left[\frac{m}{2\varepsilon}(y_{j+1}-y_j)^2-\frac{1}{2}\varepsilon m\omega^2 y_j^2\right]\overset{(y_0=0)}{=}$$
$$\frac{i}{\hbar}\sum_{j=0}^{N}\frac{m}{2\varepsilon}(y_{j+1}^2+y_j^2-y_{j+1}y_j-y_jy_{j+1})-\frac{i}{\hbar}\sum_{i,j=1}^{N}\frac{1}{2}\varepsilon m\omega^2 y_i\delta_{ij}y_j\overset{(y_{N+1}=0)}{=}$$
$$-\frac{m}{2\varepsilon i\hbar}\sum_{i,j=1}^{N}(2y_i\delta_{ij}y_j-y_i\delta_{i,j+1}y_j-y_i\delta_{i+1,j}y_j)-\frac{i\varepsilon m\omega^2}{2\hbar}\sum_{i,j=1}^{N}y_i\delta_{ij}y_j. \quad (2.96)$$

where the last step is written in such a form so that the matrix σ will be symmetric. Thus we have

$$G=\lim_{N\to\infty}\left(\frac{m}{2\pi i\hbar\varepsilon}\right)^{\frac{(N+1)}{2}}\int dy_1\dots dy_N exp(-n^T\sigma n) \quad (2.97)$$

with

$$\sigma=\frac{m}{2\varepsilon i\hbar}\begin{bmatrix}2&-1&0&\dots&0&0\\-1&2&-1&\dots&0&0\\0&-1&2&\dots&0&0\\\vdots&\vdots&\vdots&&\vdots&\vdots\\0&0&0&\dots&2&-1\\0&0&0&\dots&-1&2\end{bmatrix}+\frac{i\varepsilon m\omega^2}{2\hbar}\begin{bmatrix}1&0&0&\dots&0&0\\0&1&0&\dots&0&0\\0&0&1&\dots&0&0\\\vdots&\vdots&\vdots&&\vdots&\vdots\\0&0&0&\dots&1&0\\0&0&0&\dots&0&1\end{bmatrix} \quad (2.98)$$

(c) We can diagonalize σ by a unitary matrix U. Since σ is symmetric the following will hold

$$\sigma=U^\dagger\sigma_D U\Rightarrow\sigma^T=U^T\sigma_D(U^\dagger)^T=U^T\sigma_D U^*=\sigma\Rightarrow U=U^*. \quad (2.99)$$

So we can diagonalize σ by an orthogonal matrix R. So

$$\sigma=R^T\sigma_D R \quad \text{and} \;\det R=1 \quad (2.100)$$

which means that

$$\begin{aligned}\int d^N n e^{-n^T\sigma n} &= \int d^N n e^{-n^T R^T\sigma R n}\overset{Rn=\zeta}{=}\int d^N\zeta e^{-\zeta^T\sigma\zeta}\\ &= \left[\int d\zeta_1 e^{-\zeta_1^2 a_1}\right]\left[\int d\zeta_2 e^{-\zeta_2^2 a_2}\right]\dots\left[\int d\zeta_N e^{-\zeta_N^2 a_N}\right]\\ &= \sqrt{\frac{\pi}{a_1}}\sqrt{\frac{\pi}{a_2}}\dots\sqrt{\frac{\pi}{a_N}}=\frac{\pi^{N/2}}{\sqrt{\prod_{i=1}^N a_i}}=\frac{\pi^{N/2}}{\sqrt{\det\sigma_D}}\\ &= \frac{\pi^{N/2}}{\sqrt{\det\sigma}} \end{aligned} \quad (2.101)$$

where a_i are the diagonal elements of the matrix σ_D.

(d) From (2.98) we have

$$\left(\frac{2i\hbar\varepsilon}{m}\right)^N det\sigma =$$

$$\det\left\{\begin{bmatrix} 2 & -1 & 0 & \dots & 0 & 0 \\ -1 & 2 & -1 & \dots & 0 & 0 \\ 0 & -1 & 2 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 2 & -1 \\ 0 & 0 & 0 & \dots & -1 & 2 \end{bmatrix} - \varepsilon^2\omega^2 \begin{bmatrix} 1 & 0 & 0 & \dots & 0 & 0 \\ 0 & 1 & 0 & \dots & 0 & 0 \\ 0 & 0 & 1 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 1 & 0 \\ 0 & 0 & 0 & \dots & 0 & 1 \end{bmatrix}\right\} =$$

$$\det \sigma'_N \equiv p_N. \tag{2.102}$$

We define $j \times j$ matrices σ'_j that consist of the first j rows and j columns of σ'_N. So

$$\det \sigma'_{j+1} = \det \begin{bmatrix} 2-\varepsilon^2\omega^2 & -1 & \dots & 0 & 0 & 0 \\ -1 & 2-\varepsilon^2\omega^2 & \dots & 0 & 0 & 0 \\ 0 & -1 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & 2-\varepsilon^2\omega^2 & -1 & 0 \\ 0 & 0 & \dots & -1 & 2-\varepsilon^2\omega^2 & -1 \\ 0 & 0 & \dots & 0 & -1 & 2-\varepsilon^2\omega^2 \end{bmatrix}.$$

From the above it is obvious that

$$\begin{aligned} \det \sigma'_{j+1} &= (2-\varepsilon^2\omega^2)\det \sigma'_j - \det \sigma'_{j-1} \Rightarrow \\ p_{j+1} &= (2-\varepsilon^2\omega^2)p_j - p_{j-1} \quad \text{for } j = 2, 3, \dots, N \end{aligned} \tag{2.103}$$

with $p_0 = 1$ and $p_1 = 2 - \varepsilon^2\omega^2$.

(e) We have

$$\begin{aligned} \phi(t) \equiv \phi(t_a + j\varepsilon) &\equiv \varepsilon p_j \\ \Rightarrow \phi(t_a + (j+1)\varepsilon) &= \varepsilon p_{j+1} = (2-\varepsilon^2\omega^2)\varepsilon p_j - \varepsilon p_{j-1} \\ &= 2\phi(t_a + j\varepsilon) - \varepsilon^2\omega^2\phi(t_a + j\varepsilon) - \phi(t_a + (j-1)\varepsilon) \\ \Rightarrow \phi(t+\varepsilon) &= 2\phi(t) - \varepsilon^2\omega^2\phi(t) - \phi(t-\varepsilon). \end{aligned} \tag{2.104}$$

So

$$\phi(t+\varepsilon)-\phi(t)=\phi(t)-\phi(t-\varepsilon)-\varepsilon^2\omega^2\phi(t)\Rightarrow$$
$$\frac{\frac{\phi(t+\varepsilon)-\phi(t)}{\varepsilon}-\frac{\phi(t)-\phi(t-\varepsilon)}{\varepsilon}}{\varepsilon}=-\omega^2\phi(t)\Rightarrow$$
$$\lim_{\varepsilon\to 0}\frac{\phi'(t)-\phi'(t-\varepsilon)}{\varepsilon}=-\omega^2\phi(t)\Rightarrow\frac{d^2\phi}{dt^2}=-\omega^2\phi(t). \tag{2.105}$$

From (c) we have also that

$$\phi(t_a)=\varepsilon p_0\to 0 \tag{2.106}$$

and

$$\begin{aligned}\frac{d\phi}{dt}(t_a) &= \frac{\phi(t_a+\varepsilon)-\phi(t_a)}{\varepsilon}=\frac{\varepsilon(p_1-p_0)}{\varepsilon}=p_1-p_0\\ &= 2-\varepsilon^2\omega^2-1\to 1.\end{aligned} \tag{2.107}$$

The general solution to (2.105) is

$$\phi(t)=A\sin(\omega t+\delta) \tag{2.108}$$

and from the boundary conditions (2.106) and (2.107) we have

$$\phi(t_a)=0\Rightarrow A\sin(\omega t_a+\delta)=0\Rightarrow\delta=-\omega t_a+n\pi\quad n\in\mathcal{Z} \tag{2.109}$$

which gives that $\phi(t)=A\sin\omega(t-t_a)$, while

$$\begin{aligned}&\frac{d\phi}{dt}=A\omega\cos(t-t_a)\Rightarrow\phi'(t_a)=A\omega\overset{(2.107)}{\Rightarrow}\\ &A\omega=1\Rightarrow A=\frac{1}{\omega}\end{aligned} \tag{2.110}$$

Thus

$$\phi(t)=\frac{\sin\omega(t-t_a)}{\omega}. \tag{2.111}$$

(f) Gathering all the previous results together we get

$$G = \lim_{N\to\infty}\left[\left(\frac{m}{2\pi i\hbar\varepsilon}\right)^{(N+1)}\frac{\pi^N}{\sqrt{det\sigma}}\right]^{1/2}$$

$$= \left(\frac{m}{2\pi i\hbar}\right)^{1/2}\left[\lim_{N\to\infty}\varepsilon\left(\frac{2i\hbar\varepsilon}{m}\right)^N det\sigma\right]^{-1/2}$$

$$\stackrel{(d)}{=} \left(\frac{m}{2\pi i\hbar}\right)^{1/2}\left(\lim_{N\to\infty}\varepsilon p_N\right)^{-1/2} \stackrel{(e)}{=} \left(\frac{m}{2\pi i\hbar}\right)^{1/2}[\phi(t_b)]^{-1/2}$$

$$\stackrel{(2.111)}{=} \sqrt{\frac{m\omega}{2\pi i\hbar\sin(\omega T)}}. \qquad (2.112)$$

So from (a)

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

$$\stackrel{(2.88)}{=} \sqrt{\frac{m\omega}{2\pi i\hbar\sin(\omega T)}}exp\left[\frac{im\omega}{2\hbar\sin\omega T}\left[(x_b^2+x_a^2)\cos\omega T - 2x_b x_a\right]\right].$$

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).

We have

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

$$= \int dx_1 \sqrt{\frac{m}{2\pi i\hbar(t_2-t_1)}}\exp\left[\frac{im(x_2-x_1)^2}{2\hbar(t_2-t_1)}\right]\times$$

$$\sqrt{\frac{m}{2\pi i\hbar(t_1-t_0)}}\exp\left[\frac{im(x_1-x_0)^2}{2\hbar(t_1-t_0)}\right]$$

$$= \frac{m}{2\pi i\hbar}\sqrt{\frac{1}{(t_2-t_1)(t_1-t_0)}}\exp\frac{imx_2^2}{2\hbar(t_2-t_1)}\exp\frac{imx_0^2}{2\hbar(t_2-t_1)}\times$$

$$\int dx_1\exp\left[\frac{im}{2\hbar(t_2-t_1)}x_1^2+\frac{im}{2\hbar(t_2-t_1)}x_1^2-\frac{im}{2\hbar(t_2-t_1)}2x_1x_2-\frac{im}{2\hbar(t_2-t_1)}2x_1x_0\right]$$

$$
\begin{aligned}
&= \frac{m}{2\pi i\hbar}\sqrt{\frac{1}{(t_2-t_1)(t_1-t_0)}}\exp\left\{\frac{im}{2\hbar}\left[\frac{x_2^2}{(t_2-t_1)}+\frac{x_0^2}{(t_1-t_0)}\right]\right\}\times \\
&\quad \int dx_1 \exp\left\{\frac{im}{2\hbar}\left[\frac{1}{(t_2-t_1)}+\frac{1}{(t_1-t_0)}\right]x_1^2 - \frac{im}{\hbar}x_1\left[\frac{x_2}{(t_2-t_1)}+\frac{x_0}{(t_1-t_0)}\right]\right\} \\
&= \frac{m}{2\pi i\hbar}\sqrt{\frac{1}{(t_2-t_1)(t_1-t_0)}}\exp\left\{\frac{im}{2\hbar}\left[\frac{x_2^2}{(t_2-t_1)}+\frac{x_0^2}{(t_1-t_0)}\right]\right\}\times \\
&\quad \int dx_1 \exp\left\{\frac{-m}{2i\hbar}\left[\frac{t_2-t_0}{(t_2-t_1)(t_1-t_0)}\right]\right. \\
&\quad \left.\left[x_1^2 - \frac{2\hbar}{im}\frac{t_2-t_0}{(t_2-t_1)(t_1-t_0)}\frac{im}{\hbar}x_1\left[\frac{x_2(t_1-t_0)+x_0(t_2-t_1)}{(t_2-t_1)(t_1-t_0)}\right]\right]\right\} \\
&= \frac{m}{2\pi i\hbar}\sqrt{\frac{1}{(t_2-t_1)(t_1-t_0)}}\exp\left\{\frac{im}{2\hbar}\left[\frac{x_2^2(t_1-t_0)+x_0^2(t_2-t_1)}{(t_2-t_1)(t_1-t_0)}\right]\right\}\times \\
&\quad \left[\int dx_1 \exp\left\{\frac{-m}{2i\hbar}\left[\frac{t_2-t_0}{(t_2-t_1)(t_1-t_0)}\right]\left[x_1-\frac{x_2(t_1-t_0)+x_0(t_2-t_1)}{(t_2-t_0)}\right]^2\right\}\right]\times \\
&\quad \exp\left\{-\frac{im}{2\hbar}\frac{1}{(t_2-t_1)(t_1-t_0)}\frac{[x_2(t_1-t_0)+x_0(t_2-t_1)]^2}{(t_2-t_0)}\right\} \\
&= \frac{m}{2\pi i\hbar}\sqrt{\frac{1}{(t_2-t_1)(t_1-t_0)}}\sqrt{\frac{\pi 2i\hbar(t_2-t_1)(t_1-t_0)}{m(t_2-t_0)}}\exp\left\{\frac{im}{2\hbar}\frac{1}{(t_2-t_1)(t_1-t_0)}\right.\times \\
&\quad \left[\frac{x_2^2(t_1-t_0)(t_2-t_0)+x_0^2(t_2-t_1)(t_2-t_0)}{(t_2-t_0)}-\right. \\
&\quad \left.\left.\frac{x_2^2(t_1-t_0)^2-x_0^2(t_2-t_1)^2-2x_2x_0 2(t_1-t_0)(t_2-t_1)}{(t_2-t_0)}\right]\right\} \\
&= \sqrt{\frac{m}{2\pi i\hbar(t_2-t_1)}}\times \\
&\quad \exp\left\{\frac{im}{2\hbar}\left[\frac{x_2^2(t_1-t_0)(t_2-t_0-t_1+t_0)+x_0^2(t_2-t_1)(t_2-t_0-t_2+t_1)}{(t_2-t_0)(t_2-t_1)(t_1-t_0)}-\right.\right. \\
&\quad \left.\left.\frac{2x_2x_0 2(t_1-t_0)(t_2-t_1)}{(t_2-t_0)(t_2-t_1)(t_1-t_0)}\right]\right\} \\
&= \sqrt{\frac{m}{2\pi i\hbar(t_2-t_0)}}\exp\left[\frac{im(x_2-x_0)^2}{2\hbar(t_2-t_0)}\right] \\
&= K_f(x_2,t_2;x_0,t_0).
\end{aligned}
\tag{2.113}
$$

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**

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

(a) We have

$$\begin{aligned}
[\Pi_i, \Pi_j] &= \left[p_i - \frac{eA_i}{c}, p_j - \frac{eA_j}{c}\right] = -\frac{e}{c}[p_i, A_j] - \frac{e}{c}[A_i, p_j] \\
&= \frac{i\hbar e}{c}\frac{\partial A_j}{\partial x_i} - \frac{i\hbar e}{c}\frac{\partial A_i}{\partial x_j} = \frac{i\hbar e}{c}\left(\frac{\partial A_j}{\partial x_i} - \frac{\partial A_i}{\partial x_j}\right) \\
&= \left(\frac{i\hbar e}{c}\right) \varepsilon_{ijk} B_k. \qquad (2.114)
\end{aligned}$$

We have also that

$$\begin{aligned}
\frac{dx_i}{dt} &= \frac{1}{i\hbar}[x_i, H] = \frac{1}{i\hbar}\left[x_i, \frac{\vec{\Pi}^2}{2m} + e\phi\right] = \frac{1}{i\hbar}\left[x_i, \frac{\vec{\Pi}^2}{2m}\right] \\
&= \frac{1}{i\hbar 2m}\{[x_i, \Pi_j]\,\Pi_j + \Pi_j\,[x_i, \Pi_j]\} = \frac{1}{i\hbar 2m}\{[x_i, p_j]\,\Pi_j + \Pi_j\,[x_i, p_j]\} \\
&= \frac{2i\hbar}{2i\hbar m}\Pi_j \delta_{ij} = \frac{\Pi_i}{m} \Rightarrow
\end{aligned}$$

$$
\begin{aligned}
\frac{d^2x_i}{dt^2} &= \frac{1}{i\hbar}\left[\frac{dx_i}{dt}, H\right] = \frac{1}{i\hbar m}\left[\Pi_i, \frac{\vec{\Pi}^2}{2m} + e\phi\right] \\
&= \frac{1}{i\hbar 2m^2}\left\{[\Pi_i,\Pi_j]\,\Pi_j + \Pi_j\,[\Pi_i,\Pi_j]\right\} + \frac{e}{i\hbar m}[\Pi_i,\phi] \\
&\overset{(2.114)}{=} \frac{1}{2m^2 i\hbar}\left[\frac{i\hbar e}{c}\varepsilon_{ijk}B_k\Pi_j + \frac{i\hbar e}{c}\varepsilon_{ijk}\Pi_j B_k\right] + \frac{e}{i\hbar m}\left[p_i - \frac{eA_i}{c}, \phi\right] \\
&= \frac{e}{2m^2 c}\left(-\varepsilon_{ikj}B_k\Pi_j + \varepsilon_{ijk}\Pi_j B_k\right) + \frac{e}{i\hbar m}[p_i,\phi] \\
&= \frac{e}{2m^2 c}m\left(\varepsilon_{ijk}\frac{x_j}{dt}B_k - \varepsilon_{ikj}B_k\frac{x_j}{dt}\right) - \frac{e}{m}\frac{\partial\phi}{\partial x_i} \Rightarrow \\
m\frac{d^2x_i}{dt^2} &= eE_i + \frac{e}{2c}\left[\left(\frac{\vec{x}}{dt}\times\vec{B}\right)_i - \left(\vec{B}\times\frac{\vec{x}}{dt}\right)_i\right] \Rightarrow \\
m\frac{d^2\vec{x}}{dt^2} &= e\left[\vec{E} + \frac{1}{2c}\left(\frac{\vec{x}}{dt}\times\vec{B} - \vec{B}\times\frac{\vec{x}}{dt}\right)\right]. \qquad (2.115)
\end{aligned}
$$

(b) The time-dependent Schrödinger equation is

$$
\begin{aligned}
& i\hbar\frac{\partial}{\partial t}\langle x'|\alpha, t_0; t\rangle = \langle x'|H|\alpha, t_0; t\rangle = \langle x'|\frac{1}{2m}\left(\vec{p} - \frac{e\vec{A}}{c}\right)^2 + e\phi|\alpha, t_0; t\rangle \\
=\;& \frac{1}{2m}\left[-i\hbar\vec{\nabla}' - \frac{e\vec{A}(\vec{x}')}{c}\right]\cdot\left[-i\hbar\vec{\nabla}' - \frac{e\vec{A}(\vec{x}')}{c}\right]\langle x'|\alpha, t_0; t\rangle + e\phi(\vec{x}')\langle x'|\alpha, t_0; t\rangle \\
=\;& \frac{1}{2m}\left[-\hbar^2\vec{\nabla}'\cdot\vec{\nabla}' + \frac{e}{c}i\hbar\vec{\nabla}'\cdot\vec{A}(\vec{x}') + i\hbar\frac{e}{c}\vec{A}(\vec{x}')\cdot\vec{\nabla}' + \frac{e^2}{c^2}A^2(\vec{x}')\right]\psi(\vec{x}', t) \\
& + e\phi(\vec{x}')\psi(\vec{x}', t) \\
=\;& \frac{1}{2m}\left[-\hbar^2\nabla'^2\psi(\vec{x}', t)' + \frac{e}{c}i\hbar\left(\vec{\nabla}'\cdot\vec{A}\right)\psi(\vec{x}', t) + \frac{e}{c}i\hbar\vec{A}(\vec{x}')\cdot\vec{\nabla}'\psi(\vec{x}', t)\right. \\
+\;& \left. i\hbar\frac{e}{c}\vec{A}(\vec{x}')\cdot\vec{\nabla}'\psi(\vec{x}', t) + \frac{e^2}{c^2}A^2(\vec{x}')\psi(\vec{x}', t)\right] + e\phi(\vec{x}')\psi(\vec{x}', t) \\
=\;& \frac{1}{2m}\left[-\hbar^2\nabla'^2\psi + \frac{e}{c}i\hbar\left(\vec{\nabla}'\cdot\vec{A}\right)\psi + 2i\hbar\frac{e}{c}\vec{A}\cdot\vec{\nabla}'\psi + \frac{e^2}{c^2}A^2\psi\right] + e\phi\psi. \qquad (2.116)
\end{aligned}
$$

Multiplying the last equation by ψ^* we get

$$
i\hbar\psi^*\frac{\partial}{\partial t}\psi =
$$

$$\frac{1}{2m}\left[-\hbar^2\psi^*\nabla'^2\psi+\frac{e}{c}i\hbar\left(\vec{\nabla}'\cdot\vec{A}\right)|\psi|^2+2i\hbar\frac{e}{c}\vec{A}\cdot\psi^*\vec{\nabla}'\psi+\frac{e^2}{c^2}A^2|\psi|^2\right]+e\phi|\psi|^2.$$

The complex conjugate of this eqution is

$$-i\hbar\psi\frac{\partial}{\partial t}\psi^* =$$
$$\frac{1}{2m}\left[-\hbar^2\psi\nabla'^2\psi^*-\frac{e}{c}i\hbar\left(\vec{\nabla}'\cdot\vec{A}\right)|\psi|^2-2i\hbar\frac{e}{c}\vec{A}\cdot\psi\vec{\nabla}'\psi^*+\frac{e^2}{c^2}A^2|\psi|^2\right]+e\phi|\psi|^2.$$

Thus subtracting the last two equations we get

$$\begin{aligned}
& -\frac{\hbar^2}{2m}\left[\psi^*\nabla'^2\psi-\psi\nabla'^2\psi^*\right] \\
& +\left(\frac{e}{mc}\right)i\hbar\left(\vec{\nabla}'\cdot\vec{A}\right)|\psi|^2+\left(\frac{e}{mc}\right)i\hbar\vec{A}\cdot\left(\psi^*\vec{\nabla}'\psi+\psi\vec{\nabla}'\psi^*\right) \\
= & \; i\hbar\left(\psi^*\frac{\partial}{\partial t}\psi+\psi\frac{\partial}{\partial t}\psi^*\right)\Rightarrow \\
& -\frac{\hbar^2}{2m}\vec{\nabla}'\cdot\left[\psi^*\vec{\nabla}'\psi-\psi\vec{\nabla}'\psi^*\right]+\left(\frac{e}{mc}\right)i\hbar\left(\vec{\nabla}'\cdot\vec{A}\right)|\psi|^2+\left(\frac{e}{mc}\right)i\hbar\vec{A}\cdot\left(\vec{\nabla}'|\psi|^2\right) \\
= & \; i\hbar\frac{\partial}{\partial t}|\psi|^2\Rightarrow \\
& \frac{\partial}{\partial t}|\psi|^2=-\frac{\hbar}{m}\vec{\nabla}'\cdot\left[\Im(\psi^*\vec{\nabla}'\psi)\right]+\left(\frac{e}{mc}\right)\vec{\nabla}'\cdot\left[\vec{A}|\psi|^2\right]\Rightarrow \\
& \frac{\partial}{\partial t}|\psi|^2+\vec{\nabla}'\cdot\left[\frac{\hbar}{m}\Im(\psi^*\vec{\nabla}'\psi)-\left(\frac{e}{mc}\right)\vec{A}|\psi|^2\right]=0\Rightarrow \\
& \frac{\partial\rho}{\partial t}+\vec{\nabla}'\cdot\vec{j}=0 \qquad (2.117)
\end{aligned}$$

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

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.

The magentic field $\vec{B} = B\hat{z}$ can be derived from a vector petential $\vec{A}(\vec{x})$ of the form

$$A_x = -\frac{By}{2}, \quad A_y = \frac{Bx}{2}, \quad A_z = 0. \tag{2.118}$$

Thus we have

$$\begin{aligned} [\Pi_x, \Pi_y] &= \left[p_x - \frac{eA_x}{c}, p_y - \frac{eA_y}{c}\right] \overset{(2.118)}{=} \left[p_x + \frac{eBy}{2c}, p_y - \frac{eBx}{2c}\right] \\ &= -\frac{eB}{2c}[p_x, x] + \frac{eB}{2c}[y, p_y] = \frac{i\hbar eB}{2c} + \frac{i\hbar eB}{2c} \\ &= i\hbar\frac{eB}{c}. \end{aligned} \tag{2.119}$$

(b) The Hamiltonian for this system is given by

$$H = \frac{1}{2m}\left(\vec{p} - \frac{e\vec{A}}{c}\right)^2 = \frac{1}{2m}\Pi_x^2 + \frac{1}{2m}\Pi_y^2 + \frac{1}{2m}p_z^2 = H_1 + H_2 \tag{2.120}$$

where $H_1 \equiv \frac{1}{2m}\Pi_x^2 + \frac{1}{2m}\Pi_y^2$ and $H_2 \equiv \frac{1}{2m}p_z^2$. Since

$$[H_1, H_2] = \frac{1}{4m^2}\left[\left(p_x + \frac{eBy}{2c}\right)^2 + \left(, p_y - \frac{eBx}{2c}\right)^2, p_z^2\right] = 0 \tag{2.121}$$

there exists a set of simultaneous eigenstates $|k, n\rangle$ of the operators H_1 and H_2. So if $\hbar k$ is the continious eigegenvalue of the operator p_z and $|k, n\rangle$ its eigenstate we will have

$$H_2|k, n\rangle = \frac{p_z^2}{2m}|k, n\rangle = \frac{\hbar^2 k^2}{2m}. \tag{2.122}$$

On the other hand H_1 is similar to the Hamiltonian of the one-dimensional oscillator problem which is given by

$$H = \frac{1}{2m}p^2 + \tfrac{1}{2}m\omega^2 x^2 \tag{2.123}$$

with $[x,p] = i\hbar$. In order to use the eigenvalues of the harmonic oscillator $E_n = \hbar\omega\left(n+\frac{1}{2}\right)$ we should have the same commutator between the squared operators in the Hamiltonian. From (a) we have

$$[\Pi_x, \Pi_y] = i\hbar\frac{eB}{c} \Rightarrow [\left(\frac{\Pi_x c}{eB}\right), \Pi_y] = i\hbar. \tag{2.124}$$

So H_1 can be written in the following form

$$\begin{aligned} H_1 &\equiv \frac{1}{2m}\Pi_x^2 + \frac{1}{2m}\Pi_y^2 = \frac{1}{2m}\Pi_y^2 + \frac{1}{2m}\left(\frac{\Pi_x c}{eB}\right)^2 \frac{|eB|^2}{c^2} \\ &= \frac{1}{2m}\Pi_y^2 + \tfrac{1}{2}m\left(\frac{|eB|}{mc}\right)^2\left(\frac{\Pi_x c}{eB}\right)^2. \end{aligned} \tag{2.125}$$

In this form it is obvious that we can replace ω with $\frac{|eB|}{mc}$ to have

$$\begin{aligned} H|k,n\rangle &= H_1|k,n\rangle + H_2|k,n\rangle = \frac{\hbar^2k^2}{2m}|k,n\rangle + \left(\frac{|eB|\hbar}{mc}\right)\left(n+\frac{1}{2}\right)|k,n\rangle \\ &= \left[\frac{\hbar^2k^2}{2m} + \left(\frac{|eB|\hbar}{mc}\right)\left(n+\frac{1}{2}\right)\right]|k,n\rangle. \end{aligned} \tag{2.126}$$

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.

In the case where $\vec{B} = 0$ the Schrödinger equation of motion in the cylindrical coordinates is

$$\begin{aligned} -\tfrac{\hbar^2}{m}\left[\nabla^2\psi\right] = 2E\psi \Rightarrow \\ -\tfrac{\hbar^2}{m}\left[\tfrac{\partial^2}{\partial\rho^2} + \tfrac{1}{\rho}\tfrac{\partial}{\partial\rho} + \tfrac{1}{\rho^2}\tfrac{\partial^2}{\partial\phi^2} + \tfrac{\partial^2}{\partial z^2}\right]\Psi(\vec{x}) = 2E\Psi(\vec{x}) \end{aligned} \tag{2.127}$$

If we write $\Psi(\rho,\phi,z)=\Phi(\phi)R(\rho)Z(z)$ and $k^2=\frac{2mE}{\hbar^2}$ we will have

$$\begin{aligned}
&\Phi(\phi)Z(z)\frac{d^2R}{d\rho^2}+\Phi(\phi)Z(z)\frac{1}{\rho}\frac{dR}{d\rho}+\frac{R(\rho)Z(z)}{\rho^2}\frac{d^2\Phi}{d\phi^2}\\
&+R(\rho)\Phi(\phi)\frac{d^2Z}{dz^2}+k^2R(\rho)\Phi(\phi)Z(z)=0\Rightarrow\\
&\frac{1}{R(\rho)}\frac{d^2R}{d\rho^2}+\frac{1}{R(\rho)\rho}\frac{dR}{d\rho}+\frac{1}{\rho^2\Phi(\phi)}\frac{d^2\Phi}{d\phi^2}+\frac{1}{Z(z)}\frac{d^2Z}{dz^2}+k^2=0
\end{aligned} \tag{2.128}$$

with initial conditions $\Psi(\rho_a,\phi,z)=\Psi(R,\phi,z)=\Psi(\rho,\phi,0)=\Psi(\rho,\phi,a)=0$. So

$$\frac{1}{Z(z)}\frac{d^2Z}{dz^2}=-l^2\Rightarrow\frac{d^2Z}{dz^2}+l^2Z(z)=0\Rightarrow Z(z)=A_1e^{ilz}+B_1e^{-ilz} \tag{2.129}$$

with

$$\begin{aligned}
Z(0)&=0\Rightarrow A_1+B_1=0\Rightarrow Z(z)=A_1\left(e^{ilz}-e^{-ilz}\right)=C\sin lz\\
Z(a)&=0\Rightarrow C\sin la=0\Rightarrow la=n\pi\Rightarrow l=l_n=n\frac{\pi}{a}\quad n=\pm1,\pm2,\ldots
\end{aligned}$$

So

$$Z(z)=C\sin l_nz \tag{2.130}$$

Now we will have

$$\begin{aligned}
&\frac{1}{R(\rho)}\frac{d^2R}{d\rho^2}+\frac{1}{R(\rho)\rho}\frac{dR}{d\rho}+\frac{1}{\rho^2\Phi(\phi)}\frac{d^2\Phi}{d\phi^2}+k^2-l^2=0\\
\Rightarrow\quad&\frac{\rho^2}{R(\rho)}\frac{d^2R}{d\rho^2}+\frac{\rho}{R(\rho)}\frac{dR}{d\rho}+\frac{1}{\Phi(\phi)}\frac{d^2\Phi}{d\phi^2}+\rho^2(k^2-l^2)=0\\
\Rightarrow\quad&\frac{1}{\Phi(\phi)}\frac{d^2\Phi}{d\phi^2}=-m^2\Rightarrow\Phi(\phi)=e^{\pm im\phi}.
\end{aligned} \tag{2.131}$$

with

$$\Phi(\phi+2\pi)=\Phi(\phi)\Rightarrow m\in\mathcal{Z}. \tag{2.132}$$

So the Schrödinger equation is reduced to

$$\frac{\rho^2}{R(\rho)}\frac{d^2R}{d\rho^2}+\frac{\rho}{R(\rho)}\frac{dR}{d\rho}-m^2+\rho^2(k^2-l^2)=0$$

$$\Rightarrow \quad \frac{d^2R}{d\rho^2}+\frac{1}{\rho}\frac{dR}{d\rho}+\left[(k^2-l^2)-\frac{m^2}{\rho^2}\right]R(\rho)=0$$

$$\Rightarrow \quad \frac{d^2R}{d(\sqrt{k^2-l^2}\rho)^2}+\frac{1}{\sqrt{k^2-l^2}\rho}\frac{dR}{d(\sqrt{k^2-l^2}\rho)}+\left[1-\frac{m^2}{(k^2-l^2)\rho^2}\right]R(\rho)=0$$

$$\Rightarrow \quad R(\rho)=A_3J_m(\sqrt{k^2-l^2}\rho)+B_3N_m(\sqrt{k^2-l^2}\rho) \tag{2.133}$$

In the case at hand in which $\rho_a \to 0$ we should take $B_3=0$ since $N_m \to \infty$ when $\rho \to 0$. From the other boundary condition we get

$$R(R)=0 \Rightarrow A_3J_m(R\sqrt{k^2-l^2})=0 \Rightarrow R\sqrt{k^2-l^2}=\kappa_{m\nu} \tag{2.134}$$

where $\kappa_{m\nu}$ is the ν-th zero of the m-th order Bessel function J_m. This means that the energy eigenstates are given by the equation

$$\kappa_{m\nu}=R\sqrt{k^2-l^2} \Rightarrow k^2-l^2=\frac{\kappa_{m\nu}^2}{R^2} \Rightarrow \frac{2mE}{\hbar^2}-\left(n\frac{\pi}{a}\right)^2=\frac{\kappa_{m\nu}^2}{R^2}$$

$$\Rightarrow \quad E=\frac{\hbar^2}{2m}\left[\frac{\kappa_{m\nu}^2}{R^2}+\left(n\frac{\pi}{a}\right)^2\right] \tag{2.135}$$

while the corresponding eigenfunctions are given by

$$\psi_{nm\nu}(\vec{x})=A_cJ_m(\frac{\kappa_{m\nu}}{R}\rho)e^{im\phi}\sin\left(n\frac{\pi z}{a}\right) \tag{2.136}$$

with $n=\pm1,\pm2,\ldots$ and $m\in\mathcal{Z}$.

Now suppose that $\vec{B}=B\hat{z}$. We can then write

$$\vec{A}=\left(\frac{B\rho_a^2}{2\rho}\right)\hat{\phi}=\left(\frac{\Phi}{2\pi\rho}\right)\hat{\phi}. \tag{2.137}$$

The Schrödinger equation in the presence of the magnetic field $\vec{B}$ can be written as follows

$$\frac{1}{2m}\left[-i\hbar\vec{\nabla}-\frac{e\vec{A}(\vec{x})}{c}\right]\cdot\left[-i\hbar\vec{\nabla}-\frac{e\vec{A}(\vec{x})}{c}\right]\psi(\vec{x})=E\psi(\vec{x})$$

$$\Rightarrow \quad -\frac{\hbar^2}{2m}\left[\hat{\rho}\frac{\partial}{\partial\rho}+\hat{z}\frac{\partial}{\partial z}+\hat{\phi}\frac{1}{\rho}\left(\frac{\partial}{\partial\phi}-\frac{ie}{\hbar c}\frac{\Phi}{2\pi}\right)\right]\cdot$$

$$\left[\hat{\rho}\frac{\partial}{\partial\rho}+\hat{z}\frac{\partial}{\partial z}+\hat{\phi}\frac{1}{\rho}\left(\frac{\partial}{\partial\phi}-\frac{ie}{\hbar c}\frac{\Phi}{2\pi}\right)\right]\psi(\vec{x})=E\psi(\vec{x}). \tag{2.138}$$

Making now the transformation $D_\phi \equiv \frac{\partial}{\partial\phi} - \frac{ie}{\hbar c}\frac{\Phi}{2\pi}$ we get

$$
\begin{aligned}
& -\frac{\hbar^2}{2m}\left[\hat{\rho}\frac{\partial}{\partial\rho} + \hat{z}\frac{\partial}{\partial z} + \hat{\phi}\frac{1}{\rho}D_\phi\right] \cdot \left[\hat{\rho}\frac{\partial}{\partial\rho} + \hat{z}\frac{\partial}{\partial z} + \hat{\phi}\frac{1}{\rho}D_\phi\right]\psi(\vec{x}) = E\psi(\vec{x}) \\
\Rightarrow \quad & -\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}D_\phi^2 + \frac{\partial^2}{\partial z^2}\right]\Psi(\vec{x}) = E\Psi(\vec{x}), \qquad (2.139)
\end{aligned}
$$

where $D_\phi^2 = \left(\frac{\partial}{\partial\phi} - \frac{ie}{\hbar c}\frac{\Phi}{2\pi}\right)^2$. Leting $A = \frac{e}{\hbar c}\frac{\Phi}{2\pi}$ we get

$$
D_\phi^2 = \left(\frac{\partial^2}{\partial\phi^2} - \frac{2ie}{\hbar c}\frac{\Phi}{2\pi}\frac{\partial}{\partial\phi} - A^2\right) = \left(\frac{\partial^2}{\partial\phi^2} - 2iA\frac{\partial}{\partial\phi} - A^2\right). \qquad (2.140)
$$

Following the same procedure we used before (i.e. $\psi(\rho,\phi,z) = R(\rho)\Phi(\phi)Z(z)$) we will get the same equations with the exception of

$$
\left[\frac{\partial^2}{\partial\phi^2} - 2iA\frac{\partial}{\partial\phi} - A^2\right]\Phi = -m^2\Phi \Rightarrow \frac{d^2\Phi}{d\phi^2} - 2iA\frac{d\Phi}{d\phi} + (m^2 - A^2)\Phi = 0.
$$

The solution to this equation is of the form $e^{l\phi}$. So

$$
\begin{aligned}
& l^2 e^{l\phi} - 2iAle^{l\phi} + (m^2 - A^2)e^{l\phi} = 0 \Rightarrow l^2 - 2iAl + (m^2 - A^2) \\
\Rightarrow \quad & l = \frac{2iA \pm \sqrt{-4A^2 - 4(m^2 - A^2)}}{2} = \frac{2iA \pm 2im}{2} = i(A \pm m)
\end{aligned}
$$

which means that

$$
\Phi(\phi) = C_2 e^{i(A\pm m)\phi}. \qquad (2.141)
$$

But

$$
\begin{aligned}
& \Phi(\phi + 2\pi) = \Phi(\phi) \Rightarrow A \pm m = m' \quad m' \in \mathcal{Z} \\
\Rightarrow \quad & m = \pm(m' - A) \quad m' \in \mathcal{Z}. \qquad (2.142)
\end{aligned}
$$

This means that the energy eigenfunctions will be

$$
\psi_{nm\nu}(\vec{x}) = A_c J_m(\frac{\kappa_{m\nu}}{R}\rho)e^{im'\phi}\sin\left(n\frac{\pi z}{a}\right) \qquad (2.143)
$$

but now m is not an integer. As a result the energy of the ground state will be

$$
E = \frac{\hbar^2}{2m}\left[\frac{\kappa_{m\nu}^2}{R^2} + \left(n\frac{\pi}{a}\right)^2\right] \qquad (2.144)
$$

where now $m = m' - A$ is not zero in general but it corresponds to $m' \in \mathcal{Z}$ such that $0 \leq m' - A < 1$. Notice also that if we require the ground state to be unchanged in the presence of B, we obtain *flux quantization*

$$m' - A = 0 \Rightarrow \frac{e}{\hbar c}\frac{\Phi}{2\pi} = m' \Rightarrow \Phi = \frac{2\pi m'\hbar c}{e} \quad m' \in \mathcal{Z}. \tag{2.145}$$

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

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

(a) In the case under construction there is only a continuous spectrum and the eigenfunctions are non degenerate.

From the discussion on WKB approximation we had that for $E > V(x)$

$$\begin{aligned}
\psi_I(x) &= \frac{A}{[E-V(x)]^{1/4}} \exp\left(\frac{i}{\hbar}\int \sqrt{2m[E-V(x)]}dx\right) \\
&\quad + \frac{B}{[E-V(x)]^{1/4}} \exp\left(-\frac{i}{\hbar}\int \sqrt{2m[E-V(x)]}dx\right) \\
&= \frac{c}{[E-V(x)]^{1/4}} \sin\left(\frac{1}{\hbar}\int_x^{x'} \sqrt{2m[E-V(x)]}dx - \frac{\pi}{4}\right) \\
&= \frac{c}{[E-V(x)]^{1/4}} \sin\left(\frac{\sqrt{2m\lambda}}{\hbar}\int_x^{x'=E/\lambda} \left(\frac{E}{\lambda} - x\right)^{1/2} dx - \frac{\pi}{4}\right) \\
&= \frac{c}{[E-V(x)]^{1/4}} \sin\left[-\frac{2}{3}\left(\frac{E}{\lambda} - x\right)^{3/2}\sqrt{\frac{2m\lambda}{\hbar}} - \frac{\pi}{4}\right] \\
&= \frac{c_1}{[q]^{1/4}} \sin\left[\frac{2}{3}q^{3/2} + \frac{\pi}{4}\right]
\end{aligned} \tag{2.146}$$

where $q = \alpha\left[\frac{E}{\lambda} - x\right]$ and $\alpha = \left(\frac{2m\lambda}{\hbar^2}\right)^{1/3}$.

On the other hand when $E < V(x)$

$$\begin{aligned}
\psi_{II}(x) &= \frac{c_2}{[\lambda x - E]^{1/4}} \exp\left(-\frac{1}{\hbar}\int_{x'=E/\lambda}^{x} \sqrt{2m(\lambda x - E)}dx\right) \\
&= \frac{c_2}{[\lambda x - E]^{1/4}} \exp\left[-\frac{1}{\hbar 2m\lambda}\int_{x'=E/\lambda}^{x} \sqrt{2m(\lambda x - E)}d(2m\lambda x)\right] \\
&= \frac{c_3}{[-q]^{1/4}} \exp\left[-\frac{2}{3}(-q)^{2/3}\right]. \qquad (2.147)
\end{aligned}$$

We can find an exact solution for this problem so we can compare with the approximate solutions we got with the WKB method. We have

$$\begin{aligned}
& H|\alpha\rangle = E|\alpha\rangle \Rightarrow \langle p|H|\alpha\rangle = \langle p|E|\alpha\rangle \\
\Rightarrow\ & \langle p|\frac{p^2}{2m} + \lambda x|\alpha\rangle = E\langle p|\alpha\rangle \\
\Rightarrow\ & \frac{p^2}{2m}\alpha(p) + i\hbar\lambda\frac{d}{dp}\alpha(p) = E\alpha(p) \\
\Rightarrow\ & \frac{d}{dp}\alpha(p) = \frac{-i}{\hbar\lambda}\left(E - \frac{p^2}{2m}\right)\alpha(p) \\
\Rightarrow\ & \frac{d\alpha(p)}{\alpha(p)} = \frac{-i}{\hbar\lambda}\left(E - \frac{p^2}{2m}\right)dp \\
\Rightarrow\ & \ln\alpha(p) = \frac{-i}{\hbar\lambda}\left(Ep - \frac{p^3}{6m}\right) + c_1 \\
\Rightarrow\ & \alpha_E(p) = c\exp\left[\frac{i}{\hbar\lambda}\left(\frac{p^3}{6m} - Ep\right)\right]. \qquad (2.148)
\end{aligned}$$

We also have

$$\begin{aligned}
\delta(E - E') &= \langle E|E'\rangle = \int dp\langle E|p\rangle\langle p|E'\rangle = \int \alpha_E^*(p)\alpha_{E'}(p)dp \\
&\overset{(2.148)}{=} |c|^2 \int dp \exp\left[\frac{i}{\hbar\lambda}(E - E')p\right] |c|^2 2\pi\hbar\lambda\delta(E - E') \Rightarrow \\
c &= \frac{1}{\sqrt{2\pi\hbar\lambda}}. \qquad (2.149)
\end{aligned}$$

So

$$\alpha_E(p) = \frac{1}{\sqrt{2\pi\hbar\lambda}} \exp\left[\frac{i}{\hbar\lambda}\left(\frac{p^3}{6m} - Ep\right)\right]. \qquad (2.150)$$

These are the Hamiltonian eigenstates in momentum space. For the eigenfunctions in coordinate space we have

$$\begin{aligned}\psi(x) &= \int dp\langle x|p\rangle\langle p|E\rangle \overset{(2.150)}{=} \frac{1}{2\pi\hbar\sqrt{\lambda}}\int dp e^{\frac{ipx}{\hbar}} e^{\frac{i}{\hbar\lambda}\left(\frac{p^3}{6m}-Ep\right)} \\ &= \frac{1}{2\pi\hbar\sqrt{\lambda}}\int dp \exp\left[i\frac{p^3}{\hbar\lambda 6m} - \frac{i}{\hbar}\left(\frac{E}{\lambda}-x\right)p\right]. \qquad (2.151)\end{aligned}$$

Using now the substitution

$$u = \frac{p}{(\hbar 2m\lambda)^{1/3}} \Rightarrow \frac{p^3}{\hbar\lambda 6m} = \frac{u^3}{3} \qquad (2.152)$$

we have

$$\begin{aligned}\psi(x) &= \frac{(\hbar 2m\lambda)^{1/3}}{2\pi\hbar\sqrt{\lambda}}\int_{-\infty}^{+\infty} du \exp\left[\frac{iu^3}{3} - \frac{i}{\hbar}\left(\frac{E}{\lambda}-x\right)u(\hbar 2m\lambda)^{1/3}\right] \\ &= \frac{\alpha}{2\pi\sqrt{\lambda}}\int_{-\infty}^{+\infty} du \exp\left[\frac{iu^3}{3} - iuq\right], \qquad (2.153)\end{aligned}$$

where $\alpha = \left(\frac{2m\lambda}{\hbar^2}\right)^{1/3}$ and $q = \alpha\left[\frac{E}{\lambda} - x\right]$. So

$$\psi(x) = \frac{\alpha}{2\pi\sqrt{\lambda}}\int_{-\infty}^{+\infty} du \cos\left(\frac{u^3}{3} - uq\right) = \frac{\alpha}{\pi\sqrt{\lambda}}\int_0^{+\infty} \cos\left(\frac{u^3}{3} - uq\right) du$$

since $\int_{-\infty}^{+\infty} \sin\left(\frac{u^3}{3} - uq\right) du = 0$. In terms of the Airy functions

$$Ai(q) = \frac{1}{\sqrt{\pi}}\int_0^{+\infty} \cos\left(\frac{u^3}{3} - uq\right) du \qquad (2.154)$$

we will have

$$\psi(x) = \frac{\alpha}{\sqrt{\pi\lambda}} Ai(-q). \qquad (2.155)$$

For large $|q|$, leading terms in the asymptotic series are as follows

$$\begin{aligned}Ai(q) &\approx \frac{1}{2\sqrt{\pi}q^{1/4}}\exp\left(-\frac{2}{3}q^{3/2}\right), \quad q > 0 \qquad (2.156) \\ Ai(q) &\approx \frac{1}{\sqrt{\pi}(-q)^{1/4}}\sin\left[\frac{2}{3}(-q)^{3/2} + \frac{\pi}{4}\right], \quad q < 0 \qquad (2.157)\end{aligned}$$

Using these approximations in (2.155) we get

$$\begin{aligned}\psi(q) &\approx \frac{\alpha}{\pi\sqrt{\lambda}}\frac{1}{q^{1/4}}\sin\left[\frac{2}{3}q^{3/2}+\frac{\pi}{4}\right], \quad \text{for } E > V(x)\\ \psi(q) &\approx \frac{\alpha}{2\pi\sqrt{\lambda}}\frac{1}{(-q)^{1/4}}\exp\left[-\frac{2}{3}(-q)^{3/2}\right], \quad \text{for } E < V(x) \qquad (2.158)\end{aligned}$$

as expected from the WKB approximation.

(b) When $V = \lambda|x|$ we have bound states and therefore the energy spectrum is discrete. So in this case the energy eigenstates heve to satisfy the consistency relation

$$\int_{x_2}^{x_1} dx\sqrt{2m[E-\lambda|x|]} = \left(n+\tfrac{1}{2}\right)\pi\hbar, \quad n = 0, 1, 2, \ldots \qquad (2.159)$$

The turning points are $x_1 = -\frac{E}{\lambda}$ and $x_2 = \frac{E}{\lambda}$. So

$$\begin{aligned}\left(n+\tfrac{1}{2}\right)\pi\hbar &= \int_{-E/\lambda}^{E/\lambda} dx\sqrt{2m[E-\lambda|x|]} = 2\int_0^{E/\lambda}\sqrt{2m[E-\lambda x]}dx\\ &= -2\sqrt{2m\lambda}\int_0^{E/\lambda}\left(\frac{E}{\lambda}-x\right)^{1/2}d(-x)\\ &= -2\sqrt{2m\lambda}\frac{2}{3}\left(\frac{E}{\lambda}-x\right)^{3/2}\Bigg|_0^{E/\lambda} = 2\sqrt{2m\lambda}\frac{2}{3}\left(\frac{E}{\lambda}\right)^{3/2} \Rightarrow\\ \left(\frac{E}{\lambda}\right)^{3/2} &= \frac{3\left(n+\frac{1}{2}\right)\pi\hbar}{4\sqrt{2m\lambda}} \Rightarrow \left(\frac{E}{\lambda}\right) = \frac{[3\left(n+\frac{1}{2}\right)\pi\hbar]^{2/3}}{4^{2/3}(2m\lambda)^{1/3}} \Rightarrow\\ E_n &= \left[\frac{3\left(n+\frac{1}{2}\right)\pi\hbar\lambda}{4\sqrt{2m}}\right]^{2/3}. \qquad (2.160)\end{aligned}$$

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.

In the case of Euler angles we have

$$\mathcal{D}^{(1/2)}(\alpha,\beta,\gamma) = \begin{pmatrix} e^{-i(\alpha+\gamma)/2}\cos\frac{\beta}{2} & -e^{-i(\alpha-\gamma)/2}\sin\frac{\beta}{2}\\ e^{i(\alpha-\gamma)/2}\sin\frac{\beta}{2} & e^{i(\alpha+\gamma)/2}\cos\frac{\beta}{2}\end{pmatrix} \tag{3.1}$$

while the same rotation will be represented by

$$\mathcal{D}^{(1/2)}(\phi,\hat{n}) \stackrel{(S-3.2.45)}{=} \begin{pmatrix} \cos\left(\frac{\phi}{2}\right) - in_z\sin\left(\frac{\phi}{2}\right) & (-in_x - n_y)\sin\left(\frac{\phi}{2}\right)\\ (-in_x + n_y)\sin\left(\frac{\phi}{2}\right) & \cos\left(\frac{\phi}{2}\right) + in_z\sin\left(\frac{\phi}{2}\right)\end{pmatrix}. \tag{3.2}$$

Since these two operators must have the same effect, each matrix element should be the same. That is

$$\begin{aligned} & e^{-i(\alpha+\gamma)/2}\cos\frac{\beta}{2} = \cos\left(\frac{\phi}{2}\right) - in_z\sin\left(\frac{\phi}{2}\right)\\ \Rightarrow\quad & \cos\left(\frac{\phi}{2}\right) = \cos\frac{(\alpha+\gamma)}{2}\cos\frac{\beta}{2}\\ \Rightarrow\quad & \cos\phi = 2\cos^2\frac{\beta}{2}\cos^2\frac{(\alpha+\gamma)}{2} - 1\\ \Rightarrow\quad & \phi = \arccos\left[2\cos^2\frac{\beta}{2}\cos^2\frac{(\alpha+\gamma)}{2} - 1\right]. \end{aligned} \tag{3.3}$$

3.2 An angular-momentum eigenstate $|j, m = m_{\mathbf{max}} = j\rangle$ 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.

The rotated state is given by

$$
\begin{aligned}
|j,j\rangle_R &= R(\varepsilon,\hat{y})|j,j\rangle = d^{(j)}(\varepsilon)|j,j\rangle = \left[\exp\left(-\frac{iJ_y\varepsilon}{\hbar}\right)\right]|j,j\rangle \\
&= \left[1-\frac{iJ_y\varepsilon}{\hbar}+\frac{(-i)^2\varepsilon^2}{2\hbar^2}J_y^2\right]|j,j\rangle \qquad (3.4)
\end{aligned}
$$

up to terms of order ε^2. We can write J_y in terms of the ladder operators

$$
\left.\begin{array}{l} J_+ = J_x + iJ_y \\ J_- = J_x - iJ_y \end{array}\right\} \Rightarrow J_y = \frac{J_+ - J_-}{2i}. \qquad (3.5)
$$

Subtitution of this in (3.4), gives

$$
|j,j\rangle_R = \left[1-\frac{\varepsilon}{2\hbar}(J_+-J_-)+\frac{\varepsilon^2}{8\hbar^2}(J_+-J_-)^2\right]|j,j\rangle \qquad (3.6)
$$

We know that for the ladder operators the following relations hold

$$
\begin{aligned}
J_+|j,m\rangle &= \hbar\sqrt{(j-m)(j+m+1)}|j,m+1\rangle \qquad (3.7)\\
J_-|j,m\rangle &= \hbar\sqrt{(j+m)(j-m+1)}|j,m-1\rangle \qquad (3.8)
\end{aligned}
$$

So

$$
\begin{aligned}
(J_+-J_-)|j,j\rangle &= -J_-|j,j\rangle = -\hbar\sqrt{2j}|j,j-1\rangle \qquad (3.9)\\
(J_+-J_-)^2|j,j\rangle &= -\hbar\sqrt{2j}(J_+-J_-)|j,j-1\rangle \\
&= -\hbar\sqrt{2j}\left(J_+|j,j-1\rangle - J_-|j,j-1\rangle\right) \\
&= -\hbar\sqrt{2j}\left[\sqrt{2j}|j,j\rangle - \sqrt{2(2j-1)}|j,j-2\rangle\right]
\end{aligned}
$$

and from (3.6)

$$
\begin{aligned}
|j,j\rangle_R &= |j,j\rangle + \frac{\varepsilon}{2}\sqrt{2j}|j,j-1\rangle - \frac{\varepsilon^2}{8}2j|j,j\rangle + \frac{\varepsilon^2}{8}2\sqrt{j(2j-1)}|j,j-2\rangle \\
&= \left(1-\frac{\varepsilon^2}{4}j\right)|j,j\rangle + \frac{\varepsilon}{2}\sqrt{2j}|j,j-1\rangle + \frac{\varepsilon^2}{4}\sqrt{j(2j-1)}|j,j-2\rangle.
\end{aligned}
$$

Thus the probability for the rotated state to be found in the original state will be

$$|\langle j,j|j,j\rangle_R|^2 = \left|\left(1-\frac{\varepsilon^2}{4}j\right)\right|^2 = 1-\frac{\varepsilon^2}{2}j+O(\varepsilon^4). \tag{3.10}$$

3.3 The wave function of a particle 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 $V(r)$.

(a) We have

$$\psi(\vec{x}) \equiv \langle\vec{x}|\psi\rangle = (x+y+3z)f(r). \tag{3.11}$$

So

$$\langle\vec{x}|\vec{L}^2|\psi\rangle \stackrel{(S-3.6.15)}{=} -\hbar^2\left[\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}+\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)\right]\psi(\vec{x}). \tag{3.12}$$

If we write $\psi(\vec{x})$ in terms of spherical coordinates ($x = r\sin\theta\cos\phi, y = r\sin\theta\sin\phi, z = r\cos\theta$) we will have

$$\psi(\vec{x}) = rf(r)\left(\sin\theta\cos\phi+\sin\theta\sin\phi+3\cos\theta\right). \tag{3.13}$$

Then

$$\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\psi(\vec{x}) = \frac{rf(r)\sin\theta}{\sin^2\theta}\frac{\partial}{\partial\phi}(\cos\phi-\sin\phi) = -\frac{rf(r)}{\sin\theta}(\cos\phi+\sin\phi) \tag{3.14}$$

and

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)\psi(\vec{x}) = \frac{rf(r)}{\sin\theta}\frac{\partial}{\partial\theta}\left[-3\sin^2\theta + (\cos\phi+\sin\phi)\sin\theta\cos\theta\right] =$$
$$\frac{rf(r)}{\sin\theta}\left[-6\sin\theta\cos\theta + (\cos\phi+\sin\phi)(\cos^2\theta-\sin^2\theta)\right] \quad (3.15)$$

Substitution of (3.14) and (3.15) in (3.11) gives

$$\begin{aligned}
\langle\vec{x}|\vec{L}^2|\psi\rangle &= -\hbar^2 rf(r)\left[-\frac{1}{\sin\theta}(\cos\phi+\sin\phi)(1-\cos^2\theta+\sin^2\theta) - 6\cos\theta\right] \\
&= \hbar^2 rf(r)\left[\frac{1}{\sin\theta}2\sin^2\theta(\cos\phi+\sin\phi) + 6\cos\theta\right] \\
&= 2\hbar^2 rf(r)\left[\sin\theta\cos\phi + \sin\theta\sin\phi + 3\cos\theta\right] = 2\hbar^2\psi(\vec{x}) \Rightarrow \\
L^2\psi(\vec{x}) &= 2\hbar^2\psi(\vec{x}) = 1(1+1)\hbar^2\psi(\vec{x}) = l(l+l)\hbar^2\psi(\vec{x}) \qquad (3.16)
\end{aligned}$$

which means that $\psi(\vec{x})$ is en eigenfunction of $\vec{L}^2$ with eigenvalue $l = 1$.

(b) Since we already know that $l = 1$ we can try to write $\psi(\vec{x})$ in terms of the spherical harmonics $Y_1^m(\theta,\phi)$. We know that

$$Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta = \sqrt{\frac{3}{4\pi}}\frac{z}{r} \Rightarrow z = r\sqrt{\frac{4\pi}{3}}Y_1^0$$
$$\left.\begin{array}{lcl} Y_1^{+1} &=& -\sqrt{\frac{3}{8\pi}}\frac{(x+iy)}{r} \\ Y_1^{-1} &=& \sqrt{\frac{3}{8\pi}}\frac{(x-iy)}{r} \end{array}\right\} \Rightarrow \left\{\begin{array}{lcl} x &=& r\sqrt{\frac{2\pi}{3}}\left(Y_1^{-1} - Y_1^{+1}\right) \\ y &=& ir\sqrt{\frac{2\pi}{3}}\left(Y_1^{-1} + Y_1^{+1}\right) \end{array}\right.$$

So we can write

$$\begin{aligned}
\psi(\vec{x}) &= r\sqrt{\frac{2\pi}{3}}f(r)\left[3\sqrt{2}Y_1^0 + Y_1^{-1} - Y_1^{+1} + iY_1^{+1} + iY_1^{-1}\right] \\
&= \sqrt{\frac{2\pi}{3}}rf(r)\left[3\sqrt{2}Y_1^0 + (1+i)Y_1^{-1} + (i-1)Y_1^{+1}\right]. \qquad (3.17)
\end{aligned}$$

But this means that the part of the state that depends on the values of m can be written in the following way

$$|\psi\rangle_m = N\left[3\sqrt{2}|l=1,m=0\rangle + (1+i)|l=1,m=-1\rangle + (1-i)|l=1,m=1\rangle\right]$$

and if we want it normalized we will have

$$|N|^2(18+2+2) = 1 \Rightarrow N = \frac{1}{\sqrt{22}}. \qquad (3.18)$$

So

$$P(m=0) = |\langle l=1, m=0|\psi\rangle|^2 = \frac{9\cdot 2}{22} = \frac{9}{11}, \quad (3.19)$$

$$P(m=+1) = |\langle l=1, m=+1|\psi\rangle|^2 = \frac{2}{22} = \frac{1}{11}, \quad (3.20)$$

$$P(m=-1) = |\langle l=1, m==1|\psi\rangle|^2 = \frac{2}{22} = \frac{1}{11}. \quad (3.21)$$

(c) If $\psi_E(\vec{x})$ is an energy eigenfunction then it solves the Schrödinger equation

$$\frac{-\hbar^2}{2m}\left[\frac{\partial^2}{\partial r^2}\psi_E(\vec{x}) + \frac{2}{r}\frac{\partial}{\partial r}\psi_E(\vec{x}) - \frac{L^2}{\hbar^2 r^2}\psi_E(\vec{x})\right] + V(r)\psi_E(\vec{x}) = E\psi_E(\vec{x})$$

$$\Rightarrow \frac{-\hbar^2}{2m}Y_l^m\left[\frac{d^2}{dr^2}[rf(r)] + \frac{2}{r}\frac{d}{dr}[rf(r)] - \frac{2}{r^2}[rf(r)]\right] + V(r)rf(r)Y_l^m = Erf(r)Y_l^m \Rightarrow$$

$$V(r) = E + \frac{1}{rf(r)}\frac{\hbar^2}{2m}\left[\frac{d}{dr}[f(r)+rf'(r)] + \frac{2}{r}[f(r)+rf'(r)] - \frac{2}{r}f(r)\right] \Rightarrow$$

$$V(r) = E + \frac{1}{rf(r)}\frac{\hbar^2}{2m}\left[f'(r)+f'(r)+rf''(r)+2f'(r)\right] \Rightarrow$$

$$V(r) = E + \frac{\hbar^2}{2m}\frac{rf''(r)+4f'(r)}{rf(r)}. \quad (3.22)$$

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

$$u_{\vec{\varepsilon}} = 1 - i\frac{\vec{\varepsilon}}{\hbar}\cdot(\vec{L}+\vec{S}) \quad (3.23)$$

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.

(a) We have

$$|\varrho\rangle = \sum_{i=1}^{3} \int |\vec{x}; i\rangle\langle\vec{x}; i|\varrho\rangle = \sum_{i=1}^{3} \int |\vec{x}; i\rangle \varrho^i(\vec{x}) d^3x. \tag{3.24}$$

Under a rotation R we will have

$$\begin{aligned}
|\varrho'\rangle &= U(R)|\varrho\rangle = \sum_{i=1}^{3} \int U(R) \left[|\vec{x}\rangle \otimes |i\rangle\right] \varrho^i(\vec{x}) d^3x \\
&= \sum_{i=1}^{3} \int |R\vec{x}\rangle \otimes |i\rangle \mathcal{D}^{(1)}_{il}(R)\varrho^l(\vec{x})d^3x \overset{\det R=1}{=} \sum_{i=1}^{3} \int |\vec{x}; i\rangle \mathcal{D}^{(1)}_{il}(R)\varrho^l(R^{-1}\vec{x})d^3x \\
&= \sum_{i=1}^{3} \int |\vec{x}; i\rangle \varrho^{i\prime}\vec{x})d^3x \Rightarrow \\
\varrho^{i\prime}(\vec{x}) &= \mathcal{D}^{(1)}_{il}(R)\varrho^l(R^{-1}\vec{x}) \Rightarrow \vec{\varrho}'(\vec{x}) = R\vec{\varrho}(R^{-1}\vec{x}).
\end{aligned} \tag{3.25}$$

Under an infinitesimal rotation we will have

$$R(\delta\phi, \hat{n})\vec{r} = \vec{r} + \delta\vec{r} = \vec{r} + \delta\phi(\hat{n} \times \vec{r}) = \vec{r} + \vec{\varepsilon} \times \vec{r}. \tag{3.26}$$

So

$$\begin{aligned}
\vec{\varrho}'(\vec{x}) &= R(\delta\phi)\vec{\varrho}(R^{-1}\vec{x}) = R(\delta\phi)\vec{\varrho}(\vec{x} - \vec{\varepsilon} \times \vec{x}) \\
&= \vec{\varrho}(\vec{x} - \vec{\varepsilon} \times \vec{x}) + \vec{\varepsilon} \times \vec{\varrho}(\vec{x} - \vec{\varepsilon} \times \vec{x}).
\end{aligned} \tag{3.27}$$

On the other hand

$$\begin{aligned}
\vec{\varrho}(\vec{x} - \vec{\varepsilon} \times \vec{x}) &= \vec{\varrho}(\vec{x}) - (\vec{\varepsilon} \times \vec{x}) \cdot \vec{\nabla}\vec{\varrho}(\vec{x}) = \vec{\varrho}(\vec{x}) - \vec{\varepsilon} \cdot (\vec{x} \times \vec{\nabla})\vec{\varrho}(\vec{x}) \\
&= \vec{\varrho}(\vec{x}) - \frac{i}{\hbar}\vec{\varepsilon} \cdot \vec{L}\vec{\varrho}(\vec{x})
\end{aligned} \tag{3.28}$$

where $\vec{\nabla}\vec{\varrho}(\vec{x}) \equiv \left[\vec{\nabla}\varrho_i(\vec{x})\right]|i\rangle$. Using this in (3.27) we get

$$\begin{aligned}\vec{\varrho}'(\vec{x}) &= \vec{\varrho}(\vec{x}) - \frac{i}{\hbar}\vec{\varepsilon}\cdot\vec{L}\vec{\varrho}(\vec{x}) + \vec{\varepsilon}\times\left[\vec{\varrho}(\vec{x}) - \frac{i}{\hbar}\vec{\varepsilon}\cdot\vec{L}\vec{\varrho}(\vec{x})\right] \\ &= \vec{\varrho}(\vec{x}) - \frac{i}{\hbar}\vec{\varepsilon}\cdot\vec{L}\vec{\varrho}(\vec{x}) + \vec{\varepsilon}\times\vec{\varrho}(\vec{x}). \end{aligned} \tag{3.29}$$

But

$$\vec{\varepsilon}\times\vec{\varrho} = \left(\varepsilon_y\varrho^3 - \varepsilon_z\varrho^2\right)\hat{e}_x + \left(\varepsilon_z\varrho^1 - \varepsilon_x\varrho^1\right)\hat{e}_y + \left(\varepsilon_x\varrho^2 - \varepsilon_y\varrho^1\right)\hat{e}_z \tag{3.30}$$

or in matrix form

$$\begin{pmatrix}\varrho^{1\prime}\\ \varrho^{2\prime}\\ \varrho^{3\prime}\end{pmatrix} = \begin{pmatrix}0 & -\varepsilon_z & \varepsilon_y\\ \varepsilon_z & 0 & -\varepsilon_x\\ -\varepsilon_y & \varepsilon_x & 0\end{pmatrix}\begin{pmatrix}\varrho^1\\ \varrho^2\\ \varrho^3\end{pmatrix} =$$

$$\left[\varepsilon_x\begin{pmatrix}0&0&0\\0&0&-1\\0&1&0\end{pmatrix} + \varepsilon_y\begin{pmatrix}0&0&1\\0&0&0\\-1&0&0\end{pmatrix} + \varepsilon_z\begin{pmatrix}0&-1&0\\1&0&0\\0&0&0\end{pmatrix}\right]\begin{pmatrix}\varrho^1\\ \varrho^2\\ \varrho^3\end{pmatrix} =$$

$$-\frac{i}{\hbar}\left[\varepsilon_x\begin{pmatrix}0&0&0\\0&0&-i\hbar\\0&i\hbar&0\end{pmatrix} + \varepsilon_y\begin{pmatrix}0&0&i\hbar\\0&0&0\\-i\hbar&0&0\end{pmatrix} + \varepsilon_z\begin{pmatrix}0&-i\hbar&0\\i\hbar&0&0\\0&0&0\end{pmatrix}\right]\begin{pmatrix}\varrho^1\\ \varrho^2\\ \varrho^3\end{pmatrix}$$

which means that

$$\vec{\varepsilon}\times\vec{\varrho} = -\frac{i}{\hbar}\vec{\varepsilon}\cdot\vec{\mathcal{S}}\vec{\varrho}(\vec{x})$$

with $(\mathcal{S}_\mu)_{kl} = -i\hbar\epsilon_{\mu kl}$.

Thus we will have that

$$\vec{\varrho}'(\vec{x}) = U_{\vec{\varepsilon}}\vec{\varrho}(\vec{x}) = \left[1 - \frac{i}{\hbar}\vec{\varepsilon}\cdot(\vec{L}+\vec{\mathcal{S}})\right]\vec{\varrho}(\vec{x}) \Rightarrow U_{\vec{\varepsilon}} = 1 - \frac{i}{\hbar}\vec{\varepsilon}\cdot(\vec{L}+\vec{\mathcal{S}}). \tag{3.31}$$

(b) From their definition it is obvious that $\vec{L}$ and $\vec{\mathcal{S}}$ commute since $\vec{L}$ acts only on the $|\vec{x}\rangle$ basis and $\vec{\mathcal{S}}$ only on $|i\rangle$.

(c) $\vec{\mathcal{S}}$ is a vector operator since

$$\begin{aligned}[S_i, S_j]_{km} &= [S_iS_j - S_jS_i]_{km} = \sum\left[(-i\hbar)\epsilon_{ikl}(-i\hbar)\epsilon_{jlm} - (-i\hbar)\epsilon_{jkl}(-i\hbar)\epsilon_{ilm}\right] \\ &= \sum\left[\hbar^2\epsilon_{ikl}\epsilon_{jml} - \hbar^2\epsilon_{jkl}\epsilon_{iml}\right] \\ &= \hbar^2\sum\left(\delta_{ij}\delta_{km} - \delta_{im}\delta_{jk} - \delta_{ij}\delta_{km} + \delta_{jm}\delta_{ki}\right) \\ &= \hbar^2\sum\left(\delta_{jm}\delta_{ki} - \delta_{im}\delta_{jk}\right) \\ &= \hbar^2\sum\epsilon_{ijl}\epsilon_{kml} = \sum i\hbar\epsilon_{ijl}(-i\hbar\epsilon_{kml}) = \sum i\hbar\epsilon_{ijl}(S_l)_{km}. \end{aligned} \tag{3.32}$$

(d) It is

$$\begin{aligned}\vec{\nabla}\times\vec{\varrho}(\vec{x}) &= \frac{i}{\hbar}\vec{p}\times\vec{\varrho}(\vec{x}) = \frac{i}{\hbar}\epsilon_{i\mu l}p_\mu \varrho^l(\vec{x})|i\rangle = \frac{1}{\hbar^2}(S_\mu)^l_m p_\mu \varrho^m|i\rangle \\ &= \frac{1}{\hbar^2}(\vec{S}\cdot\vec{p})\vec{\varrho}. \end{aligned} \tag{3.33}$$

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

$$|j = 1, m = 1\rangle = \frac{1}{\sqrt{2}}|+,0\rangle - \frac{1}{\sqrt{2}}|0,+\rangle, \ldots, \tag{3.34}$$

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

We want to add the angular momenta $j_1 = 1$ and $j_2 = 1$ to form $j = |j_1 - j_2|, \ldots, j_1 + j_2 = 0, 1, 2$ states. Let us take first the state $j = 2$, $m = 2$. This state is related to $|j_1 m_1; j_2 m_2\rangle$ through the following equation

$$|j, m\rangle = \sum_{m=m_1+m_2} \langle j_1 j_2; m_1 m_2 | j_1 j_2; jm\rangle |j_1 j_2; m_1 m_2\rangle \tag{3.35}$$

So setting $j = 2$, $m = 2$ in (3.35) we get

$$|j = 2, m = 2\rangle \;=\; \langle j_1 j_2; ++|j_1 j_2; jm\rangle|++\rangle \overset{\text{norm.}}{=} |++\rangle \tag{3.36}$$

If we apply the J_- operator on this statet we will get

$$\begin{aligned} & J_-|j=2, m=2\rangle = (J_{1-} + J_{2-})|++\rangle \\ \Rightarrow\;& \hbar\sqrt{(j+m)(j-m+1)}|j=2, m=1\rangle = \\ & \hbar\sqrt{(j_1+m_1)(j_1-m_1+1)}|0+\rangle + \hbar\sqrt{(j_2+m_2)(j_2-m_2+1)}|+0\rangle \\ \Rightarrow\;& \sqrt{4}|j=2, m=1\rangle = \sqrt{2}|0+\rangle + \sqrt{2}|+0\rangle \\ \Rightarrow\;& |j=2, m=1\rangle = \frac{1}{\sqrt{2}}|0+\rangle + \frac{1}{\sqrt{2}}|+0\rangle. \end{aligned} \tag{3.37}$$

In the same way we have

$$\begin{aligned} J_-|j=2,m=1\rangle &= \frac{1}{\sqrt{2}}(J_{1-}+J_{2-})|0+\rangle + \frac{1}{\sqrt{2}}(J_{1-}+J_{2-})|+0\rangle \Rightarrow \\ \sqrt{6}|j=2,m=0\rangle &= \frac{1}{\sqrt{2}}\left[\sqrt{2}|-+\rangle + \sqrt{2}|00\rangle\right] + \frac{1}{\sqrt{2}}\left[\sqrt{2}|00\rangle + \sqrt{2}|+-\rangle\right] \Rightarrow \\ \sqrt{6}|j=2,m=0\rangle &= 2|00\rangle + |-+\rangle + |+-\rangle \Rightarrow \\ |j=2,m=0\rangle &= \sqrt{\frac{2}{3}}|00\rangle + \frac{1}{\sqrt{6}}|+-\rangle + \frac{1}{\sqrt{6}}|-+\rangle \qquad (3.38) \end{aligned}$$

$$\begin{aligned} J_-|j=2,m=0\rangle &= \sqrt{\frac{2}{3}}(J_{1-}+J_{2-})|00\rangle \\ &\quad + \frac{1}{\sqrt{6}}(J_{1-}+J_{2-})|+-\rangle + \frac{1}{\sqrt{6}}(J_{1-}+J_{2-})|-+\rangle \Rightarrow \\ \sqrt{6}|j=2,m=-1\rangle &= \sqrt{\frac{2}{3}}\left[\sqrt{2}|-0\rangle + \sqrt{2}|0-\rangle\right] + \frac{1}{\sqrt{6}}\sqrt{2}|0-\rangle + \frac{1}{\sqrt{6}}\sqrt{2}|-0\rangle \Rightarrow \\ |j=2,m=-1\rangle &= \frac{2}{6}\sqrt{2}|0-\rangle + \frac{2}{6}\sqrt{2}|-0\rangle + \frac{1}{6}\sqrt{2}|0-\rangle + \frac{1}{6}\sqrt{2}|-0\rangle \Rightarrow \\ |j=2,m=-1\rangle &= \frac{1}{\sqrt{2}}|0-\rangle + \frac{1}{\sqrt{2}}|-0\rangle \qquad (3.39) \end{aligned}$$

$$\begin{aligned} J_-|j=2,m=-1\rangle &= \frac{1}{\sqrt{2}}(J_{1-}+J_{2-})|0-\rangle + \frac{1}{\sqrt{2}}(J_{1-}+J_{2-})|-0\rangle \Rightarrow \\ \sqrt{4}|j=2,m=-2\rangle &= \frac{1}{\sqrt{2}}\sqrt{2}|--\rangle + \frac{1}{\sqrt{2}}\sqrt{2}|--\rangle \Rightarrow \\ |j=2,m=-2\rangle &= |--\rangle. \qquad (3.40) \end{aligned}$$

Now let us return to equation (3.35). If $j=1$, $m=1$ we will have

$$|j=1,m=1\rangle = a|+0\rangle + b|0+\rangle \qquad (3.41)$$

This state should be orthogonal to all $|j,m\rangle$ states and in particular to $|j=2,m=1\rangle$. So

$$\begin{aligned} \langle j=2,m=1|j=1,m=1\rangle = 0 \Rightarrow \tfrac{1}{\sqrt{2}}a + \tfrac{1}{\sqrt{2}}b = 0 \Rightarrow \\ a+b=0 \Rightarrow a=-b \qquad . \qquad (3.42) \end{aligned}$$

In addition the state $|j=1,m=1\rangle$ should be normalized so

$$\langle j=1,m=1|j=1,m=1\rangle = 1 \Rightarrow |a|^2+|b|^2 = 1 \stackrel{(3.42)}{\Rightarrow} 2|a|^2 = 1 \Rightarrow |a| = \frac{1}{\sqrt{2}}.$$

By convention we take a to be real and positive so $a=\frac{1}{\sqrt{2}}$ and $b=-\frac{1}{\sqrt{2}}$. That is

$$|j=1,m=1\rangle = \frac{1}{\sqrt{2}}|+0\rangle - \frac{1}{\sqrt{2}}|0+\rangle. \quad (3.43)$$

Using the same procedure we used before

$$\begin{aligned}
J_-|j=1,m=1\rangle &= \frac{1}{\sqrt{2}}(J_{1-}+J_{2-})|+0\rangle - \frac{1}{\sqrt{2}}(J_{1-}+J_{2-})|0+\rangle \Rightarrow \\
\sqrt{2}|j=1,m=0\rangle &= \frac{1}{\sqrt{2}}\left[\sqrt{2}|00\rangle + \sqrt{2}|+-\rangle\right] - \frac{1}{\sqrt{2}}\left[\sqrt{2}|-+\rangle + \sqrt{2}|00\rangle\right] \Rightarrow \\
|j=1,m=0\rangle &= \frac{1}{\sqrt{2}}|+-\rangle - \frac{1}{\sqrt{2}}|-+\rangle \quad (3.44)
\end{aligned}$$

$$\begin{aligned}
J_-|j=1,m=0\rangle &= \frac{1}{\sqrt{2}}(J_{1-}+J_{2-})|+-\rangle - \frac{1}{\sqrt{2}}(J_{1-}+J_{2-})|-+\rangle \Rightarrow \\
\sqrt{2}|j=1,m=-1\rangle &= \frac{1}{\sqrt{2}}\sqrt{2}|0-\rangle - \frac{1}{\sqrt{2}}\sqrt{2}|-0\rangle \Rightarrow \\
|j=1,m=-1\rangle &= \frac{1}{\sqrt{2}}|0-\rangle - \frac{1}{\sqrt{2}}|-0\rangle. \quad (3.45)
\end{aligned}$$

Returning back to (3.35) we see that the state $|j=0,m=0\rangle$ can be written as

$$|j=0,m=0\rangle = c_1|00\rangle + c_2|+-\rangle + c_3|-+\rangle. \quad (3.46)$$

This state should be orthogonal to all states $|j,m\rangle$ and in particulat to $|j=2,m=0\rangle$ and to $j=1,m=0\rangle$. So

$$\begin{aligned}
&\langle j=2,m=0|j=0,m=0\rangle = 0 \Rightarrow \sqrt{\frac{2}{3}}c_1 + \frac{1}{\sqrt{6}}c_2 + \frac{1}{\sqrt{6}}c_3 \\
\Rightarrow\ & 2c_1 + c_2 + c_3 = 0 \quad (3.47) \\
&\langle j=1,m=0|j=0,m=0\rangle = 0 \Rightarrow \frac{1}{\sqrt{2}}c_2 - \frac{1}{\sqrt{2}}c_3 \\
\Rightarrow\ & c_2 = c_3. \quad (3.48)
\end{aligned}$$

Using the last relation in (3.47), we get

$$2c_1 + 2c_2 = 0 \Rightarrow c_1 + c_2 = 0 \Rightarrow c_1 = -c_2. \tag{3.49}$$

The state $|j = 0, m = 0\rangle$ should be normalized so

$$\langle j = 0, m = 0|j = 0, m = 0\rangle = 1 \Rightarrow |c_1|^2 + |c_2|^2 + |c_3|^2 = 1 \Rightarrow 3|c_2|^2 = 1$$
$$\Rightarrow \quad |c_2| = \frac{1}{\sqrt{3}}. \tag{3.50}$$

By convention we take c_2 to be real and positive so $c_2 = c_3 = \frac{1}{\sqrt{3}}$ and $c_1 = -\frac{1}{\sqrt{3}}$. Thus

$$|j = 0, m = 0\rangle = \frac{1}{\sqrt{3}}|+-\rangle + \frac{1}{\sqrt{3}}|-+\rangle - \frac{1}{\sqrt{3}}|00\rangle. \tag{3.51}$$

So gathering all the previous results together

$$\begin{array}{lcl}
|j = 2, m = 2\rangle & = & |++\rangle \\
|j = 2, m = 1\rangle & = & \frac{1}{\sqrt{2}}|0+\rangle + \frac{1}{\sqrt{2}}|+0\rangle \\
|j = 2, m = 0\rangle & = & \sqrt{\frac{2}{3}}|00\rangle + \frac{1}{\sqrt{6}}|+-\rangle + \frac{1}{\sqrt{6}}|-+\rangle \\
|j = 2, m = -1\rangle & = & \frac{1}{\sqrt{2}}|0-\rangle + \frac{1}{\sqrt{2}}|-0\rangle \\
|j = 2, m = -2\rangle & = & |--\rangle \\
|j = 1, m = 1\rangle & = & \frac{1}{\sqrt{2}}|+0\rangle - \frac{1}{\sqrt{2}}|0+\rangle \\
|j = 1, m = 0\rangle & = & \frac{1}{\sqrt{2}}|+-\rangle - \frac{1}{\sqrt{2}}|-+\rangle \\
|j = 1, m = -1\rangle & = & \frac{1}{\sqrt{2}}|0-\rangle - \frac{1}{\sqrt{2}}|-0\rangle \\
|j = 0, m = 0\rangle & = & \frac{1}{\sqrt{3}}|+-\rangle + \frac{1}{\sqrt{3}}|-+\rangle - \frac{1}{\sqrt{3}}|00\rangle.
\end{array} \tag{3.52}$$

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 $V_{x,y,z}$.

(a) Since $\vec{U}$ and $\vec{V}$ are vector operators they will satisfy the following commutation relations

$$[U_i, J_j] = i\hbar\varepsilon_{ijk}U_k \quad [V_i, J_j] = i\hbar\varepsilon_{ijk}V_k. \tag{3.53}$$

From the components of a vector operator we can construct a spherical tensor of rank 1 in the following way. The defining properties of a spherical tensor of rank 1 are the following

$$[J_z, U_q^{(1)}] = \hbar q U_q^{(1)}, \qquad [J_\pm, U_q^{(1)}] = \hbar\sqrt{(1 \mp q)(2 \pm q)}U_{q\pm 1}^{(1)}. \tag{3.54}$$

It is

$$\begin{aligned}
[J_z, U_z] &\stackrel{(3.53)}{=} 0\hbar U_z \stackrel{(3.54)}{\Rightarrow} \\
& U_z = U_0 && (3.55)\\
[J_+, U_0] &\stackrel{(3.54)}{=} \sqrt{2}\hbar U_{+1} = [J_+, U_z] = [J_x + iJ_y, U_z] \\
&\stackrel{(3.53)}{=} -i\hbar U_y + i(i\hbar)U_x = -\hbar(U_x + iU_y) \Rightarrow \\
& U_{+1} = -\frac{1}{\sqrt{2}}(U_x + iU_y) && (3.56)\\
[J_-, U_0] &\stackrel{(3.54)}{=} \sqrt{2}\hbar U_{-1} = [J_-, U_z] = [J_x - iJ_y, U_z] \\
&\stackrel{(3.53)}{=} -i\hbar U_y - i(i\hbar)U_x = \hbar(U_x - iU_y) \Rightarrow \\
& U_{-1} = \frac{1}{\sqrt{2}}(U_x - iU_y) && (3.57)
\end{aligned}$$

So from the vector operators $\vec{U}$ and $\vec{V}$ we can construct spherical tensors with components

$$\begin{array}{lll} U_0 = U_z & & V_0 = V_z \\ U_{+1} = -\frac{1}{\sqrt{2}}(U_x + iU_y) & & V_{+1} = -\frac{1}{\sqrt{2}}(V_x + IV_y) \\ U_{-1} = \frac{1}{\sqrt{2}}(U_x - iU_y) & & V_{-1} = \frac{1}{\sqrt{2}}(V_x - iV_y) \end{array} \tag{3.58}$$

It is known (S-3.10.27) that if $X_{q_1}^{(k_1)}$ and $Z_{q_2}^{(k_2)}$ are irreducible spherical tensors of rank k_1 and k_2 respectively then we can construct a spherical tensor of rank k

$$T_q^{(k)} = \sum_{q_1 q_2} \langle k_1 k_2; q_1 q_2 | k_1 k_2; kq\rangle X_{q_1}^{(k_1)} Z_{q_2}^{(k_2)} \tag{3.59}$$

In this case we have

$$\begin{aligned}
T^{(1)}_{+1} &= \langle 11;+10|11;11\rangle U_{+1}V_0 + \langle 11;0+1|11;11\rangle U_0V_{+1} \\
&\overset{(3.52)}{=} \frac{1}{\sqrt{2}}U_{+1}V_0 - \frac{1}{\sqrt{2}}U_0V_{+1} \\
&= -\tfrac{1}{2}(U_x+iU_y)V_z + \tfrac{1}{2}U_z(V_x+iV_y) \qquad (3.60)
\end{aligned}$$

$$\begin{aligned}
T^{(1)}_{0} &= \langle 11;00|11;10\rangle U_0V_0 + \langle 11;-1+1|11;10\rangle U_{-1}V_{+1} \\
&\quad +\langle 11;+1-1|11;10\rangle U_{+1}V_{-1} \\
&\overset{(3.52)}{=} -\frac{1}{\sqrt{2}}U_{-1}V_{+1} + \frac{1}{\sqrt{2}}U_{+1}V_{-1} \\
&= \frac{1}{\sqrt{2}}\tfrac{1}{2}(U_x-iU_y)(V_x+iV_y) - \frac{1}{\sqrt{2}}\tfrac{1}{2}(U_x+iU_y)(V_x-iV_y) \\
&= \frac{1}{2\sqrt{2}}\left[U_xV_x+iU_xV_y-iU_yV_x+U_yV_y-U_xV_x+iU_xV_y-iU_yV_x-U_yV_y\right] \\
&= \frac{i}{\sqrt{2}}(U_xV_y-U_yV_x) \qquad (3.61)
\end{aligned}$$

$$\begin{aligned}
T^{(1)}_{-1} &= \langle 11;-10|11;11\rangle U_{-1}V_0 + \langle 11;0-1|11;11\rangle U_0V_{-1} \\
&\overset{(3.52)}{=} -\frac{1}{\sqrt{2}}U_{-1}V_0 + \frac{1}{\sqrt{2}}U_0V_{-1} \\
&= -\tfrac{1}{2}(U_x-iU_y)V_z + \tfrac{1}{2}U_z(V_x-iV_y). \qquad (3.62)
\end{aligned}$$

(b) In the same manner we will have

$$\begin{aligned}
T^{(2)}_{+2} &= \langle 11;+1+1|11;2+2\rangle U_{+1}V_{+1} \overset{(3.52)}{=} U_{+1}V_{+1} = \tfrac{1}{2}(U_x+iU_y)(V_x+iV_y) \\
&= -\tfrac{1}{2}(U_xV_x-U_yV_y+iU_xV_y+iU_yV_x) \qquad (3.63)
\end{aligned}$$

$$\begin{aligned}
T^{(2)}_{+1} &= \langle 11;0+1|11;2+1\rangle U_0V_{+1} + \langle 11;+10|11;2+1\rangle U_{+1}V_0 \\
&\overset{(3.52)}{=} \frac{1}{\sqrt{2}}U_0V_{+1} + \frac{1}{\sqrt{2}}U_{+1}V_0 \\
&= -\tfrac{1}{2}(U_zV_x+U_xV_z+iU_zV_y+iU_yV_z) \qquad (3.64)
\end{aligned}$$

$$\begin{aligned}
T^{(2)}_{0} &= \langle 11;00|11;20\rangle U_0V_0 + \langle 11;-1+1|11;20\rangle U_{-1}V_{+1} \\
&\quad +\langle 11;+1-1|11;20\rangle U_{+1}V_{-1}
\end{aligned}$$

$$
\begin{aligned}
&\overset{(3.52)}{=} \sqrt{\frac{2}{3}}U_0V_0 + \sqrt{\frac{1}{6}}U_{-1}V_{+1} + \sqrt{\frac{1}{6}}U_{+1}V_{-1} \\
&= \sqrt{\frac{2}{3}}U_zV_z - \sqrt{\frac{1}{6}}\tfrac{1}{2}(U_x - iU_y)(V_x + iV_y) - \sqrt{\frac{1}{6}}\frac{1}{\sqrt{2}}\tfrac{1}{2}(U_x + iU_y)(V_x - iV_y) \\
&= \sqrt{\frac{1}{6}}\Big[2U_zV_z - \tfrac{1}{2}U_xV_x - \frac{i}{2}U_xV_y + \frac{i}{2}U_yV_x \\
&\quad -\tfrac{1}{2}U_yV_y - \tfrac{1}{2}U_xV_x + \frac{i}{2}U_xV_y - \frac{i}{2}U_yV_x - \tfrac{1}{2}U_yV_y\Big] \\
&= \sqrt{\frac{1}{6}}(2U_zV_z - U_xV_x - U_yV_y) \qquad (3.65)
\end{aligned}
$$

$$
\begin{aligned}
T^{(2)}_{-1} &= \langle 11; 0-1|11; 2-1\rangle U_0V_{-1} + \langle 11; -10|11; 2+1\rangle U_{-1}V_0 \\
&\overset{(3.52)}{=} \frac{1}{\sqrt{2}}U_0V_{-1} + \frac{1}{\sqrt{2}}U_{-1}V_0 \\
&= \tfrac{1}{2}(U_zV_x + U_xV_z - iU_zV_y - iU_yV_z) \qquad (3.66)
\end{aligned}
$$

$$
\begin{aligned}
T^{(2)}_{-2} &= \langle 11; -1-1|11; 2-2\rangle U_{-1}V_{-1} \overset{(3.52)}{=} U_{-1}V_{-1} = \tfrac{1}{2}(U_x - iU_y)(V_x - iV_y) \\
&= \tfrac{1}{2}(U_xV_x - U_yV_y - iU_xV_y - iU_yV_x). \qquad (3.67)
\end{aligned}
$$

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.]

(a) We have

$$
\begin{aligned}
&\sum_{m=-j}^{j} |d^{(j)}_{mm'}(\beta)|^2 m \\
= &\sum_{m=-j}^{j} m|\langle jm|e^{-iJ_y\beta/\hbar}|jm'\rangle|^2 \\
= &\sum_{m=-j}^{j} m\langle jm|e^{-iJ_y\beta/\hbar}|jm'\rangle \left(\langle jm|e^{-iJ_y\beta/\hbar}|jm'\rangle\right)^* \\
= &\sum_{m=-j}^{j} m\langle jm|e^{-iJ_y\beta/\hbar}|jm'\rangle\langle jm'|e^{iJ_y\beta/\hbar}|jm\rangle \\
= &\sum_{m=-j}^{j} \langle jm'|e^{iJ_y\beta/\hbar} m|jm\rangle\langle jm|e^{-iJ_y\beta/\hbar}|jm'\rangle \\
= &\frac{1}{\hbar}\langle jm'|e^{iJ_y\beta/\hbar}J_z\left[\sum_{m=-j}^{j}|jm\rangle\langle jm|\right]e^{-iJ_y\beta/\hbar}|jm'\rangle \\
= &\frac{1}{\hbar}\langle jm'|e^{iJ_y\beta/\hbar}J_z e^{-iJ_y\beta/\hbar}|jm'\rangle \\
= &\frac{1}{\hbar}\langle jm'|\mathcal{D}^*(\beta;\hat{e}_y)J_z\mathcal{D}(\beta;\hat{e}_y)|jm'\rangle. \qquad (3.68)
\end{aligned}
$$

But the momentum $\vec{J}$ is a vector operator so from (S-3.10.3) we will have that

$$
\mathcal{D}^*(\beta;\hat{e}_y)J_z\mathcal{D}(\beta;\hat{e}_y) = \sum_j R_{zj}(\beta;\hat{e}_y)J_j. \qquad (3.69)
$$

On the other hand we know (S-3.1.5b) that

$$
R(\beta;\hat{e}_y) = \begin{pmatrix} \cos\beta & 0 & \sin\beta \\ 0 & 1 & 0 \\ -\sin\beta & 0 & \cos\beta \end{pmatrix}. \qquad (3.70)
$$

So

$$
\begin{aligned}
\sum_{m=-j}^{j} |d^{(j)}_{mm'}(\beta)|^2 m &= \frac{1}{\hbar}\left[-\sin\beta\langle jm'|J_x|jm'\rangle + \cos\beta\langle jm'|J_z|jm'\rangle\right] \\
&= \frac{1}{\hbar}\left[-\sin\beta\langle jm'|\frac{J_+ + J_-}{2}|jm'\rangle + \hbar m'\cos\beta\right] \\
&= m'\cos\beta. \qquad (3.71)
\end{aligned}
$$

For $j = 1/2$ we know from (S-3.2.44) that

$$d^{(1/2)}_{mm'}(\beta) = \begin{pmatrix} \cos\frac{\beta}{2} & -\sin\frac{\beta}{2} \\ \sin\frac{\beta}{2} & \cos\frac{\beta}{2} \end{pmatrix}. \tag{3.72}$$

So for $m' = 1/2$

$$\begin{aligned} \sum_{m=-1/2}^{1/2} |d^{(j)}_{m1/2}(\beta)|^2 m &= -\tfrac{1}{2}\sin^2\frac{\beta}{2} + \tfrac{1}{2}\cos^2\frac{\beta}{2} \\ &= \tfrac{1}{2}\cos\beta = m'\cos\beta \end{aligned} \tag{3.73}$$

while for $m' = -1/2$

$$\begin{aligned} \sum_{m=-1/2}^{1/2} |d^{(j)}_{m1/2}(\beta)|^2 m &= -\tfrac{1}{2}\cos^2\frac{\beta}{2} + \tfrac{1}{2}\sin^2\frac{\beta}{2} \\ &= -\tfrac{1}{2}\cos\beta = m'\cos\beta. \end{aligned} \tag{3.74}$$

(b) We have

$$\begin{aligned} &\sum_{m=-j}^{j} m^2 |d^{(j)}_{m'm}(\beta)|^2 \\ = &\sum_{m=-j}^{j} m^2 |\langle jm'|e^{-iJ_y\beta/\hbar}|jm\rangle|^2 \\ = &\sum_{m=-j}^{j} m^2 \langle jm'|e^{-iJ_y\beta/\hbar}|jm\rangle \left(\langle jm'|e^{-iJ_y\beta/\hbar}|jm\rangle\right)^* \\ = &\sum_{m=-j}^{j} m^2 \langle jm'|e^{-iJ_y\beta/\hbar}|jm\rangle\langle jm|e^{iJ_y\beta/\hbar}|jm'\rangle \\ = &\sum_{m=-j}^{j} \langle jm'|e^{-iJ_y\beta/\hbar} m^2 |jm\rangle\langle jm|e^{iJ_y\beta/\hbar}|jm'\rangle \\ = &\frac{1}{\hbar^2}\langle jm'|e^{-iJ_y\beta/\hbar} J_z^2 \left[\sum_{m=-j}^{j} |jm\rangle\langle jm|\right] e^{iJ_y\beta/\hbar}|jm'\rangle \\ = &\frac{1}{\hbar^2}\langle jm'|e^{-iJ_y\beta/\hbar} J_z^2 e^{iJ_y\beta/\hbar}|jm'\rangle \\ = &\frac{1}{\hbar}\langle jm'|\mathcal{D}(\beta;\hat{e}_y) J_z^2 \mathcal{D}^\dagger(\beta;\hat{e}_y)|jm'\rangle. \end{aligned} \tag{3.75}$$

From (3.65) we know that

$$T_0^{(2)} = \sqrt{\frac{1}{6}}(3J_z^2 - J^2) \tag{3.76}$$

where $T_0^{(2)}$ is the 0-component of a second rank tensor. So

$$J_z^2 = \frac{\sqrt{6}}{3}T_0^{(2)} + \frac{1}{3}J^2 \tag{3.77}$$

and since $\mathcal{D}(R)J^2\mathcal{D}^\dagger(R) = J^2\mathcal{D}(R)\mathcal{D}^\dagger(R) = J^2$ we will have

$$\begin{aligned}\textstyle\sum_{m=-j}^{j} \quad & m^2|d_{mm'}^{(j)}(\beta)|^2 = \\ & \frac{1}{\hbar^3}\frac{1}{3}\langle jm'|J^2|jm'\rangle + \sqrt{\frac{2}{3}}\frac{1}{\hbar^2}\langle jm'|\mathcal{D}(\beta;\hat{e}_y)J_z^2\mathcal{D}^\dagger(\beta;\hat{e}_y)|jm'\rangle\end{aligned} \tag{3.78}$$

We know that for a spherical tensor (S-3.10.22b)

$$\mathcal{D}(R)T_q^{(k)}\mathcal{D}^\dagger(R) = \sum_{q'=-k}^{k}\mathcal{D}_{q'q}^{(k)}(R)T_{q'}^{(k)} \tag{3.79}$$

which means in our case that

$$\begin{aligned}\langle jm'|\mathcal{D}(\beta;\hat{e}_y)J_z^2\mathcal{D}^\dagger(\beta;\hat{e}_y)|jm'\rangle &= \langle jm'|\sum_{q'=-2}^{2}T_{q'}^{(2)}\mathcal{D}_{q'0}^{(2)}(\beta;\hat{e}_y)|jm'\rangle \\ = \sum_{q'=-2}^{2}\mathcal{D}_{q'0}^{(2)}(\beta;\hat{e}_y)\langle jm'|T_{q'}^{(2)}|jm'\rangle.\end{aligned} \tag{3.80}$$

But we know from the Wigner-Eckart theorem that $\langle jm'|T_{q'\neq 0}^{(2)}|jm'\rangle = 0$. So

$$\begin{aligned}&\sum_{m=-j}^{j} m^2|d_{mm'}^{(j)}(\beta)|^2 \\ =\; & \frac{1}{3\hbar^2}\hbar^2 j(j+1) + \frac{1}{\hbar^2}\sqrt{\frac{2}{3}}\mathcal{D}_{00}^{(2)}(\beta;\hat{e}_y)\langle jm'|T_0^{(2)}|jm'\rangle \\ =\; & \frac{1}{3}j(j+1) + \frac{1}{2}d_{00}^{(2)}(\beta)\langle jm'|J_z^2 - \frac{1}{3}J^2|jm'\rangle \\ =\; & \frac{1}{3}j(j+1) + \frac{1}{2}d_{00}^{(2)}(\beta)\left[m'^2 - \frac{1}{3}j(j+1)\right]\end{aligned}$$

$$\begin{aligned}
&= \frac{1}{3}j(j+1) + \frac{1}{2}(3\cos^2\beta - 1)\left[m'^2 - \frac{1}{3}j(j+1)\right] \\
&= -\frac{1}{2}j(j+1)\cos^2\beta + \frac{1}{6}j(j+1) + \frac{1}{3}j(j+1) + \frac{m'^2}{2}(3\cos^2\beta - 1) \\
&= \tfrac{1}{2}j(j+1)\sin^2\beta + m'^2\tfrac{1}{2}(3\cos^2\beta - 1) \qquad (3.81)
\end{aligned}$$

where we have used $d_{00}^{(2)}(\beta) = P_2(\cos\beta) = \frac{1}{2}(3\cos^2\beta - 1)$.

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.

(a) Using the relations (3.63-3.67) we can find that in the case where $\vec{U} = \vec{V} = \vec{x}$ the components of a spherical tensor of rank 2 will be

$$\begin{aligned}
T_{+2}^{(2)} &= \tfrac{1}{2}(x^2 - y^2) + ixy & T_{-2}^{(2)} &= \tfrac{1}{2}(x^2 - y^2) - ixy \\
T_{+1}^{(2)} &= -(xz + izy) & T_{-1}^{(2)} &= xz - izy \qquad (3.82) \\
T_{0}^{(2)} &= \sqrt{\tfrac{1}{6}}(2z^2 - x^2 - y^2) = \sqrt{\tfrac{1}{6}}(3z^2 - r^2)
\end{aligned}$$

So from the above we have

$$\left(x^2 - y^2\right) = T_{+2}^{(2)} + T_{-2}^{(2)}, \quad xy = \frac{T_{+2}^{(2)} - T_{-2}^{(2)}}{2i}, \quad xz = \frac{T_{-1}^{(2)} - T_{+1}^{(2)}}{2}. \quad (3.83)$$

(b) We have

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

$$\stackrel{(3.82)}{=} \quad \sqrt{6}e\langle\alpha, j, m = j|T_0^{(2)}|\alpha, j, m = j\rangle \stackrel{(W.-E.)}{=} \langle j2; j0|j2; jj\rangle \frac{\langle\alpha j\|T^{(2)}\|\alpha j\rangle}{\sqrt{2j+1}}\sqrt{6}e$$

$$\Rightarrow \quad \langle\alpha j\|T^{(2)}\|\alpha j\rangle = \frac{Q}{\sqrt{6}e}\frac{\sqrt{2j+1}}{\langle j2; j0|j2; jj\rangle}. \tag{3.84}$$

So

$$\begin{aligned} e \quad & \langle\alpha, j, m'|(x^2 - y^2)|\alpha, j, m = j\rangle \\ & \stackrel{(3.83)}{=} e\langle\alpha, j, m'|T_{+2}^{(2)}|\alpha, j, m = j\rangle + e\langle\alpha, j, m'|T_{-2}^{(2)}|\alpha, j, m = j\rangle \\ & = e\overbrace{\langle j2; j2|j2; jm'\rangle}^{0}\frac{\langle\alpha j\|T^{(2)}\|\alpha j\rangle}{\sqrt{2j+1}} + e\delta_{m',j-2}\langle j2; j-2|j2; jj-2\rangle\frac{\langle\alpha j\|T^{(2)}\|\alpha j\rangle}{\sqrt{2j+1}} \\ & \stackrel{(3.84)}{=} \frac{Q}{\sqrt{6}}\frac{\langle j2; j, -2|j2; j, j-2\rangle}{\langle j2; j, 0|j2; j, j\rangle}\delta_{m',j-2}. \end{aligned} \tag{3.85}$$

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?

(a) Suppose that $|n\rangle$ in a nondegenerate energy eigenstate. Then

$$
\begin{aligned}
& H\Theta|n\rangle = \Theta H|n\rangle = E_n|n\rangle \Rightarrow \Theta|n\rangle = e^{i\delta}|n\rangle \\
\Rightarrow\; & \Theta|n, t_0 = 0; t\rangle = \Theta e^{-itH/\hbar}|n\rangle = \Theta e^{-itE_n/\hbar}|n\rangle = \\
& e^{itE_n/\hbar}\Theta|n\rangle = e^{i\left(\frac{E_n t}{\hbar}+\delta\right)}|n\rangle = e^{i\left(\frac{2E_n t}{\hbar}+\delta\right)}|n, t_0 = 0; t\rangle \\
\Rightarrow\; & \Theta\left[\int d^3x|\vec{x}\rangle\langle\vec{x}|\right]|n, t_0 = 0; t\rangle = e^{i\left(\frac{2E_n t}{\hbar}+\delta\right)}\left[\int d^3x|\vec{x}\rangle\langle\vec{x}|\right]|n, t_0 = 0; t\rangle \\
\Rightarrow\; & \int d^3x\langle\vec{x}|n, t_0 = 0; t\rangle^*|\vec{x}\rangle = \int d^3x e^{i\left(\frac{2E_n t}{\hbar}+\delta\right)}\langle\vec{x}|n, t_0 = 0; t\rangle|\vec{x}\rangle \\
\Rightarrow\; & \phi_n^*(\vec{x}, t) = e^{i\left(\frac{2E_n t}{\hbar}+\delta\right)}\phi_n(\vec{x}, t). \qquad (4.1)
\end{aligned}
$$

So if we choose at any instant of time $\delta = -\frac{2E_n t}{\hbar}$ the wave function will be real.

(b) In the case of a free particle the Schrödinger equation is

$$
\begin{aligned}
& \frac{p^2}{2m}|n\rangle = E|n\rangle \Rightarrow -\frac{\hbar^2}{2m}\vec{\nabla}\phi_n(x) = E\phi_n(x) \\
\Rightarrow\; & \phi_n(x) = Ae^{i\vec{p}\cdot\vec{x}/\hbar} + Be^{-i\vec{p}\cdot\vec{x}/\hbar} \qquad (4.2)
\end{aligned}
$$

The wave functions $\phi_n(x) = e^{-i\vec{p}\cdot\vec{x}/\hbar}$ and $\phi_n'(x) = e^{i\vec{p}\cdot\vec{x}/\hbar}$ correspond to the same eigenvalue $E = \frac{p^2}{2m}$ and so there is degeneracy since these correspond to different state kets $|\vec{p}\rangle$ and $|-\vec{p}\rangle$. So we cannot apply the previous result.

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.

In the momentum space we have

$$|\alpha\rangle = \int d^3p' \langle\vec{p}'|\alpha\rangle|\vec{p}'\rangle \Rightarrow |\alpha\rangle = \int d^3p' \phi(\vec{p}')|\vec{p}'\rangle$$
$$\Rightarrow \quad \Theta|\alpha\rangle = \int d^3p' \Theta\left[\langle\vec{p}'|\alpha\rangle|\vec{p}'\rangle\right] = \int d^3p' \langle\vec{p}'|\alpha\rangle^* \Theta|\vec{p}'\rangle. \tag{4.3}$$

For the momentum it is natural to require

$$\langle\alpha|\vec{p}|\alpha\rangle = -\langle\tilde{\alpha}|\vec{p}|\tilde{\alpha}\rangle \Rightarrow$$
$$\langle\tilde{\alpha}|\Theta\vec{p}\Theta^{-1}|\tilde{\alpha}\rangle \Rightarrow \Theta\vec{p}\Theta^{-1} = -\vec{p} \tag{4.4}$$

So

$$\Theta\vec{p}|\vec{p}'\rangle \overset{(4.4)}{=} -\vec{p}\Theta|\vec{p}'\rangle \Rightarrow \Theta|\vec{p}'\rangle = |-\vec{p}'\rangle \tag{4.5}$$

up to a phase factor. So finally

$$\Theta|\alpha\rangle = \int d^3p' \langle\vec{p}'|\alpha\rangle^* |-\vec{p}'\rangle = \int d^3p' \langle-\vec{p}'|\alpha\rangle^* |\vec{p}'\rangle$$
$$\Rightarrow \quad \langle\vec{p}'|\Theta|\alpha\rangle = \tilde{\phi}(\vec{p}') = \langle-\vec{p}'|\alpha\rangle^* = \phi^*(-\vec{p}'). \tag{4.6}$$

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.

The defining property of a Bloch function $\psi_{n,k}(x)$ is

$$\psi_{n,k}(x + a) = e^{ika}\psi_{n,k}(x). \tag{4.7}$$

We can show that the functions $\sum_{R_i} \phi_n(x - R_i)e^{ikR_i}$ satisfy the same relation

$$\begin{aligned}\sum_{R_i} \phi_n(x + a - R_i)e^{ikR_i} &= \sum_{R_i} \phi_n[x - (R_i - a)]e^{ik(R_i-a)}e^{ika} \\ \overset{R_i-a=R_j}{=} \quad & e^{ika}\sum_{R_j} \phi_n(x - R_j)e^{ikR_j}\end{aligned} \tag{4.8}$$

which means that it is a Bloch function

$$\psi_{n,k}(x) = \sum_{R_i} \phi_n(x - R_i)e^{ikR_i}. \tag{4.9}$$

The last relation gives the Bloch functions in terms of Wannier functions. To find the expansion of a Wannier function in terms of Bloch functions we multiply this relation by e^{-ikR_j} and integrate over k.

$$\begin{aligned}\psi_{n,k}(x) &= \sum_{R_i} \phi_n(x - R_i)e^{ikR_i} \\ \Rightarrow \quad \int_{-\pi/a}^{\pi/a} dk e^{-ikR_j}\psi_{n,k}(x) &= \sum_{R_i} \phi_n(x - R_i) \int_{-\pi/a}^{\pi/a} e^{ik(R_i-R_j)}dk\end{aligned} \tag{4.10}$$

But

$$\int_{-\pi/a}^{\pi/a} e^{ik(R_i-R_j)}dk = \left.\frac{e^{ik(R_i-R_j)}}{i(R_i-R_j)}\right|_{-\pi/a}^{\pi/a} = \frac{2\sin\left[\pi/a(R_i-R_j)\right]}{R_i-R_j}$$
$$= \delta_{ij}\frac{2\pi}{a} \tag{4.11}$$

where in the last step we used that $R_i - R_j = na$, with $n \in \mathcal{Z}$. So

$$\int_{-\pi/a}^{\pi/a} dke^{-ikR_j}\psi_{n,k}(x) = \sum_{R_i}\phi_n(x-R_i)\delta_{ij}\frac{2\pi}{a}$$
$$\Rightarrow \quad \phi_n(x-R_i) = \frac{a}{2\pi}\int_{-\pi/a}^{\pi/a} e^{-ikR_i}\psi_{n,k}(x)dk \tag{4.12}$$

So using the orthonormality properties of the Bloch functions

$$\int dx\phi_m^*(x-R_i)\phi_n(x-R_j)$$
$$= \int\int\int \frac{a^2}{(2\pi)^2}e^{ikR_i}\psi_{m,k}^*(x)e^{-ik'R_j}\psi_{n,k'}(x)dkdk'dx$$
$$= \int\int \frac{a^2}{(2\pi)^2}e^{ikR_i-ik'R_j}\int \psi_{m,k}^*(x)\psi_{n,k'}(x)dxdkdk'$$
$$= \int\int \frac{a^2}{(2\pi)^2}e^{ikR_i-ik'R_j}\delta_{mn}\delta(k-k')dkdk'$$
$$= \frac{a^2}{(2\pi)^2}\delta_{mn}\int_{-\pi/a}^{\pi/a} e^{ik(R_i-R_j)}dk = \frac{a}{2\pi}\delta_{mn}\delta_{ij}. \tag{4.13}$$

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 $F_{lm}(r)$?

Since the Hamiltonian is invariant under time reversal

$$H\Theta = \Theta H. \tag{4.14}$$

So if $|n\rangle$ is an energy eigenstate with eigenvalue E_n we will have

$$H\Theta|n\rangle = \Theta H|n\rangle = E_n\Theta|n\rangle. \tag{4.15}$$

If there is no degeneracy $|n\rangle$ and $\Theta|n\rangle$ can differ at most by a phase factor. Hence

$$|\tilde{n}\rangle \equiv \Theta|n\rangle = e^{i\delta}|n\rangle. \tag{4.16}$$

For the angular-momentum operator we have from (S-4.4.53)

$$\begin{array}{c} \langle n|\vec{L}|n\rangle = -\langle \tilde{n}|\vec{L}|\tilde{n}\rangle \overset{(4.16)}{=} -\langle n|\vec{L}|n\rangle \Rightarrow \\ \langle n|\vec{L}|n\rangle = 0 \end{array} \quad . \tag{4.17}$$

We have

$$\begin{aligned} \Theta|n\rangle &= \Theta\int d^3x|\vec{x}\rangle\langle\vec{x}|n\rangle = \int d^3x\langle\vec{x}|n\rangle^*\Theta|\vec{x}\rangle \\ &= \int d^3x\langle\vec{x}|n\rangle^*|\vec{x}\rangle \overset{(4.16)}{=} e^{i\delta}|n\rangle \Rightarrow \\ \langle\vec{x'}|\Theta|n\rangle &= \langle\vec{x'}|n\rangle^* = e^{i\delta}\langle\vec{x'}|n\rangle. \end{aligned} \tag{4.18}$$

So if we use $\langle\vec{x}|n\rangle = \sum_l\sum_m F_{lm}(r)Y_l^m(\theta,\phi)$

$$\begin{aligned} & \sum_{ml} F^*_{lm}(r)Y_l^{m*}(\theta,\phi) = e^{i\delta}\sum_{ml} F_{lm}(r)Y_l^m(\theta,\phi) \\ \overset{(S-4.4.57)}{\Rightarrow} \quad & \sum_{ml} F^*_{lm}(r)(-1)^m Y_l^{-m}(\theta,\phi) = e^{i\delta}\sum_{ml} F_{lm}(r)Y_l^m(\theta,\phi) \\ \Rightarrow \quad & \int Y_{l'}^{m'*}\sum_{ml} F^*_{lm}(r)(-1)^m Y_l^{-m}(\theta,\phi)d\Omega = e^{i\delta}\int Y_{l'}^{m'*}\sum_{ml} F_{lm}(r)Y_l^m(\theta,\phi)d\Omega \\ \Rightarrow \quad & \sum_{ml} F^*_{lm}(r)(-1)^m\delta_{m',-m}\delta_{l'l} = e^{i\delta}\sum_{ml} F_{lm}(r)\delta_{m',m}\delta_{l'l} \\ \Rightarrow \quad & F^*_{l',-m'}(r)(-1)^{-m'} = e^{i\delta}F_{l'm'}(r) \Rightarrow F^*_{l',-m'}(r) = (-1)^{m'}F_{l'm'}(r)e^{i\delta}. \end{aligned} \tag{4.19}$$

4.5 The Hamiltonian for a spin 1 system is given by

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

Solve this problem *exactly* to find the normalized energy eigenstates and eigenvalues. (A spin-dependent Hamiltonian of this kind actually appears in crystal physics.) Is this Hamiltonian invariant under time reversal? How do the normalized eigenstates you obtained transform under time reversal?

For a spin 1 system $l = 1$ and $m = -1, 0, +1$. For the operator S_z we have

$$S_z|l,m\rangle = \hbar m|l,m\rangle \Rightarrow \langle ln|S_z|l,m\rangle = \hbar m\langle n|m\rangle \Rightarrow (S_z)_{nm} = \hbar m\delta_{nm} \quad (4.20)$$

So

$$S_z \doteq \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \Rightarrow S_z^2 \doteq \hbar^2 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

For the operator S_x we have

$$\begin{aligned} S_x|l,m\rangle &= \frac{S_+ + S_-}{2}|1,m\rangle = \tfrac{1}{2}S_+|1,m\rangle + \tfrac{1}{2}S_-|1,m\rangle \rightarrow \\ \langle 1,n|S_x|1,m\rangle &= \tfrac{1}{2}\langle 1,n|S_+|1,m\rangle + \tfrac{1}{2}\langle 1,n|S_-|1,m\rangle \\ &\overset{(S-3.5.39)}{=} \tfrac{1}{2}\hbar\sqrt{(1-m)(2+m)}\delta_{n,m+1} + \tfrac{1}{2}\hbar\sqrt{(1+m)(2-m)}\delta_{n,m-1}. \end{aligned}$$

So

$$\begin{aligned} S_x &\doteq \frac{\hbar}{2}\begin{pmatrix} 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{pmatrix} + \frac{\hbar}{2}\begin{pmatrix} 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 \end{pmatrix} \\ &= \frac{\hbar}{2}\begin{pmatrix} 0 & \sqrt{2} & 0 \\ \sqrt{2} & 0 & \sqrt{2} \\ 0 & \sqrt{2} & 0 \end{pmatrix} \Rightarrow \\ S_x^2 &= \frac{\hbar^2}{4}\begin{pmatrix} 2 & 0 & 2 \\ 0 & 4 & 0 \\ 2 & 0 & 2 \end{pmatrix} = \hbar^2 \begin{pmatrix} \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 1 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix}. \end{aligned} \quad (4.21)$$

In the same manner for the operator $S_y = \frac{S_+ - S_-}{2i}$ we find

$$
\begin{aligned}
S_x &\doteq \frac{\hbar}{2i}\begin{pmatrix} 0 & \sqrt{2} & 0 \\ -\sqrt{2} & 0 & \sqrt{2} \\ 0 & -\sqrt{2} & 0 \end{pmatrix} \Rightarrow \\
S_x^2 &\doteq -\frac{\hbar^2}{4}\begin{pmatrix} -2 & 0 & 2 \\ 0 & -4 & 0 \\ 2 & 0 & -2 \end{pmatrix} = \hbar^2 \begin{pmatrix} \frac{1}{2} & 0 & -\frac{1}{2} \\ 0 & 1 & 0 \\ -\frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix}. \qquad (4.22)
\end{aligned}
$$

Thus the Hamiltonian can be represented by the matrix

$$
H \doteq \hbar^2 \begin{pmatrix} A & 0 & B \\ 0 & 0 & 0 \\ B & 0 & A \end{pmatrix}. \qquad (4.23)
$$

To find the energy eigenvalues we have to solve the secular equation

$$
\begin{aligned}
&\det(H - \lambda I) = 0 \Rightarrow \det \begin{pmatrix} A\hbar^2 - \lambda & 0 & B\hbar^2 \\ 0 & -\lambda & 0 \\ B\hbar^2 & 0 & A\hbar^2 - \lambda \end{pmatrix} = 0 \\
\Rightarrow\ & (A\hbar^2 - \lambda)^2(-\lambda) + (B\hbar^2)^2\lambda = 0 \Rightarrow \lambda\left[(A\hbar^2 - \lambda)^2 - (B\hbar^2)^2\right] = 0 \\
\Rightarrow\ & \lambda(A\hbar^2 - \lambda - B\hbar^2)(A\hbar^2 - \lambda + B\hbar^2) = 0 \\
\Rightarrow\ & \lambda_1 = 0, \quad \lambda_2 = \hbar^2(A+B), \quad \lambda_3 = \hbar^2(A-B). \qquad (4.24)
\end{aligned}
$$

To find the eigenstate $|n_{\lambda_c}\rangle$ that corresponds to the eigenvalue λ_c we have to solve the following equation

$$
\hbar^2 \begin{pmatrix} A & 0 & B \\ 0 & 0 & 0 \\ B & 0 & A \end{pmatrix}\begin{pmatrix} a \\ b \\ c \end{pmatrix} = \lambda_c \begin{pmatrix} a \\ b \\ c \end{pmatrix}. \qquad (4.25)
$$

For $\lambda_1 = 0$

$$
\begin{aligned}
&\hbar^2 \begin{pmatrix} A & 0 & B \\ 0 & 0 & 0 \\ B & 0 & A \end{pmatrix}\begin{pmatrix} a \\ b \\ c \end{pmatrix} = 0 \Rightarrow \begin{cases} aA + cB = 0 \\ aB + cA = 0 \end{cases} \\
&\Rightarrow \begin{cases} a = -c\frac{B}{A} \\ -c\frac{B^2}{A} + cA = 0 \end{cases} \Rightarrow \begin{cases} a = 0 \\ c = 0 \end{cases} \qquad (4.26)
\end{aligned}
$$

So

$$
\begin{aligned}
|n_0\rangle &\doteq \begin{pmatrix} 0 \\ b \\ 0 \end{pmatrix} \overset{norm.}{=} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \Rightarrow \\
|n_0\rangle &= |10\rangle.
\end{aligned} \tag{4.27}
$$

In the same way for $\lambda = \hbar^2(A+B)$

$$
\begin{pmatrix} A & 0 & B \\ 0 & 0 & 0 \\ B & 0 & A \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = (A+B) \begin{pmatrix} a \\ b \\ c \end{pmatrix} \Rightarrow \left\{ \begin{aligned} aA + cB &= a(A+B) \\ 0 &= b(A+B) \\ aB + cA &= c(A+B) \end{aligned} \right.
$$

$$
\Rightarrow \left\{ \begin{array}{l} a = c \\ b = 0 \end{array} \right. \tag{4.28}
$$

So

$$
\begin{aligned}
|n_{A+B}\rangle &\doteq \begin{pmatrix} c \\ 0 \\ c \end{pmatrix} \overset{norm.}{=} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} \Rightarrow \\
|n_{A+B}\rangle &= \frac{1}{\sqrt{2}}|1,+1\rangle + \frac{1}{\sqrt{2}}|1,-1\rangle.
\end{aligned} \tag{4.29}
$$

For $\lambda = \hbar^2(A-B)$ we have

$$
\begin{pmatrix} A & 0 & B \\ 0 & 0 & 0 \\ B & 0 & A \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = (A-B) \begin{pmatrix} a \\ b \\ c \end{pmatrix} \Rightarrow \left\{ \begin{aligned} aA + cB &= a(A-B) \\ 0 &= b(A-B) \\ aB + cA &= c(A-B) \end{aligned} \right.
$$

$$
\Rightarrow \left\{ \begin{array}{r} a = -c \\ b = 0 \end{array} \right. \tag{4.30}
$$

So

$$
\begin{aligned}
|n_{A+B}\rangle &\doteq \begin{pmatrix} c \\ 0 \\ -c \end{pmatrix} \overset{norm.}{=} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} \Rightarrow \\
|n_{A-B}\rangle &= \frac{1}{\sqrt{2}}|1,+1\rangle - \frac{1}{\sqrt{2}}|1,-1\rangle.
\end{aligned} \tag{4.31}
$$

Now we are going to check if the Hamiltonian is invariant under time reversal

$$\begin{aligned}\Theta H \Theta^{-1} &= A\Theta S_z^2 \Theta^{-1} + B(\Theta S_x^2 \Theta^{-1} - \Theta S_y^2 \Theta^{-1}) \\ &= A\Theta S_z \Theta^{-1} \Theta S_z \Theta^{-1} + B(\Theta S_x \Theta^{-1} \Theta S_x \Theta^{-1} - \Theta S_y \Theta^{-1} \Theta S_y \Theta^{-1}) \\ &= A S_z^2 + B(S_x^2 - S_y^2) = H. \end{aligned} \tag{4.32}$$

To find the transformation of the eigenstates under time reversal we use the relation (S-4.4.58)

$$\Theta |l, m\rangle = (-1)^m |l, -m\rangle. \tag{4.33}$$

So

$$\begin{aligned}\Theta |n_0\rangle &= \Theta |10\rangle \overset{(4.33)}{=} |10\rangle \\ &= |n_0\rangle \end{aligned} \tag{4.34}$$

$$\tag{4.35}$$

$$\begin{aligned}\Theta |n_{A+B}\rangle &= \frac{1}{\sqrt{2}} \Theta |1, +1\rangle + \frac{1}{\sqrt{2}} \Theta |1, -1\rangle \\ &\overset{(4.33)}{=} -\frac{1}{\sqrt{2}} |1, -1\rangle - \frac{1}{\sqrt{2}} |1, +1\rangle \\ &= -|n_{A+B}\rangle \end{aligned} \tag{4.36}$$

$$\tag{4.37}$$

$$\begin{aligned}\Theta |n_{A-B}\rangle &= \frac{1}{\sqrt{2}} \Theta |1, +1\rangle - \frac{1}{\sqrt{2}} \Theta |1, -1\rangle \\ &\overset{(4.33)}{=} -\frac{1}{\sqrt{2}} |1, -1\rangle + \frac{1}{\sqrt{2}} |1, +1\rangle \\ &= |n_{A-B}\rangle. \end{aligned} \tag{4.38}$$

5 Approximation Methods

5.1 Consider an isotropic harmonic oscillator in *two* dimensions. The Hamiltonian is given by

$$H_0 = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{m\omega^2}{2}(x^2 + y^2)$$

(a) What are the energies of the three lowest-lying states? Is there any degeneracy?

(b) We now apply a perturbation

$$V = \delta m\omega^2 xy$$

where δ is a dimensionless real number much smaller than unity. Find the zeroth-order energy eigenket and the corresponding energy to first order [that is the unperturbed energy obtained in (a) plus the first-order energy shift] for each of the three lowest-lying states.

(c) Solve the $H_0 + V$ problem *exactly*. Compare with the perturbation results obtained in (b).
[You may use $\langle n'|x|n\rangle = \sqrt{\hbar/2m\omega}(\sqrt{n+1}\delta_{n',n+1} + \sqrt{n}\delta_{n',n-1})$.]

Define step operators:

$$\begin{aligned}
a_x &\equiv \sqrt{\frac{m\omega}{2\hbar}}(x + \frac{ip_x}{m\omega}), \\
a_x^\dagger &\equiv \sqrt{\frac{m\omega}{2\hbar}}(x - \frac{ip_x}{m\omega}), \\
a_y &\equiv \sqrt{\frac{m\omega}{2\hbar}}(y + \frac{ip_y}{m\omega}), \\
a_y^\dagger &\equiv \sqrt{\frac{m\omega}{2\hbar}}(y - \frac{ip_y}{m\omega}).
\end{aligned} \tag{5.1}$$

From the fundamental commutation relations we can see that

$$[a_x, a_x^\dagger] = [a_y, a_y^\dagger] = 1.$$

Defining the number operators

$$N_x \equiv a_x^\dagger a_x, \qquad N_y \equiv a_y^\dagger a_y$$

we find

$$\begin{aligned} N &\equiv N_x + N_y = \frac{H_0}{\hbar\omega} - 1 \Rightarrow \\ H_0 &= \hbar\omega(N+1). \end{aligned} \tag{5.2}$$

I.e. energy eigenkets are also eigenkets of N:

$$\begin{aligned} N_x \,|\, m,n \,\rangle &= m \,|\, m,n \,\rangle, \\ N_y \,|\, m,n \,\rangle &= n \,|\, m,n \,\rangle \Rightarrow \\ N \,|\, m,n \,\rangle &= (m+n) \,|\, m,n \,\rangle \end{aligned} \tag{5.3}$$

so that

$$H_0 \,|\, m,n \,\rangle = E_{m,n} \,|\, m,n \,\rangle = \hbar\omega(m+n+1) \,|\, m,n \,\rangle.$$

(a) The lowest lying states are

state	degeneracy
$E_{0,0} = \hbar\omega$	1
$E_{1,0} = E_{0,1} = 2\hbar\omega$	2
$E_{2,0} = E_{0,2} = E_{1,1} = 3\hbar\omega$	3

(b) Apply the perturbation $V = \delta m\omega^2 xy$.

Full problem:	$(H_0 + V) \,|\, l \,\rangle = E \,|\, l \,\rangle$
Unperturbed problem:	$H_0 \,|\, l^0 \,\rangle = E^0 \,|\, l^0 \,\rangle$

Expand the energy levels and the eigenkets as

$$\begin{aligned} E &= E^0 + \Delta^1 + \Delta^2 + \ldots \\ |\, l \,\rangle &= |\, l^0 \,\rangle + |\, l^1 \,\rangle + \ldots \end{aligned} \tag{5.4}$$

so that the full problem becomes

$$(E^0 - H_0)\left[\,|\, l^0 \,\rangle + |\, l^1 \,\rangle + \ldots\right] = (V - \Delta^1 - \Delta^2 \ldots)\left[\,|\, l^0 \,\rangle + |\, l^1 \,\rangle + \ldots\right].$$

To 1'st order:

$$(E^0 - H_0)\,|\,l^1\,\rangle = (V - \Delta^1)\,|\,l^0\,\rangle. \tag{5.5}$$

Multiply with $\langle\, l^0\,|$ to find

$$\begin{aligned} \langle\, l^0\,|\,E^0 - H_0\,|\,l^1\,\rangle &= 0 = \langle\, l^0\,|\,V - \Delta^1\,|\,l^0\,\rangle \Rightarrow \\ \Delta^1\langle\, l^0\,|\,l^0\,\rangle &= \Delta^1 = \langle\, l^0\,|\,V\,|\,l^0\,\rangle \end{aligned} \tag{5.6}$$

In the degenerate case this does not work since we're not using the right basis kets. Wind back to (5.5) and multiply it with another degenerate basis ket

$$\begin{aligned} \langle\, m^0\,|\,E^0 - H_0\,|\,l^1\,\rangle &= 0 = \langle\, m^0\,|\,V - \Delta^1\,|\,l^0\,\rangle \Rightarrow \\ \Delta^1\langle\, m^0\,|\,l^0\,\rangle &= \langle\, m^0\,|\,V\,|\,l^0\,\rangle. \end{aligned} \tag{5.7}$$

Now, $\langle\, m^0\,|\,l^0\,\rangle$ is not necessarily δ_{kl} since only states corresponding to different eigenvalues have to be orthogonal!

Insert a **1**:

$$\sum_{k\in D}\langle\, m^0\,|\,V\,|\,k^0\,\rangle\langle\, k^0\,|\,l^0\,\rangle = \Delta^1\langle\, m^0\,|\,l^0\,\rangle.$$

This is the eigenvalue equation which gives the correct zeroth order eigenvectors!

Let us use all this:

1. The ground state is non-degenerate $\Rightarrow$

$$\Delta^1_{00} = \langle\, 0,0\,|\,V\,|\,0,0\,\rangle = \delta m\omega^2\langle\, 0,0\,|\,xy\,|\,0,0\,\rangle \sim \langle\, 0,0\,|\,(a_x + a_x^\dagger)(a_y + a_y^\dagger)\,|\,0,0\,\rangle = 0$$

2. First excited state is degenerate $|\,1,0\,\rangle$, $|\,0,1\,\rangle$. We need the matrix elements $\langle\, 1,0\,|\,V\,|\,1,0\,\rangle$, $\langle\, 1,0\,|\,V\,|\,0,1\,\rangle$, $\langle\, 0,1\,|\,V\,|\,1,0\,\rangle$, $\langle\, 0,1\,|\,V\,|\,0,1\,\rangle$.

$$V = \delta m\omega^2 xy = \delta m\omega^2\frac{\hbar}{2m\omega}(a_x + a_x^\dagger)(a_y + a_y^\dagger) = \frac{\delta\hbar\omega}{2}(a_x a_y + a_x^\dagger a_y + a_x a_y^\dagger + a_x^\dagger a_y^\dagger)$$

and

$$a_x\,|\,m,n\,\rangle = \sqrt{m}\,|\,m-1,n\,\rangle \qquad a_x^\dagger\,|\,m,n\,\rangle = \sqrt{m+1}\,|\,m+1,n\,\rangle \quad \textit{etc.}$$

Together this gives

$$\begin{aligned} V_{10,10} &= V_{01,01} = 0, \\ V_{10,01} &= \frac{\delta\hbar\omega}{2}\langle\, 1,0 \,|\, a_x a_y^\dagger \,|\, 0,1 \,\rangle = \frac{\delta\hbar\omega}{2}, \\ V_{01,10} &= \frac{\delta\hbar\omega}{2}\langle\, 1,0 \,|\, a_x^\dagger a_y \,|\, 0,1 \,\rangle = \frac{\delta\hbar\omega}{2}. \end{aligned} \tag{5.8}$$

The V-matrix becomes

$$\frac{\delta\hbar\omega}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

and so the eigenvalues ($= \Delta^1$) are

$$\Delta^1 = \pm\frac{\delta\hbar\omega}{2}.$$

To get the eigenvectors we solve

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix} = \pm\begin{pmatrix} x \\ y \end{pmatrix}$$

and get

$$\begin{aligned} |\cdots\rangle_+ &= \frac{1}{\sqrt{2}}(\,|\,0,1\,\rangle + |\,1,0\,\rangle), \qquad E_+ = \hbar\omega(2 + \frac{\delta}{2}), \\ |\cdots\rangle_- &= \frac{1}{\sqrt{2}}(\,|\,0,1\,\rangle - |\,1,0\,\rangle), \qquad E_- = \hbar\omega(2 - \frac{\delta}{2}). \end{aligned} \tag{5.9}$$

3. The second excited state is also degenerate $|\,2,0\,\rangle$, $|\,1,1\,\rangle$, $|\,0,2\,\rangle$, so we need the corresponding 9 matrix elements. However the only non-vanishing ones are:

$$V_{11,20} = V_{20,11} = V_{11,02} = V_{02,11} = \frac{\delta\hbar\omega}{\sqrt{2}} \tag{5.10}$$

(where the $\sqrt{2}$ came from going from level 1 to 2 in either of the oscillators) and thus to get the eigenvalues we evaluate

$$0 = det\begin{pmatrix} -\lambda & 1 & 0 \\ 1 & -\lambda & 1 \\ 0 & 1 & -\lambda \end{pmatrix} = -\lambda(\lambda^2 - 1) + \lambda = \lambda(2 - \lambda^2)$$

which means that the eigenvalues are $\{0, \pm\delta\hbar\omega\}$. By the same method as above we get the eigenvectors

$$\begin{aligned}
|\cdots\rangle_+ &= \tfrac{1}{2}(|2,0\rangle + \sqrt{2}|1,1\rangle + |0,2\rangle), & E_+ &= \hbar\omega(3+\delta),\\
|\cdots\rangle_0 &= \frac{1}{\sqrt{2}}(-|2,0\rangle + |0,2\rangle), & E_0 &= 3\hbar\omega,\\
|\cdots\rangle_- &= \tfrac{1}{2}(|2,0\rangle - \sqrt{2}|1,1\rangle + |0,2\rangle), & E_- &= \hbar\omega(3-\delta).
\end{aligned}$$

(c) To solve the problem exactly we will make a variable change. The potential is

$$\begin{aligned}
& m\omega^2\left[\tfrac{1}{2}(x^2+y^2)+\delta xy\right] = \\
= \; & m\omega^2\left[\frac{1}{4}((x+y)^2+(x-y)^2)+\frac{\delta}{4}(x+y)^2-(x-y)^2)\right]. \quad (5.11)
\end{aligned}$$

Now it is natural to introduce

$$\begin{aligned}
x' &\equiv \frac{1}{\sqrt{2}}(x+y), & p'_x &\equiv \frac{1}{\sqrt{2}}(p'_x+p'_y),\\
y' &\equiv \frac{1}{\sqrt{2}}(x-y), & p'_y &\equiv \frac{1}{\sqrt{2}}(p'_x-p'_y). \quad (5.12)
\end{aligned}$$

Note: $[x', p'_x] = [y', p'_y] = i\hbar$, so that $(x',\ p'_x)$ and $(y',\ p'_y)$ are canonically conjugate.

In these new variables the problem takes the form

$$H = \frac{1}{2m}(p'^2_x + p'^2_y) + \frac{m\omega^2}{2}[(1+\delta)x'^2 + (1-\delta)y'^2].$$

So we get one oscillator with $\omega'_x = \omega\sqrt{1+\delta}$ and another with $\omega'_y = \omega\sqrt{1-\delta}$. The energy levels are:

$$\begin{aligned}
E_{0,0} &= \hbar\omega,\\
E_{1,0} &= \hbar\omega + \hbar\omega'_x = \hbar\omega(1+\sqrt{1+\delta}) =\\
&= \hbar\omega(1+1+\tfrac{1}{2}\delta+\ldots) = \hbar\omega(2+\tfrac{1}{2}\delta)+O(\delta^2),
\end{aligned}$$

$$\begin{aligned}
E_{0,1} &= \hbar\omega + \hbar\omega_y' = \ldots = \hbar\omega(2 - \tfrac{1}{2}\delta) + O(\delta^2), \\
E_{2,0} &= \hbar\omega + 2\hbar\omega_x' = \ldots = \hbar\omega(3 + \delta) + O(\delta^2), \\
E_{1,1} &= \hbar\omega + \hbar\omega_x' + \hbar\omega_y' = \ldots = 3\hbar\omega + O(\delta^2), \\
E_{0,2} &= \hbar\omega + 2\hbar\omega_y' = \ldots = \hbar\omega(3 - \delta) + O(\delta^2).
\end{aligned} \tag{5.13}$$

So first order perturbation theory worked!

5.2 A system that has three unperturbed states can be represented by the perturbed Hamiltonian matrix

$$\begin{pmatrix} E_1 & 0 & a \\ 0 & E_1 & b \\ a^* & b^* & E_2 \end{pmatrix}$$

where $E_2 > E_1$. The quantities a and b are to be regarded as perturbations that are of the same order and are small compared with $E_2 - E_1$. Use the second-order nondegenerate perturbation theory to calculate the perturbed eigenvalues. (Is this procedure correct?) Then diagonalize the matrix to find the exact eigenvalues. Finally, use the second-order degenerate perturbation theory. Compare the three results obtained.

(a) First, find the exact result by diagonalizing the Hamiltonian:

$$\begin{aligned}
0 &= \begin{vmatrix} E_1 - E & 0 & a \\ 0 & E_1 - E & b \\ a^* & b^* & E_2 - E \end{vmatrix} = \\
&= (E_1 - E)\left[(E_1 - E)(E_2 - E) - |b|^2\right] + a\left[0 - a^*(E_1 - E)\right] = \\
&= (E_1 - E)^2(E_2 - E) - (E_1 - E)(|b|^2 + |a|^2).
\end{aligned} \tag{5.14}$$

So, $E = E_1$ or $(E_1 - E)(E_2 - E) - (|b|^2 + |a|^2) = 0$ i.e.

$$\begin{aligned}
E^2 &- (E_1 + E_2)E + E_1E_2 - (|a|^2 + |b|^2) = 0 \Rightarrow \\
E &= \frac{E_1 + E_2}{2} \pm \sqrt{\frac{E_1 + E_2}{2}^2 - E_1E_2 + |a|^2 + |b|^2} =
\end{aligned}$$

$$= \frac{E_1 + E_2}{2} \pm \sqrt{\frac{E_1 - E_2}{2}^2 + |a|^2 + |b|^2}. \tag{5.15}$$

Since $|a|^2 + |b|^2$ is small we can expand the square root and write the three energy levels as:

$$\begin{aligned} E &= E_1, \\ E &= \frac{E_1 + E_2}{2} + \frac{E_1 - E_2}{2}\left(1 + \tfrac{1}{2}(|a|^2 + |b|^2)(\frac{2}{E_1 - E_2})^2 + \ldots\right) = \\ &= E_1 + \frac{|a|^2 + |b|^2}{E_1 - E_2}, \\ E &= \frac{E_1 + E_2}{2} - \frac{E_1 - E_2}{2}(\ldots) = E_2 - \frac{|a|^2 + |b|^2}{E_1 - E_2}. \end{aligned} \tag{5.16}$$

(b) Non degenerate perturbation theory to 2'nd order. The basis we use is

$$|\,1\,\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \qquad |\,2\,\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \qquad |\,3\,\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

The matrix elements of the perturbation $V = \begin{pmatrix} 0 & 0 & a \\ 0 & 0 & b \\ a^* & b^* & 0 \end{pmatrix}$ are

$$\langle\,1\,|\,V\,|\,3\,\rangle = a, \qquad \langle\,2\,|\,V\,|\,3\,\rangle = b, \qquad \langle\,1\,|\,V\,|\,2\,\rangle = \langle\,k\,|\,V\,|\,k\,\rangle = 0.$$

Since $\Delta_k^{(1)} = \langle\,k\,|\,V\,|\,k\,\rangle = 0$ 1'st order gives nothing. But the 2'nd order shifts are

$$\begin{aligned} \Delta_1^{(2)} &= \sum_{k \neq 1} \frac{|V_{k1}|^2}{E_1^0 - E_k^0} = \frac{|\langle\,3\,|\,V\,|\,1\,\rangle|^2}{E_1 - E_2} = \frac{|a|^2}{E_1 - E_2}, \\ \Delta_2^{(2)} &= \sum_{k \neq 2} \frac{|V_{k2}|^2}{E_2^0 - E_k^0} = \frac{|\langle\,3\,|\,V\,|\,2\,\rangle|^2}{E_1 - E_2} = \frac{|b|^2}{E_1 - E_2}, \\ \Delta_3^{(2)} &= \sum_{k \neq 3} \frac{|V_{k3}|^2}{E_3^0 - E_k^0} = \frac{|a|^2}{E_2 - E_1} + \frac{|b|^2}{E_2 - E_1} = -\frac{|a|^2 + |b|^2}{E_1 - E_2}. \end{aligned} \tag{5.17}$$

The unperturbed problem has two (degenerate) states $|1\rangle$ and $|2\rangle$ with energy E_1, and one (non-degenerate) state $|3\rangle$ with energy E_2. Using non-degenerate perturbation theory we expect only the correction to E_2 (i.e. $\Delta_3^{(2)}$) to give the correct result, and indeed this turns out to be the case.

(c) To find the correct energy shifts for the two degenerate states we have to use degenerate perturbation theory. The V-matrix for the degenerate subspace is $\begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$, so 1'st order pert.thy. will again give nothing. We have to go to 2'nd order. The problem we want to solve is $(H_0 + V)\,|\,l\,\rangle = E\,|\,l\,\rangle$ using the expansion

$$|\,l\,\rangle = |\,l^0\,\rangle + |\,l^1\,\rangle + \ldots \qquad E = E^0 + \Delta^{(1)} + \Delta^{(2)} + \ldots \tag{5.18}$$

where $H_0\,|\,l^0\,\rangle = E^0\,|\,l^0\,\rangle$. Note that the superscript index in a bra or ket denotes which order it has in the perturbation expansion. Different solutions to the full problem are denoted by different l's. Since the (sub-) problem we are now solving is 2-dimensional we expect to find two solutions corresponding to $l = 1, 2$. Inserting the expansions in (5.18) leaves us with

$$\begin{aligned} &(E^0 - H_0)\left[\,|\,l^0\,\rangle + |\,l^1\,\rangle + \ldots\right] = \\ &\qquad (V - \Delta^{(1)} - \Delta^{(2)}\ldots)\left[\,|\,l^0\,\rangle + |\,l^1\,\rangle + \ldots\right]. \end{aligned} \tag{5.19}$$

At first order in the perturbation this says:

$$(E^0 - H_0)\,|\,l^1\,\rangle = (V - \Delta^{(1)})\,|\,l^0\,\rangle,$$

where of course $\Delta^{(1)} = 0$ as noted above. Multiply this from the left with a bra $\langle\,k^0\,|$ from outside the deg. subspace

$$\begin{aligned} &\langle\,k^0\,|\,E^0 - H_0\,|\,l^1\,\rangle = \langle\,k^0\,|\,V\,|\,l^0\,\rangle \\ &\Rightarrow |\,l^1\,\rangle = \sum_{k \neq D} \frac{|\,k^0\,\rangle\langle\,k^0\,|\,V\,|\,l^0\,\rangle}{E^0 - E_k}. \end{aligned} \tag{5.20}$$

This expression for $|\,l^1\,\rangle$ we will use in the 2'nd order equation from (5.19)

$$(E^0 - H_0)\,|\,l^2\,\rangle = V\,|\,l^1\,\rangle - \Delta^{(2)}\,|\,l^0\,\rangle.$$

To get rid of the left hand side, multiply with a degenerate bra $\langle\,m^0\,|$ $(H_0\,|\,m^0\,\rangle = E^0\,|\,m^0\,\rangle)$

$$\langle\,m^0\,|\,E^0 - H_0\,|\,l^2\,\rangle = 0 = \langle\,m^0\,|\,V\,|\,l^1\,\rangle - \Delta^{(2)}\langle\,m^0\,|\,l^0\,\rangle.$$

Inserting the expression (5.20) for $|\, l^1 \rangle$ we get

$$\sum_{k\neq D} \frac{\langle\, m^0 \,|\, V \,|\, k^0 \,\rangle\langle\, k^0 \,|\, V \,|\, l^0 \,\rangle}{E^0 - E_k} = \Delta^{(2)}\langle\, m^0 \,|\, l^0 \,\rangle.$$

To make this look like an eigenvalue equation we have to insert a **1**:

$$\sum_{n\in D}\sum_{k\neq D} \frac{\langle\, m^0 \,|\, V \,|\, k^0 \,\rangle\langle\, k^0 \,|\, V \,|\, n^0 \,\rangle}{E^0 - E_k}\langle\, n^0 \,|\, l^0 \,\rangle = \Delta^{(2)}\langle\, m^0 \,|\, l^0 \,\rangle.$$

Maybe it looks more familiar in matrix form

$$\sum_{n\in D} M_{mn} x_n = \Delta^{(2)} x_m$$

where

$$\begin{aligned} M_{mn} &= \sum_{k\neq D} \frac{\langle\, m^0 \,|\, V \,|\, k^0 \,\rangle\langle\, k^0 \,|\, V \,|\, n^0 \,\rangle}{E^0 - E_k}, \\ x_m &= {}^0\langle\, m \,|\, l^0 \,\rangle \end{aligned}$$

are expressed in the basis defined by $|\, l^0 \,\rangle$. Evaluate M in the degenerate subspace basis $D = \{\,|\,1\,\rangle,\,|\,2\,\rangle\}$

$$\begin{aligned} M_{11} &= \frac{V_{13}V_{31}}{E_1 - E_3^0} = \frac{|a|^2}{E_1 - E_2}, \qquad M_{12} = \frac{V_{13}V_{32}}{E_1 - E_3^0} = \frac{ab^*}{E_1 - E_2}, \\ M_{21} &= \frac{V_{23}V_{31}}{E_1 - E_3^0} = \frac{a^*b}{E_1 - E_2}, \qquad M_{22} = \frac{|V_{23}|^2}{E_1 - E_3^0} = \frac{|b|^2}{E_1 - E_2}. \end{aligned}$$

With this explicit expression for M, solve the eigenvalue equation (define $\lambda = \Delta^{(2)}(E_1 - E_2)$, and take out a common factor $\frac{1}{E_1 - E_2}$)

$$\begin{aligned} 0 &= det \begin{pmatrix} |a|^2 - \lambda & ab^* \\ a^*b & |b|^2 - \lambda \end{pmatrix} = \\ &= (|a|^2 - \lambda)(|b|^2 - \lambda) - |a|^2|b|^2 = \\ &= \lambda^2 - (|a|^2 + |b|^2)\lambda \\ &\Rightarrow \lambda = 0, |a|^2 + |b|^2 \\ &\Rightarrow \Delta_1^{(2)} = 0 \qquad \Delta_2^{(2)} = \frac{|a|^2 + |b|^2}{E_1 - E_2}. \end{aligned} \tag{5.21}$$

From before we knew the non-degenerate energy shift, and now we see that degenerate perturbation theory leads to the correct shifts for the other two levels. Everything is as we would have expected.

5.3 A one-dimensional harmonic oscillator is in its ground state for $t < 0$. For $t \geq 0$ it is subjected to a time-dependent but spatially uniform *force* (not potential!) in the x-direction,

$$F(t) = F_0 e^{-t/\tau}$$

(a) Using time-dependent perturbation theory to first order, obtain the probability of finding the oscillator in its first excited state for $t > 0$. Show that the $t \to \infty$ (τ finite) limit of your expression is independent of time. Is this reasonable or surprising?

(b) Can we find higher excited states?
[**You may use** $\langle n'|x|n\rangle = \sqrt{\hbar/2m\omega}(\sqrt{n+1}\delta_{n',n+1} + \sqrt{n}\delta_{n',n-1})$.]

(a) The problem is defined by

$$H_0 = \frac{p^2}{2m} + \frac{m\omega 2x^2}{2} \qquad V(t) = -F_0 x e^{-t/\tau} \quad (F = -\frac{\partial V}{\partial x})$$

At $t = 0$ the system is in its ground state $|\,\alpha, 0\,\rangle = |\,0\,\rangle$. We want to calculate

$$\begin{aligned} |\,\alpha, t\,\rangle &= \sum_n c_n(t) e^{-E_n t/\hbar}\,|\,n\,\rangle \\ E_n^0 &= \hbar\omega(n + \tfrac{1}{2}) \end{aligned}$$

where we get $c_n(t)$ from its diff. eqn. (S. 5.5.15):

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}c_n(t) &= \sum_m V_{nm} e^{i\omega_{nm}t} c_m(t) \\ V_{nm} &= \langle\, n\,|\,V\,|\,m\,\rangle \\ \omega_{nm} &= \frac{E_n - E_m}{\hbar} = \omega(n-m) \end{aligned} \tag{5.22}$$

We need the matrix elements V_{nm}

$$\begin{aligned} V_{nm} &= \langle\, n\,| - F_0 x e^{-t/\tau}\,|\,m\,\rangle = -F_0 e^{-t/\tau}\langle\, n\,|\,x\,|\,m\,\rangle = \\ &= -F_0 e^{-t/\tau}\sqrt{\frac{\hbar}{2m\omega}}(\sqrt{m}\delta_{n,m-1} + \sqrt{m+1}\delta_{n,m+1}). \end{aligned}$$

Put it back into (5.22)

$$i\hbar\frac{\partial}{\partial t}c_n(t) = -F_0 e^{-t/\tau}\sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n+1}e^{-i\omega t}c_{n+1}(t) + \sqrt{n}e^{i\omega t}c_{n-1}(t)\right).$$

Perturbation theory means expanding $c_n(t) = c_n^{(0)} + c_n^{(1)} + \ldots$, and to zeroth order this is

$$\frac{\partial}{\partial t}c_n^{(0)}(t) = 0 \quad \Rightarrow c_n^{(0)} = \delta_{n0}$$

To first order we get

$$\begin{aligned} c_n^{(1)}(t) &= \frac{1}{i\hbar}\int_0^t dt' \sum_m V_{nm}(t')e^{i\omega_{nm}t'}c_m^{(0)} = \\ &= -\frac{F_0}{i\hbar}\sqrt{\frac{\hbar}{2m\omega}}\int_0^t dt' e^{-t/\tau}\left(\sqrt{n+1}e^{-i\omega t'}c_{n+1}^{(0)}(t) + \sqrt{n}e^{i\omega t'}c_{n-1}^{(0)}(t)\right) \end{aligned}$$

We get one non-vanishing term for $n = 1$, i.e. at first order in perturbation theory with the H.O. in the ground state at $t = 0$ there is just one non-zero expansion coefficient

$$\begin{aligned} c_1^{(1)}(t) &= -\frac{F_0}{i\hbar}\sqrt{\frac{\hbar}{2m\omega}}\int_0^t dt' e^{i\omega t' - t'/\tau}\sqrt{1}\delta_{1-1,0} = \\ &= -\frac{F_0}{i\hbar}\sqrt{\frac{\hbar}{2m\omega}}\left[\frac{1}{i\omega - \frac{1}{\tau}}e^{(i\omega - \frac{1}{\tau})t'}\right]_0^t \\ &= \frac{F_0}{i\hbar}\sqrt{\frac{\hbar}{2m\omega}}\frac{1}{i\omega - \frac{1}{\tau}}\left(1 - e^{(i\omega - \frac{1}{\tau})t}\right) \end{aligned}$$

and

$$|\,\alpha, t\,\rangle = \sum_n c_n^{(1)}(t)e^{\frac{-iE_n t}{\hbar}}\,|\,n\,\rangle = c_1^{(1)}(t)e^{\frac{-iE_1 t}{\hbar}}\,|\,1\,\rangle.$$

The probability of finding the H.O. in $|\,1\,\rangle$ is

$$|\langle\,1\,|\,\alpha, t\,\rangle|^2 = |c_1^{(1)}(t)|^2.$$

As $t \to \infty$

$$c_1^{(1)} \to \frac{F_0}{i\hbar}\sqrt{\frac{\hbar}{2m\omega}}\frac{1}{i\omega - \frac{1}{\tau}} = const.$$

This is of course reasonable since applying a static force means that the system asymptotically finds a new equilibrium.

(b) As remarked earlier there are no other non-vanishing c_n's at first order, so no higher excited states can be found. However, going to higher order in perturbation theory such states will be excited.

5.4 Consider a composite system made up of two spin $\frac{1}{2}$ objects. for $t < 0$, the Hamiltonian does not depend on spin and can be taken to be zero by suitably adjusting the energy scale. For $t > 0$, the Hamiltonian is given by

$$H = \left(\frac{4\Delta}{\hbar^2}\right) \vec{S}_1 \cdot \vec{S}_2.$$

Suppose the system is in $|+-\rangle$ for $t \leq 0$. Find, as a function of time, the probability for being found in each of the following states $|++\rangle$, $|+-\rangle$, $|-+\rangle$, $|--\rangle$:

(a) By solving the problem exactly.

(b) By solving the problem assuming the validity of first-order time-dependent perturbation theory with H as a perturbation switched on at $t = 0$. Under what condition does (b) give the correct results?

(a) The basis we are using is of course $|S_{1z}, S_{2z}\rangle$. Expand the interaction potential in this basis:

$$\begin{aligned}
\vec{S}_1 \cdot \vec{S}_2 &= S_{1x}S_{2x} + S_{1y}S_{2y} + S_{1z}S_{2z} = \{\text{in this basis}\} \\
&= \frac{\hbar^2}{4}\Big[(|+\rangle\langle-| + |-\rangle\langle+|)_1(|+\rangle\langle-| + |-\rangle\langle+|)_2 + \\
&+ i^2(-|+\rangle\langle-| + |-\rangle\langle+|)_1(-|+\rangle\langle-| + |-\rangle\langle+|)_2 + \\
&+ (|+\rangle\langle+| - |-\rangle\langle-|)_1(|+\rangle\langle+| - |-\rangle\langle-|)_2\Big] = \\
&= \frac{\hbar^2}{4}\Big[|++\rangle\langle--| + |+-\rangle\langle-+| + \\
&\qquad + |-+\rangle\langle+-| + |--\rangle\langle++| + \\
&+ i^2(|++\rangle\langle--| - |+-\rangle\langle-+| + \\
&\qquad - |-+\rangle\langle+-| + |--\rangle\langle++|) +
\end{aligned}$$

$$
\begin{aligned}
+ \quad & |++\rangle\langle++| - |+-\rangle\langle+-| + \\
& -|-+\rangle\langle-+| + |--\rangle\langle--| \Big] =
\end{aligned}
$$

In matrix form this is (using $|1\rangle = |++\rangle$ $|2\rangle = |+-\rangle$ $|3\rangle = |-+\rangle$ $|4\rangle = |--\rangle$)

$$
H = \Delta \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{5.23}
$$

This basis is nice to use, since even though the problem is 4-dimensional we get a 2-dimensional matrix to diagonalize. Lucky us! (Of course this luck is due to the rotational invariance of the problem.)

Now diagonalize the 2×2 matrix to find the eigenvalues and eigenkets

$$
\begin{aligned}
0 \quad = \quad & det \begin{pmatrix} -1-\lambda & 2 \\ 2 & -1-\lambda \end{pmatrix} = (-1-\lambda)^2 - 4 = \lambda^2 + 2\lambda - 3 \\
& \Rightarrow \lambda = 1, -3
\end{aligned}
$$

<u>$\lambda = 1$:</u>

$$
\begin{pmatrix} -1 & 2 \\ 2 & -1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} x \\ y \end{pmatrix}
$$

$$
\Rightarrow -x + 2y = x \Rightarrow x = y = \frac{1}{\sqrt{2}}
$$

<u>$\lambda = -3$:</u>

$$
\begin{pmatrix} -1 & 2 \\ 2 & -1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = -3 \begin{pmatrix} x \\ y \end{pmatrix}
$$

$$
\Rightarrow -x + 2y = -3x \Rightarrow x = -y = \frac{1}{\sqrt{2}}
$$

So, the complete spectrum is:

$$
\begin{cases}
|++\rangle, |--\rangle, \frac{1}{\sqrt{2}}(|+-\rangle + |-+\rangle & \text{with energy } \Delta \\[2ex]
\frac{1}{\sqrt{2}}(|+-\rangle - |-+\rangle & \text{with energy } -3\Delta
\end{cases}
$$

This was a cumbersome but straightforward way to calculate the spectrum. A smarter way would have been to use $\vec{S} = \vec{S}_1 + \vec{S}_2$ to find

$$\vec{S}^2 \;=\; S^2 = \vec{S}_1^2 + \vec{S}_2^2 + 2\vec{S}_1 \cdot \vec{S}_2 \quad \Rightarrow \quad \vec{S}_1 \cdot \vec{S}_2 = \tfrac{1}{2}\left(\vec{S}^2 - \vec{S}_1^2 - \vec{S}_2^2\right)$$

We know that $\vec{S}_1^2 = \vec{S}_2^2 = \hbar^2 \frac{1}{2}\left(\frac{1}{2}+1\right) = \frac{3\hbar^2}{4}$ so

$$\vec{S}_1 \cdot \vec{S}_2 = \tfrac{1}{2}\left(S^2 - \frac{3\hbar^2}{2}\right)$$

Also, we know that two spin$\frac{1}{2}$ systems add up to one triplet (spin 1) and one singlet (spin 0), i.e.

$$\begin{array}{ll} S = 1\,(3 \text{ states}) \Rightarrow & \vec{S}_1 \cdot \vec{S}_2 = \frac{1}{2}(\hbar^2 1(1+1) - \frac{3\hbar^2}{2}) = \frac{1}{4}\hbar^2 \\ S = 0\,(1 \text{ state}) \Rightarrow & \vec{S}_1 \cdot \vec{S}_2 = \frac{1}{2}(-\frac{3\hbar^2}{2}) = -\frac{3}{4}\hbar^2 \end{array} . \tag{5.24}$$

Since $H = \frac{4\Delta}{\hbar^2}\vec{S}_1 \cdot \vec{S}_2$ we get

$$\begin{aligned} \text{E(spin=1)} &= \frac{4\Delta}{\hbar^2}\frac{1\hbar^2}{4} = \Delta, \\ \text{E(spin=0)} &= \frac{4\Delta}{\hbar^2}\frac{-3\hbar^2}{4} = -3\Delta. \end{aligned} \tag{5.25}$$

From Clebsch-Gordan decomposition we know that $\Big\{ |\,++\,\rangle, |\,--\,\rangle, \frac{1}{\sqrt{2}}(|\,+-\,\rangle + |\,-+\,\rangle) \Big\}$ are spin 1, and $\frac{1}{\sqrt{2}}(|\,+-\,\rangle - |\,-+\,\rangle)$ is spin 0!

Let's get back on track and find the *dynamics*. In the new basis H is diagonal and time-independent, so we can use the simple form of tthe time-evolution operator:

$$\mathcal{U}(t, t_0) = exp\left\{-\frac{i}{\hbar}H(t-t_0)\right\}.$$

The initial state was $|\,+-\,\rangle$. In the new basis

$$\Big\{ \,|\,1\,\rangle = |\,++\,\rangle, |\,2\,\rangle = |\,--\,\rangle, |\,3\,\rangle = \frac{1}{\sqrt{2}}(|\,+-\,\rangle + |\,-+\,\rangle), \\ |\,4\,\rangle = \frac{1}{\sqrt{2}}(|\,+-\,\rangle - |\,-+\,\rangle)\,\Big\}$$

the initial state is

$$|\,+-\,\rangle = \frac{1}{\sqrt{2}}(\,|\,3\,\rangle + \,|\,4\,\rangle).$$

Acting with $\mathcal{U}(t,0)$ on that we get

$$\begin{aligned}
|\,\alpha,t\,\rangle &= \frac{1}{\sqrt{2}}exp\left\{-\frac{i}{\hbar}Ht\right\}(\,|\,3\,\rangle + \,|\,4\,\rangle) = \\
&= \frac{1}{\sqrt{2}}\left[exp\left\{-\frac{i}{\hbar}\Delta t\right\}\,|\,3\,\rangle + exp\left\{\frac{3i}{\hbar}\Delta t\right\}\,|\,4\,\rangle\right] = \\
&= \left[exp\left\{\frac{-i\Delta t}{\hbar}\right\}\frac{1}{\sqrt{2}}(\,|\,+-\,\rangle + \,|\,-+\,\rangle)+\right. \\
&\qquad \left. +exp\left\{\frac{3i\Delta t}{\hbar}\right\}\frac{1}{\sqrt{2}}(\,|\,+-\,\rangle - \,|\,-+\,\rangle)\right] = \\
&= \tfrac{1}{2}\left[(e^{-i\omega t} + e^{3i\omega t})\,|\,+-\,\rangle + (e^{-i\omega t} + e^{3i\omega t})\,|\,-+\,\rangle\right]
\end{aligned}$$

where

$$\omega \equiv \frac{\Delta}{\hbar}. \tag{5.26}$$

The probability to find the system in the state $|\,\beta\,\rangle$ is as usual $|\langle\,\beta\,|\,\alpha,t\,\rangle|^2$

$$\begin{cases}
\langle\,++\,|\,\alpha,t\,\rangle = \langle\,--\,|\,\alpha,t\,\rangle = 0 \\
|\langle\,+-\,|\,\alpha,t\,\rangle|^2 = \frac{1}{4}\left(2 + e^{4i\omega t} + e^{-4i\omega t}\right) = \frac{1}{2}\left(1 + cos4\omega t\right) \simeq 1 - 4(\omega t)^2\ldots \\
|\langle\,-+\,|\,\alpha,t\,\rangle|^2 = \frac{1}{4}\left(2 - e^{4i\omega t} - e^{-4i\omega t}\right) = \frac{1}{2}\left(1 - cos4\omega t\right) \simeq 4(\omega t)^2\ldots
\end{cases}$$

(b) First order perturbation theory (use S. 5.6.17):

$$\begin{aligned}
c_n^{(0)} &= \delta_{ni}, \\
c_n^{(1)}(t) &= \frac{-i}{\hbar}\int_{t_0}^{t} dt' e^{i\omega_{ni}t'}V_{ni}(t').
\end{aligned} \tag{5.27}$$

Here we have (using the original basis) $H_0 = 0$, V given by (5.23)

$$|\,i\,\rangle = |\,+-\,\rangle,$$

$$\begin{aligned} |\, f\,\rangle &= |\, -+\rangle, \\ \omega_{ni} &= \frac{E_n - E_i}{\hbar} = \{E_n = 0\} = 0, \\ V_{fi} &= 2\Delta, \\ V_{ni} &= 0, \quad n \neq f. \end{aligned}$$

Inserting this into (5.27) yields

$$\begin{aligned} c_i^{(0)} &= c_{|+-\rangle}^{(0)} = 1, \\ c_f^{(1)} &= c_{|-+\rangle}^{(1)} = -\frac{i}{\hbar}\int_0^t dt 2\Delta = -2i\omega t. \end{aligned} \tag{5.28}$$

as the only non-vanishing coefficients up to first order. The probability of finding the system in $|\, --\rangle$ or $|\, ++\rangle$ is thus obviously zero, whereas for the other two states

$$\begin{aligned} P(|\, +-\rangle) &= 1 \\ P(|\, -+\rangle) &= |c_f^{(1)}(t) + c_f^{(2)}(t) + \ldots|^2 = |2i\omega t|^2 = 4(\omega t)^2 \end{aligned}$$

to first order, in correspondence with the exact result.

The approximation breaks down when $\omega t \ll 1$ is no longer valid, so for a given t:

$$\omega t \ll 1 \Rightarrow \Delta \ll \frac{\hbar}{t}.$$

5.5 The ground state of a hydrogen atom ($n = 1, l = 0$) is subjected to a time-dependent potential as follows:

$$V(\vec{x}, t) = V_0 \cos(kz - \omega t).$$

Using time-dependent perturbation theory, obtain an expression for the transition rate at which the electron is emitted with momentum $\vec{p}$. Show, in particular, how you may compute the angular distribution of the ejected electron (in terms of θ and ϕ defined with respect to the z-axis). Discuss *briefly* the similarities and the differences between this problem and the (more realistic) photoelectric effect. (*note:* For the initial wave function use

$$\Psi_{n=1,l=0}(\vec{x}) = \frac{1}{\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{\frac{3}{2}} e^{-Zr/a_0}.$$

If you have a normalization problem, the final wave function may be taken to be

$$\Psi_f(\vec{x}) = \left(\frac{1}{L^{\frac{3}{2}}}\right) e^{i\vec{p}\cdot\vec{x}/\hbar}$$

with L very large, but you should be able to show that the observable effects are independent of L.)

To begin with the atom is in the $n = 1, l = 0$ state. At $t = 0$ the perturbation

$$V = V_0 \, cos(kz - \omega t)$$

is turned on. We want to find the transition rate at which the electron is emitted with momentum $\vec{p}_f$. The initial wave-function is

$$\Psi_i(\vec{x}) = \frac{1}{\sqrt{\pi}} \left(\frac{1}{a_0}\right)^{3/2} e^{-r/a_0}$$

and the final wave-function is

$$\Psi_f(\vec{x}) = \left(\frac{1}{L^{3/2}}\right) e^{i\vec{p}\cdot\vec{x}/\hbar}.$$

The perturbation is

$$\begin{aligned} V &= V_0 \left[e^{i(kz-\omega t)} + e^{-i(kz-\omega t)} \right] \\ &= \mathcal{V} e^{i\omega t} + \mathcal{V}^\dagger e^{-i\omega t}. \end{aligned} \tag{5.29}$$

Time-dependent perturbation theory (S.5.6.44) gives us the transition rate

$$\mathrm{w}_{i\to n} = \frac{2\pi}{\hbar} \left| \mathcal{V}^\dagger_{ni} \right|^2 \delta(E_n - (E_i + \hbar\omega))$$

because the atom absorbs a photon $\hbar\omega$. The matrix element is

$$\left| \mathcal{V}^\dagger_{ni} \right|^2 = \frac{V_0^2}{4} \left| \left(e^{ikz} \right)_{ni} \right|^2$$

and

$$\begin{aligned} \left(e^{ikz} \right)_{ni} &= \langle \vec{k}_f \,|\, e^{ikz} \,|\, n = 1, l = 0 \,\rangle = \int d^3x \langle \vec{k}_f \,|\, e^{ikz} \,|\, x \,\rangle \langle \, x \,|\, n = 1, l = 0 \,\rangle = \\ &= \int d^3x \frac{e^{-i\vec{k}_f\cdot\vec{x}}}{L^{3/2}} e^{ikx_3} \frac{1}{\sqrt{\pi}} \left(\frac{1}{a_0}\right)^{3/2} e^{-r/a_0} = \\ &= \frac{1}{L^{3/2}\sqrt{\pi} a_0^{3/2}} \int d^3x e^{-i(\vec{k}_f\cdot\vec{x} - kx_3) - r/a_0}. \end{aligned} \tag{5.30}$$

So $\left(e^{ikz}\right)_{ni}$ is the 3D Fourier transform of the initial wave-function (and some constant) with $\vec{q} = \vec{k}_f - k\vec{e}_z$. That can be extracted from (Sakurai problem 5.39)

$$\left(e^{ikz}\right)_{ni} = \frac{64\pi^2}{L^3 a_0^5} \frac{1}{\left[\frac{1}{a_0^2} + (\vec{k}_f - k\vec{e}_z)^2\right]^4}$$

The transition rate is understood to be integrated over the density of states. We need to get that as a function of $\vec{p}_f = \hbar\vec{k}_f$. As in (S.5.7.31), the volume element is

$$n^2 dn d\Omega = n^2 d\Omega \frac{dn}{dp_f} dp_f.$$

Using

$$k_f^2 = \frac{p_f^2}{\hbar^2} = \frac{n^2(2\pi)^2}{L^2}$$

we get

$$\frac{dn}{dp_f} = \frac{1}{2n}\frac{2L^2 p_f}{(2\pi\hbar)^2} = \frac{2\pi\hbar}{Lp_f}\frac{L^2 p_f}{(2\pi\hbar)^2} = \frac{L}{2\pi\hbar}$$

which leaves

$$n^2 dn d\Omega = \frac{L^3 k_f^2}{(2\pi)^3\hbar} d\Omega dp_f = \frac{L^3 p_f^2}{(2\pi\hbar)^3} d\Omega dp_f$$

and this is the sought density.
Finally,

$$\mathrm{w}_{i\to\vec{p}_f} = \frac{2\pi}{\hbar}\frac{V_0^2}{4}\frac{64\pi^2}{L^3 a_0^5}\frac{1}{\left[\frac{1}{a_0^2} + (\vec{k}_f - k\vec{e}_z)^2\right]^4}\frac{L^3 p_f^2}{(2\pi\hbar)^3} d\Omega dp_f.$$

Note that the L's cancel. The angular dependence is in the denominator:

$$\begin{aligned}\left(\vec{k}_f - k\vec{e}_z\right)^2 &= \left[\left(|k_f|cos\theta - k\right)\vec{e}_z + |k_f|sin\theta\left(cos\varphi\vec{e}_x + sin\varphi\vec{e}_y\right)\right]^2 = \\ &= |k_f|^2 cos^2\theta + k^2 - 2k|k_f|cos\theta + |k_f|^2 sin^2\theta = \\ &= k_f^2 + k^2 - 2k|k_f|cos\theta. \qquad (5.31)\end{aligned}$$

In a comparison between this problem and the photoelectric effect as discussed in (S. 5.7) we note that since there is no polarization vector involved, w has no dependence on the azimuthal angle ϕ. On the other hand we did not make any dipole approximation but performed the x-integral exactly.