Chapter 5 problems

Problem 5.1

(a) Write down the Hamiltonian for a particle of mass m in a one-dimensional harmonic oscillator potential in terms of momentum $\hat{p}_x$ and position $\hat{x}$.

(b) If operators

$$\hat{b} = \left(\frac{m\omega}{2\hbar}\right)^{1/2}\left(\hat{x} + \frac{i\hat{p}_x}{m\omega}\right)$$

$$\hat{b}^\dagger = \left(\frac{m\omega}{2\hbar}\right)^{1/2}\left(\hat{x} - \frac{i\hat{p}_x}{m\omega}\right)$$

are defined show that the Hamiltonian can be expressed as

$$\hat{H} = \frac{\hbar\omega}{2}(\hat{b}\hat{b}^\dagger + \hat{b}^\dagger\hat{b})$$

(c) Derive the commutation relation $[\hat{b}, \hat{b}^\dagger]$ by writing out the differential form of $\hat{b}$ and $\hat{b}^\dagger$ and operating on a dummy wave function.

(d) Using the result from (c) show that the Hamiltonian is

$$\hat{H} = \hbar\omega\left(\hat{b}^\dagger\hat{b} + \frac{1}{2}\right)$$

Problem 5.2

(a) Find the expectation value of position and momentum for the first excited state for a particle of mass m in a one-dimensional harmonic oscillator potential.

(b) Find the value of the product in uncertainty in position Δx and momentum Δp_x for the first excited state of a particle of mass m in a one-dimensional harmonic oscillator potential.

Problem 5.3

Often an operator $\hat{A}$ is time-independent but the corresponding numerical value of the observable A has a spread in values ΔA about an average value $\langle A(t)\rangle$ and varies with time because the system is described by a wave function $\psi(x, t)$ which is not an eigenstate. The change in $\langle A(t)\rangle$ during the time interval Δt is the slope $\frac{d}{dt}\langle A(t)\rangle$ multiplied by Δt. Hence, the exact time t at which the numerical value of the observable A passes through a specific value will actually have a spread in values Δt such that

$$\Delta t = \Delta A / \left|\frac{d}{dt}\langle A\rangle\right|$$

(a) Use the generalized uncertainty relation $\Delta A \Delta B \geq \left|\frac{1}{2}\langle[\hat{A}, \hat{B}]\rangle\right|$ for time independent operators $\hat{A}$ and $\hat{B}$ to show that $\Delta E \Delta t \geq \frac{\hbar}{2}$.

(b) Show that the spread in photon number Δn and phase $\Delta\phi$ for light of frequency ω is

$$\Delta n \Delta\phi \geq \frac{1}{2}$$

and that for a Poisson distribution of such photons

$$\Delta\phi \geq \frac{1}{2\sqrt{\langle n\rangle}}$$

(c) Apply the results in (b) and determine Δn and $\Delta\phi$ for a 100 ps pulse of λ = 1500 nm wavelength light from a 10 μW source.

Problem 5.4

A particle of charge e, mass m, and momentum p oscillates in a one-dimensional harmonic potential $V(x) = m\omega_0^2x^2/2$ and is subject to an oscillating electric field $|\mathbf{E}|\cos(\omega t)$.

(a) Write down the Hamiltonian of the system.

(b) Find $\frac{\mathrm{d}}{\mathrm{d}t}\langle x\rangle$.

(c) Find $\frac{\mathrm{d}}{\mathrm{d}t}\langle p\rangle$ and show that $\frac{\mathrm{d}}{\mathrm{d}t}\langle p\rangle = -\langle\frac{\mathrm{d}}{\mathrm{d}x}V(x)\rangle$. Describe the conditions when the quantum mechanical result $m\frac{\mathrm{d}^2}{\mathrm{d}t^2}\langle x\rangle = -\langle\frac{\mathrm{d}}{\mathrm{d}x}V(x)\rangle$ is the same as Newton's second law in which force on a particle is $F = m\frac{\mathrm{d}^2x}{\mathrm{d}t^2} = -\frac{\mathrm{d}}{\mathrm{d}x}V(x)$

(d) Find $\frac{\mathrm{d}}{\mathrm{d}t}\langle H\rangle$.

(e) Use your results in (b) and (c) to find the time dependence of the expectation value of position. What happens to the maximum value of $\langle x\rangle$ as a function of time when $\omega_0 = \omega$ and when ω is close in value to ω_0?

Problem 5.5

Express the total ground state energy of a one dimensional harmonic oscillator as the sum of potential and kinetic energy terms involving displacement Δx and momentum Δp_x. Assume the minimum uncertainty relation $\Delta x\Delta p_x = \hbar/2$ and find the ground state energy of the system.

Problem 5.6

(a) What is the minimum energy E_0 stored in a resonant LC circuit?

(b) Find an expression for the value of capacitance C if the charging energy associated with the coulomb blockade for the capacitor is the same as E_0.

(c) If the inductor has value $L = 10^{-8}$ H, what is the resonant oscillation frequency of the circuit and what is the value of the capacitance C?

(d) If the current in the circuit can be measured to an accuracy of one electron per oscillation, how accurately can the voltage of the circuit be determined?

Problem 5.7

An electron is confined by a one-dimensional harmonic potential.

(a) What is the value of the mean electric-field dipole moment when the electron is in eigenstate $|\phi_n\rangle$?

(b) What is the value of the mean electric-field dipole moment in the presence of a uniform static electric field **E** in the *x* direction?

(c) What is the static electric susceptibility and permittivity of the system?

(d) Estimate the frequency dependent electric susceptibility of the system.

Problem 5.8

The annihilation operator for a particle of mass *m* in a one dimensional harmonic oscillator potential is

$$\hat{b} = \left(\frac{m\omega}{2\hbar}\right)^{1/2}\left(\hat{x} + \frac{i\hat{p}_x}{m\omega}\right)$$

where $\hat{x}$ is the position operator and $\hat{p}_x$ is the momentum operator.

(a) Show that $\langle n|\hat{b}^{\dagger}|m\rangle = \langle m|\hat{b}|n\rangle^*$ and $\langle \hat{b}^{\dagger} n|\hat{b}^{\dagger} n\rangle = \langle n|\hat{b}\hat{b}^{\dagger} n\rangle$.

(b) Show that $\langle m|\hat{b}^{\dagger}|n\rangle \neq \langle n|\hat{b}^{\dagger}|m\rangle^*$ and hence that $\hat{b}^{\dagger}$ is *not* a Hermitian operator.

(c) Show that the number operator $\hat{n} = \hat{b}^{\dagger}\hat{b}$ is Hermitian.

(d) Show that the position operator $\hat{x}$ and the momentum operator $\hat{p}_x$ are Hermitian operators.

Problem 5.9

(a) Numerically evaluate and plot the time evolution of expectation value of position $\langle x(t)\rangle$, probability $|\psi(x, t)|^2$, and current density $J(x, t)$, for a superposition of the ground-state, ψ_0, and first excited state, ψ_1, of an electron confined to motion in a one-dimensional rectangular potential well of thickness *L* and infinite potential elsewhere. The superposition state is

$$\psi = \frac{1}{\sqrt{N+1}}\sum_{n=0}^{N}\psi_n$$

where $N = 1$. Repeat the calculation but now for a superposition state in which $N = 9$ and explain the differences in the results of the two calculations.

What is the value of the guaranteed full revival time and what is the smallest possible time between full revivals?

(b) Numerically evaluate the time evolution of $\langle x(t)\rangle$ and $|\psi(x, t)|^2$ for a superposition of the ground-state and first excited state of the harmonic oscillator.

(c) Numerically evaluate the time evolution of $\langle x(t)\rangle$ and $|\psi(x, t)|^2$ for $N = 18$ and $\Delta N = 2$ in which the superposition state of a harmonic oscillator with eigenfunctions $\psi_n(x, t)$ is

$$\psi(x, t) = \frac{1}{\sqrt{2\Delta N}}\sum_{n=N-\Delta N}^{n=N+\Delta N}\psi_n(x, t)$$

(d) The coherent quantum superposition of harmonic oscillator eigenstates $\psi_n(x)$ that best describes the classical harmonic oscillator is

$$\psi_\alpha(x, t) = e^{\frac{-|\alpha|^2}{2}}\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}\psi_n(x)e^{-i\omega_n t}$$

where $\omega_n = \omega\left(n + \frac{1}{2}\right)$ and α is an eigenvalue of the annihilation operator $\hat{b}$ acting on the state $|\alpha\rangle$. Numerically evaluate the time evolution of $\langle x(t)\rangle$ and $|\psi_\alpha(x, t)|^2$ for $\alpha = 1$, $\alpha = 2$ and $\alpha = 9$. Find analytic expressions for time evolution of expectation value of position and momentum.

Problem 5.10

Pure exponential decay $e^{-t/\tau}$ starting from a constant value at time $t = 0$ is *forbidden* in a closed unitary system evolving due to a Hermitian time-independent Hamiltonian $\hat{H}$.

(a) The probability amplitude that an initial state $|j\rangle$ is observed in state $|k\rangle$ at time t is $A_{kj}(t) = \langle k|\hat{U}(t)|j\rangle$, where $\hat{U}(t)$ is the unitary time evolution operator. Analytically show that the probability of measuring and observing state $|j\rangle$ is symmetric in time.

(b) Show analytically that any measurable state of the system cannot evolve as a simple exponential, $e^{-t/\tau}$, for either short times ($t \ll \tau$) or long times ($t \gg \tau$), thereby proving that exponential decay is incompatible with unitary evolution.

(c) Show numerically that the initial change in expectation value of position for the closed unitary system described in Problem 5.9(a) with $N \gg 2$ does not evolve as a simple exponential.

Problem 5.11

(a) Consider the wave function in Problem 5.9(a) with $N = 4$. Calculate numerically the real part of ψ as a function of time at position $x_0 = L/5$ and find the value of the full revival time (the time it takes for the wave function to return to its original state). Show that peaks in the FFT spectrum are energy eigenvalues of the system. Show that this result generalizes to states of an arbitrary potential, $V(x)$, so long as x_0 is not an eigenfunction node.

(b) Demonstrate how to use the information in (a) to find the eigenfunctions ψ_n. Show that the numerical approach generalizes and so may be used to find the eigenstates of an arbitrary potential, $V(x)$.

(c) Consider the wave function in Problem 5.9(d) with $\alpha = 2$. Calculate numerically the real part of ψ as a function of time at position $x_0 = 0$. Show that peaks in the FFT spectrum are energy eigenvalues of the system.

Comment on anything learned.

Problem 5.12

Find the eigenenergies, eigenfunctions, and degeneracy of an isotropic two-dimensional harmonic oscillator by separation into Cartesian coordinates.

Problem 5.13

Numerical methods exist to solve dynamics of a classical particle of mass *m* with position *x* and momentum *p* described by Hamiltonian of the form $H = T(p) + V(x)$. For the simple harmonic oscillator with spring constant κ the kinetic energy $T = p^2/2m$ and potential energy $V = m\omega^2 x^2/2$, where angular frequency $\omega = \sqrt{\kappa/m}$.

(a) Defining canonical relations $-\frac{dH}{dx} = \frac{dp}{dt}$ and $\frac{dH}{dp} = \frac{dx}{dt}$, show that

$$\dot{x} = \upsilon \equiv \frac{dx}{dt}$$

$$\dot{\upsilon} = -\omega^2 x$$

and that the analytic solution for position is $x(t) = x(0)\cos(\omega t) + (\upsilon(0)/\omega)\sin(\omega t)$.

(b) A phase-space plot of p as a function of x is an ellipse whose area is constant because energy is conserved. Rewrite equations for $\dot{x}$ and $\dot{\upsilon}$ in (a) using discretization of space and time where $dx = \Delta x$ and $dt = \Delta t$, such that $x_n = n\Delta x$ and $t_n = n\Delta t$, to obtain a set of equations for x_{n+1} and υ_{n+1} in terms of x_n, υ_n, Δt, and ω. Write the set of linear equations in matrix form $z_{n+1} = \mathbf{A}z_n$, such that $z_n = \mathbf{A}z_{n-1} = \ldots\mathbf{A}^n z_0$.

(c) Numerical stability implies that the phase-space vector norm $\|z_n\|$ remains bounded for all n. For any consistent matrix norm

$$\rho(\mathbf{A}) = \max_i(|\lambda_i|) = \lim_{n\to\infty}\|\mathbf{A}^n\|^{1/n}$$

where λ_i are the eigenvalues of $\mathbf{A}$. The spectral radius theorem states that given a matrix $\mathbf{A}$ over the complex numbers, the iterations $z_n = \mathbf{A}^n z_0$ are bounded if $\rho(\mathbf{A}) \le 1$. Show under Euler discretization in part (b), energy is not conserved by explicitly demonstrating that $\rho(\mathbf{A}) > 1$. Thus the phase-space area is not conserved over time.

(d) In addition to the utility of the Baker-Campbell-Hausdorff formula in quantum mechanics (see Problem 4.15(b)), the identity can be exploited to integrate Hamiltonians of the form $H = T(p) + V(x)$. By constructing explicit and time-reversible symplectic integrators of higher order that maintain the structure of the Hamiltonian, it is possible to suppress numerical error stemming from the energy non-conserving discretization of sets of coupled equations. If $e^{\hat{A}+\hat{B}} = e^{-\frac{1}{2}[\hat{A},\hat{B}]}e^{\hat{A}}e^{\hat{B}}$ is true, show that $e^{2\hat{A}+\hat{B}} = e^{\hat{A}}e^{\hat{B}}e^{\hat{A}}$.

(e) For Hamiltonians of the form $H = T(p) + V(x) = p^2/2m + V(x)$, show that $e^{t\frac{d}{dt}} = e^{t(P+X)}$, where $P = -\frac{dV}{dx}\frac{d}{dp}$ and $X = \frac{dT}{dp}\frac{d}{dx}$.

(f) Since $[\hat{A}, [\hat{A}, \hat{B}]] \ne 0$ in general, show that to order $O(\Delta t^2)$, the symmetric symplectic integrator can be written as $U(\Delta t)^{t/\Delta t} = e^{t(P+X)} + O(\Delta t^2)$, where $U(\Delta t)^{t/\Delta t} = (e^{\Delta tP/2}e^{\Delta tX}e^{\Delta tP/2})^{t/\Delta t}$. What does this result indicate about the energy conserving properties of a symplectic integrator?

Problem 5.14

(a) Show that the Hamiltonian for a parallel LC circuit with current flow I and voltage V may be written as $\hat{H} = \frac{\hat{Q}^2}{2C} + \frac{\hat{\phi}_B^2}{2L}$ for which the commutator for charge, $\hat{Q}$, and magnetic flux, $\hat{\phi}_B$, operators is $[\hat{Q}, \hat{\phi}_B] = i\hbar$ and resonant frequency $\omega_0 = 1/\sqrt{LC}$.

(b) Define operators

$$\hat{b} = \left(\frac{1}{2\hbar}\sqrt{\frac{C}{L}}\right)^{1/2}\hat{\phi}_B + i\left(\frac{1}{2\hbar}\sqrt{\frac{L}{C}}\right)^{1/2}\hat{Q}$$

and show that

$$\hat{\phi}_B = \left(\frac{\hbar}{2}\sqrt{\frac{L}{C}}\right)^{1/2}(\hat{b} + \hat{b}^\dagger),\ \hat{Q} = i\left(\frac{\hbar}{2}\sqrt{\frac{C}{L}}\right)^{1/2}(\hat{b}^\dagger - \hat{b}),\ \text{and}\ \hat{H} = \hbar\omega_0\left(\hat{b}^\dagger\hat{b} + \frac{1}{2}\right).$$

(c) For number states $|n\rangle$ and deviations in observable A such that $(\Delta A)^2 = \langle A^2\rangle - \langle A\rangle^2$, show and explain why $\langle \phi_B\rangle = \langle Q\rangle = 0$,

$$(\Delta\phi_B)^2 = \hbar\sqrt{\frac{L}{C}}\left(n + \frac{1}{2}\right),\ (\Delta Q)^2 = \hbar\sqrt{\frac{C}{L}}\left(n + \frac{1}{2}\right),\ \text{and}\ \Delta\phi_B\Delta Q = \hbar\left(n + \frac{1}{2}\right).$$

(d) Using results from (c) show that $\langle I\rangle = \langle V\rangle = 0$,

$$(\Delta I)^2 = \frac{\hbar\omega_0}{L}\left(n + \frac{1}{2}\right),\ (\Delta V)^2 = \frac{\hbar\omega_0}{C}\left(n + \frac{1}{2}\right),\ \text{and}\ \Delta I\Delta V = \hbar\omega_0^2\left(n + \frac{1}{2}\right).$$

(e) If the current in a resonant circuit with inductance $L = 1$ nH and capacitance $C = 100$ fF can be measured to an accuracy of one electron per oscillation, how accurately can the voltage be determined? Compare the result with capacitor thermal voltage noise $\sqrt{k_B T/C}$ at room-temperature ($T = 300$ K).

Problem 5.15

The eigenstate representation uses matrix elements $\langle m|\hat{A}|n\rangle$ for operator $\hat{A}$ where $|n\rangle$ and $|m\rangle$ are eigenstates. For a particle mass m_0 in a one-dimensional harmonic oscillator potential show that:

(a) $\langle m|\hat{H}|n\rangle = \hbar\omega\left(n + \frac{1}{2}\right)\delta_{m,n}$

and form the matrix H associated with the Hamiltonian whose rows and columns are labeled by m and n respectively.

(b) Find the matrix $\mathbf{b}^\dagger$ associated with the creation operator.

(c) Find the matrix $\mathbf{b}$ associated with the annihilation operator.

(d) Find the matrix $\mathbf{x}$ associated with the position operator.

(e) Find the matrix $\mathbf{p}$ associated with the momentum operator.

(f) By multiplying the matrix $\mathbf{x}$ and $\mathbf{p}$ find the matrix $\mathbf{xp} - \mathbf{px}$ associated with the commutator for position and momentum.

(g) What is the expectation value $\langle x\rangle$ and $\langle x^2\rangle$ of a pure state $|n\rangle$.

(h) What is the expectation value $\langle x\rangle$ and $\langle x^2\rangle$ of a mixed state $\frac{|n\rangle + |m\rangle}{\sqrt{2}}$.

Problem 5.16

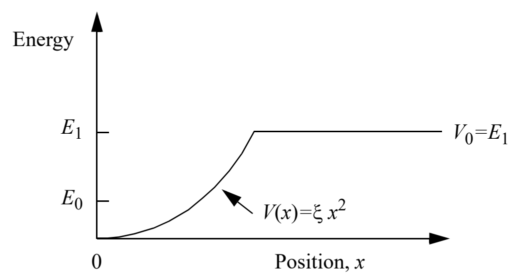
(a) The ground state, $|n = 0\rangle$, of an electron mass m_0 moving in a one-dimensional potential $V(x) = \xi\hat{x}^2$ is defined by $\hat{b}|n = 0\rangle = 0$, where the annihilation operator is

$$\hat{b} = \left(\frac{m_0\xi}{2\hbar^2}\right)^{\frac{1}{4}}\left(\hat{x} + \frac{\mathrm{i}\hat{p}}{\sqrt{2m_0\xi}}\right),$$

$\hat{x}$ is the position operator, $\hat{p}$ is the momentum operator, and ξ is a constant. Find the normalized wave function and numerical value of the energy eigenvalue for the ground state $|n = 0\rangle$ when $\xi = 4.6 \times 10^{-3}\ \mathrm{kg\ rad^2\ s^{-2}}$.

(b) State the value of the lowest three energy eigenvalues and sketch the corresponding wave functions if the potential in (a) is *modified* so that $V(x < 0) = \infty$.

(c) Sketch the wave function for the ground state with energy eigenvalue E_0 and first excited state with energy eigenvalue E_1 if the potential in (b) is *modified* as shown in the following figure.



In answering part (a) of this question, use may be made of the standard integral $\int_{-\infty}^{\infty} \mathrm{e}^{-ax^2}\mathrm{d}x = \sqrt{\frac{\pi}{a}}$.

Problem 5.17

The Hamiltonian of a particle mass m moving in a one-dimensional harmonic oscillator potential may be written

$$\hat{H} = \hbar\omega\left(\hat{b}^\dagger\hat{b} + \frac{1}{2}\right)$$

where ω is the angular frequency of oscillation and the operator

$$\hat{b} = \left(\frac{m\omega}{2\hbar}\right)^{1/2}\left(\hat{x} + \frac{\mathrm{i}\hat{p}}{m\omega}\right)$$

satisfies the commutation relations $[\hat{b}, \hat{b}^\dagger] = 1$ and $[\hat{b}, \hat{b}] = [\hat{b}^\dagger, \hat{b}^\dagger] = 0$.

(a) Show that the ground-state wave function $\psi_{n=0}$ is defined by $\hat{b}|0\rangle = 0$.

(b) Find the normalized ground-state and first-excited state wave function.

(c) The operator $\frac{1}{\sqrt{2}}\left(1+\frac{\hat{b}^{\dagger}}{\sqrt{n+1}}\right)$ acts on the state $|n\rangle$ and creates a new wave function $\psi(x, t)$. Find the probability density $|\psi(x, t)|^2$, the expectation value of energy, the expectation value of position $\langle x(t)\rangle$, the value of $\langle x^2\rangle$, the uncertainty in position $\Delta x(t)$, and the minimum and maximum values of position-momentum uncertainty product $\Delta x \Delta p$.

Problem 5.18

Expressed in terms of orthonormal Fock states $|n\rangle$, the normalized coherent state is

$$|\alpha\rangle = e^{-|\alpha|^2/2}\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}|n\rangle$$

(a) Show that coherent states α_1 and α_2 are not orthogonal and have overlap such that

$$|\langle\alpha_1|\alpha_2\rangle|^2 = e^{-|\alpha_1-\alpha_2|^2}$$

so that orthogonality occurs as $|\alpha_1-\alpha_2| \to \infty$.

(b) Show that coherent states are complete by integrating $\frac{1}{\pi}\int d^2\alpha\ |\alpha\rangle\langle\alpha| = 1$ over the complex plane.

(c) Show that coherent states form an over-complete set of states.

Problem 5.19

A stationary superposition non-separable state of the two-dimensional isotropic harmonic oscillator is $\psi(x, y) = a_0\left(\phi_2(x)\phi_3(y)+\frac{2}{3}\phi_3(x)\phi_2(y)\right)$ where x and y are Cartesian coordinates.

(a) Plot $\psi(\xi_x, \xi_y)$, where position is normalized to units of $\xi_x = x\sqrt{m\omega/\hbar}$ and $\xi_y = y\sqrt{m\omega/\hbar}$.

(b) Plot probability $P(\xi_y) = \int_{-\infty}^{\infty}|\psi(\xi_x, \xi_y)|^2 d\xi_x$ for the state in (a) before measuring position ξ_x. If ξ_x is measured first with the result $\xi_{x0} = 2$, plot the probability $P(\xi_y)|_{\xi_{x0}} = |\psi(\xi_{x0}, \xi_y)|^2$.

Problem 5.20

An objective fidelity measure $F_{\text{obj}} = |\cos(\pi t/\tau)|^{\beta}$ with a full revival (Poincaré recurrence) period τ is sought for a conservative system that has an initial wave function $\psi(x, t=0)$ and a quantum fidelity measure

$$F_{\text{sim}}(t) = |\langle\psi^*(x, t)|\psi(x, 0)\rangle|^2 = \int_0^L \psi^*(x, t)\psi(x, 0)dx$$

A particle of mass m_0 in a domain of thickness L with periodic boundary conditions experiences motion in the x-direction. The potential is zero except for N rectangular potential wells each of thickness $L_w = 0.4$ nm and potential energy $V_0 = -0.2$ eV. If $\psi(x, t = 0) = \frac{1}{\sqrt{N}}\sum_n^N \phi_n(x)$ for the first N lowest energy eigenstates ϕ_n and the minimum allowed separation between wells is 0.1 nm, find the energy eigenvalues E_n and separation in optimal potential well positions that satisfy the objective when

(a) $N = 2$, $\tau = 75$ fs, $\beta = 2$, and $L = 10$ nm.

(b) $N = 4$, $\tau = 100$ fs, $\beta = 4$, and $L = 20$ nm.

For each case plot objective $F_{obj}(t)$ and optimal $F_{sim}(t)$ for time $0 \leq t \leq 3\tau$ and plot the optimal potential $V_{opt}(x)$. Explain your results and why the objective in part (b) is not accessible if $\beta = 6$.