Applied Quantum Mechanics

Chapter 5 problems

LAST NAME FIRST NAME

Problem 5.1

An electron is constrained to motion in the x-direction by a potential $V(x) = 0$ for $-\frac{L}{2} < x < \frac{L}{2}$ and $V(x) = \infty$ elsewhere. The electron is in the simple superposition state consisting of the ground and third excited state so that

$$\psi(x, t) = \frac{1}{\sqrt{2}}(\psi_1(x, t) + \psi_4(x, t))$$

Find expressions for:

(a) The probability density, $|\psi(x, t)|^2$.

(b) The average particle position, $\langle x(t)\rangle$.

(c) The momentum probability density, $|\psi(p_x, t)|^2$

(d) The average momentum, $\langle p_x(t)\rangle$.

(e) The current flux, $J_x(x, t)$.

Problem 5.2

(a) Show that the density of states for a free-particle of mass m in two-dimensions is

$$D_2(E) = \frac{m}{2\pi\hbar^2}$$

(b) At low temperature, electrons in two electrodes occupy states up to the Fermi energy, E_F. The two closely spaced electrodes are connected by a two dimensional conductance region. Derive an expression for the conductance of electrons flowing between the two electrodes as a function of applied voltage V_{bias}, assuming the transmission coefficient through the two-dimensional region is unity. Consider the two limiting cases $eV_{bias} >> E_F$ and $eV_{bias} << E_F$.

Problem 5.3

Derive expressions for the two-dimensional $D_2^{opt}(\omega)$ and one-dimensional $D_1^{opt}(\omega)$ density of photon states in a homogeneous dielectric medium characterized by refractive index, n_r.

Problem 5.4

(a) In a particular system the dispersion relation for electrons in one-dimension is $E_k = \hbar\omega_k = 2t\cos(k_xL)$, where t and L are constants and the wave vector in the x-direction is $0 \le k_x < \pi/L$. This dispersion relation can be derived using a nearest neighbor tight binding model where t is the overlap integral between atomic orbitals. Choosing one hundred equally spaced discrete values of k_x, write a computer program and plot the electron density of states $N(E) = \sum_k \frac{|\Gamma|/\pi}{(E-E_k)^2 + (\Gamma/2)^2}$ using $\Gamma = t/10$ and $t = -1$.

(b) If one includes next nearest neighbor interactions, the dispersion relation in (a) can, to within a scaling factor, be written $E_k = 2t\cos(k_xL) + 2t'\cos(2k_xL)$. Write a computer program to plot the dispersion relation. Then calculate and plot the electron density of states using $\Gamma = t/10$, $t = -1$, $t' = -0.1$ and compare with the result you obtained in (a) including a comparison with the effective electron mass at the band edges.

(c) Calculate and plot the electron density of states for a square lattice with lattice constant L and the following different dispersion relations:

(i) $E_k = 2t(\cos(k_xL) + \cos(k_yL))$

and

(ii) $E_k = (2t\cos(k_xL) + 2t'\cos(2k_xL) + 2t\cos(k_yL) + 2t'\cos(2k_yL))$.

Use parameters $\Gamma = t/10$, $t = -1$, $t' = t/10$ and explain the differences in the density of states you obtain for case (i) and (ii).

(d) Calculate and plot the electron density of states for a cubic lattice with lattice constant L and the following different dispersion relations:

(i) $E_k = 2t(\cos(k_xL) + \cos(k_yL) + \cos(k_zL))$

and

(ii) $$E_k = (2t\cos(k_xL) + 2t'\cos(2k_xL) + 2t\cos(k_yL) + 2t'\cos(2k_yL) + 2t\cos(k_zL) + 2t'\cos(2k_zL)) .$$

Use parameters $\Gamma = t/10$, $t = -1$, $t' = t/10$ and explain the differences in the density of states you obtain for case (i) and (ii).

Submit the code used for your solutions.

Problem 5.5

A hydrogen atom is in its ground state with electron wave function

$$\phi = \frac{2}{a_B^{3/2}} e^{-r/a_B}\left(\frac{1}{4\pi}\right)^{1/2}$$

In this expression a_B is the Bohr radius and r is a radial coordinate.

Use spherical coordinates to find the expectation value of position r and momentum p_r for the electron in this state. You should use the fact that in radial coordinates the Hermitian momentum operator is $\hat{p}_r = -i\hbar\frac{1}{r}\frac{\partial}{\partial r}r$.

Problem 5.6

Using the fact that the Hamiltonian appearing in the Schrödinger equation

$$\frac{-i}{\hbar}\hat{H}|\psi(\mathbf{r}, t)\rangle = |\frac{\partial}{\partial t}\psi(\mathbf{r}, t)\rangle$$

is Hermitian, (i.e., $\langle\psi|\hat{H}\psi\rangle = \langle\hat{H}\psi|\psi\rangle$), show that the time dependence of the average value of the observable A associated with the operator $\hat{A}$ is

$$\frac{d}{dt}\langle A\rangle = \frac{i}{\hbar}\langle[\hat{H},\hat{A}]\rangle + \langle\frac{\partial}{\partial t}\hat{A}\rangle$$

Problem 5.7

Show that:

(a) The position operator $\hat{x}$ acting on wave function $\psi(x)$ is Hermitian (i.e., $\hat{x}^\dagger = \hat{x}$).

(b) The operator $\frac{\mathrm{d}}{\mathrm{d}x}$ acting on the wave function $\psi(x)$ is anti-Hermitian (i.e., $\left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^{\dagger} = -\frac{\mathrm{d}}{\mathrm{d}x}$).

(c) The momentum operator $-i\hbar\frac{\mathrm{d}}{\mathrm{d}x}$ acting on the wave function $\psi(x)$ is Hermitian.

Problem 5.8

A particle mass m is confined to motion in a one-dimensional potential $V(x)$. The Hamiltonian is

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)$$

and the momentum operator is

$$\hat{p} = -i\hbar\frac{\mathrm{d}}{\mathrm{d}x}$$

(a) Find the commutator $[\hat{H}, \hat{p}]$.

(b) For what potentials, $V(x)$, are solutions of the time-independent Schrödinger equation also eigenstates of momentum?

Problem 5.9

Classical electromagnetic theory uses real magnetic and electric fields coupled via Maxwell's equations. The magnetic and electric fields each have physical meaning. Both fields are needed to describe the instantaneous state and time evolution of the system. Quantum mechanics uses one complex wave function to describe both the instantaneous state and time evolution of the system. It is also possible to describe quantum mechanics using two coupled real wave functions corresponding to the real and imaginary parts of the complex wave function. Why isn't this done?

Problem 5.10

A classical bit of information has state 0 or 1 which in quantum mechanics corresponds to the orthonormal basis states $|0\rangle$ and $|1\rangle$. The difference between classical bits and quantum bits (q-bits) is that a q-bit can exist in a continuum of states between $|0\rangle$ and $|1\rangle$ as a superposition state $|\psi\rangle = a_0|0\rangle + a_1|1\rangle$ where $|a_0|^2 + |a_1|^2 = 1$.

(a) Two q-bits have a normalized linear superposition state $|\psi\rangle = a_{00}|00\rangle + a_{01}|01\rangle + a_{10}|10\rangle + a_{11}|11\rangle$ where $|00\rangle$, $|01\rangle$, $|10\rangle$, and $|11\rangle$ are the basis states. Measuring just the first q-bit gives eigenvalue 0 with probability $|a_{00}|^2 + |a_{01}|^2$. What is the renormalized post-measurement state $|\psi'\rangle$?

(b) The first q-bit in a two q-bit Bell state $|\psi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$ is measured. It has probability ½ that the post-state is $|\psi'\rangle = |00\rangle$ and probability ½ that the post-state is $|\psi'\rangle = |11\rangle$. What is the result of measuring the second q-bit when initially in state $|\psi\rangle$ and when initially in the state $|\psi'\rangle$?

Problem 5.11

A function $|f\rangle$ can be expressed as an expansion of complete orthonormal basis functions $|\phi_n\rangle$.

(a) Show that the identity operator $\hat{I} \equiv \sum_n |\phi_n\rangle\langle\phi_n|$ acting on the function $|f\rangle$ leaves it unchanged.

(b) The sum of diagonal elements of an operator $\hat{A}$ expressed as a matrix is called a trace operator, $\mathrm{Tr}(\hat{A})$. Show that the trace operator is independent of the basis used.

(c) A unitary operator satisfies $\hat{U}^{-1} = \hat{U}^{\dagger}$. Show that the inner product of functions $|f_1\rangle$ and $|g_1\rangle$ is invariant under unitary transformation such that $|f_2\rangle = \hat{U}|f_1\rangle$ and $|g_2\rangle = \hat{U}|g_1\rangle$.

(d) Demonstrate a unitary transformation can be used to change the representation of an operator from $\hat{A}$ to $\hat{B} = \hat{U}\hat{A}\hat{U}^{\dagger}$ by showing that the matrix elements satisfy $\langle g_1|\hat{A}|f_1\rangle = \langle g_2|\hat{B}|f_2\rangle$.

Problem 5.12

The non-zero state $|n, t\rangle$ evolves in time according to the Schrödinger equation $i\hbar\frac{\partial}{\partial t}|n, t\rangle = \hat{H}|n, t\rangle$, where $\hat{H}$ is the Hamiltonian. A unitary time-evolution operator $\hat{U}(t, t_0)$ evolves the state from time t_0 such that $|n, t\rangle = \hat{U}(t, t_0)|n, t_0\rangle$. For $\hat{H} \neq \hat{H}(t)$ show that

$$|n, t\rangle = e^{-i\hat{H}(t-t_0)/\hbar}|n, t_0\rangle$$

and for $\hat{H} = \hat{H}(t)$, such that $[\hat{H}(t), \hat{H}(t')] = 0$ and $t \neq t'$, show that

$$|n, t\rangle = e^{\frac{-i}{\hbar}\int\limits_{t'=t_0}^{t'=t}\hat{H}(t')dt'}|n, t_0\rangle .$$

Problem 5.13

Suppose the Hamiltonian H_λ describing a particle mass m constrained to motion in the x-direction contains an adjustable parameter λ that may appear in the kinetic energy T, potential energy V, or both. The energy eigenvalue E_λ and eigenstate ψ_λ also depend on λ. For any λ one may write $E_\lambda = \langle\psi_\lambda|H_\lambda|\psi_\lambda\rangle$.

(a) Show that $\frac{\mathrm{d}E_\lambda}{\mathrm{d}\lambda} = \langle\psi_\lambda|\frac{\mathrm{d}H_\lambda}{\mathrm{d}\lambda}|\psi_\lambda\rangle$

(b) Starting from the time-independent Schrödinger equation

$$\left(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)\right)\psi(x) = E\psi(x)$$

scale x such that $x \to \lambda x$ and apply the result in (a) to show that for any bound state one obtains the generalized Virial theorem

$$2\langle\psi|\frac{p^2}{2m}|\psi\rangle = \langle\psi|x\frac{\partial}{\partial x}V(x)|\psi\rangle$$

when $\lambda \to 1$, so that if $V(x) \propto x^{\gamma}$ then $2\langle T\rangle = \gamma\langle V\rangle$.

Problem 5.14

(a) Show that one may expand

$$e^{\alpha\hat{A}}\hat{B}e^{-\alpha\hat{A}} = \hat{B} + \alpha[\hat{A},\hat{B}] + \frac{\alpha^2}{2!}[\hat{A},[\hat{A},\hat{B}]] + \frac{\alpha^3}{3!}[\hat{A},[\hat{A},[\hat{A},\hat{B}]]] + \ldots$$

where $\hat{A}$ and $\hat{B}$ are operators and α is a scalar.

(b) If $[\hat{A}, [\hat{A}, \hat{B}]] = [\hat{B}, [\hat{A}, \hat{B}]] = 0$, show that

$$e^{\hat{A}+\hat{B}} = e^{-\frac{1}{2}[\hat{A},\hat{B}]}e^{\hat{A}}e^{\hat{B}} = e^{\frac{1}{2}[\hat{A},\hat{B}]}e^{\hat{B}}e^{\hat{A}}$$

(c) If $[\hat{A}, [\hat{A}, \hat{B}]] = [\hat{B}, [\hat{A}, \hat{B}]] = 0$, rewrite $e^{\hat{A}}e^{\hat{B}}e^{\hat{A}}$ as a single exponential.

Problem 5.15

If Hamiltonian $\hat{H}$ does not depend on time the system is stationary and the Schrödinger equation $i\hbar\frac{\partial}{\partial t}|n, t\rangle = \hat{H}|n, t\rangle$ can be integrated to give $|n, t\rangle = e^{-i\hat{H}t/\hbar}|n, t = 0\rangle$.

(a) Expand $e^{-i\hat{H}t/\hbar}$, take the time derivative, and show that $i\hbar\frac{\partial}{\partial t}|n, t\rangle = \hat{H}e^{-i\hat{H}t/\hbar}|n, t = 0\rangle = \hat{H}|n, t\rangle$.

(b) The unitary operator $\hat{U}(t) = e^{-i\hat{H}t/\hbar}$ is the generator of time development and belongs to the unitary Lie group $U(1)$. If the system evolves for a short time interval, Δt, show that $|n, t\rangle = U(\Delta t)|n, t = 0\rangle$, where $\hat{U}(\Delta t) = \hat{I} - \frac{i\hat{H}\Delta t}{\hbar} + O(\Delta t)^2$.

(c) From the group property of the operator in (b) one can build up finite time evolution from a product of N small time steps such that $t = N\Delta t$ where $\Delta t = t/N \to 0$. Making use of the fact that in the limit $N \to \infty$ one may use the binomial theorem to write $e^x = \left(1 + \frac{x}{N}\right)^N$, show that $\hat{U}(t) = e^{-i\hat{H}t/\hbar}$.

Problem 5.16

The active region of a new design of a single-walled carbon nanotube transistor is modeled as a conducting channel nanotube 2 nm in diameter that is coated in a 2 nm thick dielectric of relative permittivity $\varepsilon_{r0} = 10$ and a wrap-around metal gate of length $L = 100$ nm. Electrical conduction is via 4 quantized conductance channels (two electron paths each with spin up and down). What is the maximum characteristic frequency of operation of the device when configured to drive a fan-out of 4 identical transistors?

Problem 5.17

A particle moving in one dimension has stationary wave function

$$\psi(-L < x < L) = A\left(1 + \cos\left(\frac{\pi x}{L}\right)\right)$$

and

$$\psi(-L \geq x \geq L) = 0$$

(a) Determine the normalization constant A.

(b) Find the position uncertainty Δx and the momentum uncertainty Δp and show that $\Delta x \Delta p \geq \frac{\hbar}{2}$.

(c) Determine the spatial extent of the classically allowed region.