Applied Quantum Mechanics

Chapter 5 problems

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

In a particular system the symmetric dispersion relation for propagating electrons in one-dimension is $E_k = \hbar\omega_k = 2t_{hop,\,1}\cos(k_x L)$, where $t_{hop,\,1}$ 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 $t_{hop,\,1}$ is the overlap integral between atomic orbitals.

(a) Find the complex band structure for non-propagating electron states.

(b) Choosing one hundred equally spaced discrete values of k_x, plot the density of propagating electron states

$$N(E) = \sum_k \frac{\gamma/\pi}{(E - E_k)^2 + (\gamma/2)^2}$$

using $\gamma = |t_{hop,\,1}|/10$ and $t_{hop,\,1} = -1$.

(c) If next nearest-neighbor interactions are included, the dispersion relation in (a) can, to within a scaling factor, be written $E_k = 2t_{\text{hop, 1}}\cos(k_x L) + 2t_{\text{hop, 2}}\cos(2k_x L)$. Write a computer program to plot the dispersion relation. Then calculate and plot the electron density of states using $\gamma = |t_{\text{hop, 1}}|/10$, $t_{\text{hop, 1}} = -1$, $t_{\text{hop, 2}} = -0.1$ and compare with the result you obtained in (a) including a comparison with the effective electron mass at the band edges.

(d) Calculate and plot the electron density of states for a square lattice with lattice constant L and a tight-binding nearest-neighbor dispersion relation given by $E_k = 2t_{\text{hop, 1}}(\cos(k_x L) + \cos(k_y L))$. Find an expression for electron dispersion E_k when an additional next-nearest-neighbor hopping term $t_{\text{hop, 2}}$ is included and calculate the electron density of states. Use parameters $\gamma = |t_{\text{hop, 1}}|/10$, $t_{\text{hop, 1}} = -1$, $t_{\text{hop, 2}} = t_{\text{hop, 1}}/10$ and explain the differences in the density of states you obtain for the two cases.

(e) Calculate and plot the electron density of states for a cubic lattice with lattice constant L and a tight-binding nearest-neighbor dispersion relation given by $E_k = 2t_{\text{hop, 1}}(\cos(k_x L) + \cos(k_y L) + \cos(k_z L))$. Find an expression for electron dispersion E_k when an additional next-nearest-neighbor hopping term $t_{\text{hop, 2}}$ is included and calculate the electron density of states. Use parameters $\gamma = |t_{\text{hop, 1}}|/10$, $t_{\text{hop, 1}} = -1$, $t_{\text{hop, 2}} = t_{\text{hop, 1}}/10$ and explain the differences in the density of states you obtain for the two cases.

Submit the code used for your solutions.

Problem 5.5

(a) Explain why a one-dimensional tight-binding model of N atoms on a lattice with nearest-neighbor spacing L, periodic boundary conditions, and nearest-neighbor hopping integral $t_{\text{hop, 1}}$ between atomic s-orbital sites at x_j and $x_i = x_j \pm nL$ has a symmetric electron density of states.

(b) In general, the electron dispersion relation for a one-dimensional tight-binding model describing atoms on a lattice with nearest-neighbor spacing L and periodic boundary conditions is

$$E_k = -2\sum_{n}^{N_{\text{atom}}} t_{\text{hop}, n}\cos(nkL)$$

where $t_{\text{hop}, n}$ is the overlap integral between atomic s-orbital sites at x_j and $x_i = x_j \pm nL$ with n a positive non-zero integer and N_{atom} is the number of atoms in the lattice. What values of electron hopping integral $t_{\text{hop}, n}$ result in a *linear* dispersion relation and what is the corresponding density of states?

Problem 5.6

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

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

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 5.7
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 5.8
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 5.9
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 5.10
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 5.11

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 5.12

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 5.13

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

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

Problem 5.14

Suppose the Hamiltonian $\hat{H}_\lambda$ 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 $E_\lambda = \langle\psi_\lambda|\hat{H}_\lambda|\psi_\lambda\rangle$.

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

(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 5.15

(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

$e^{\hat{A}+\hat{B}} = e^{-\frac{1}{2}[\hat{A},\hat{B}]}e^{\hat{A}}e^{\hat{B}} = e^{\frac{1}{2}[\hat{A},\hat{B}]}e^{\hat{B}}e^{\hat{A}}$ so if $[\hat{A},\hat{B}] = 0$ then $e^{\hat{A}+\hat{B}} = e^{\hat{A}}e^{\hat{B}}$.

(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 5.16

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 $|n, t\rangle = \hat{U}(\Delta t)|n, t = 0\rangle$, 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) a finite time evolution may be built up 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 5.17

The active region 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 5.18

An electron of eigenenergy E in a one-dimensional potential $V(x)$ 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.

(d) Find and plot an analytic expression for the potential $V(x)$ and calculate the numerical value of E expressed in eV when $L = 1$ nm.

Problem 5.19

(a) Solve the Schrödinger equation and find the normalized bound-state wave functions and corresponding eigenenergies for a single particle of mass m trapped in a two-dimensional (2D) rectangular potential well with infinite barrier energy such that

$$V(0 < x < L_x, 0 < y < L_y) = 0$$

and

$$V(0 \geq x \geq L_x, 0 \geq y \geq L_y) = \infty$$

(b) Assuming that $L_x = L_y = 1$ nm and ignoring degeneracy, plot the ground state wave function $\psi_0(x, y)$ as well as the first three excited-state wave functions $\psi_1(x, y)$,

$\psi_2(x, y)$, and $\psi_3(x, y)$ in the same figure by using MATLAB's "subplot" function. Do the same for the corresponding probability densities, functions $|\psi_0(x, y)|^2$, $|\psi_1(x, y)|^2$, $|\psi_2(x, y)|^2$ and $|\psi_3(x, y)|^2$. Use either "surf" or "imagesc" for the plots and make sure to label everything, including the corresponding bound-state energies in each subplot title (in units of $\hbar^2\pi^2/2mL_x^2$).

(c) In units of $\hbar^2\pi^2/2mL_x^2$, use MATLAB's "imagesc" function to plot the particle's energy as a function of the energy indices n_x and n_y, for the range $1 \le n_x \le 100$ and $1 \le n_y \le 100$. Generate three separate figures for the cases when $L_x = L_y$, $L_x = 2L_y$, and $L_x = 10L_y$. Comment on what you observe in and between each of these geometries.

Problem 5.20

N_{atom} atoms with s-orbital atomic states exist in a one-dimensional domain of length L. A physical model of the system includes periodic boundary conditions and a hopping integral whose value is $-t_{\text{hop}}/|x_i - x_j|^\alpha$ between an atom at position x_i and an atom at position x_j. The value of $\alpha = 3$ and $t_{\text{hop}} = 1$.

(a) Write an optimization algorithm in which values of x_i are chosen at random to find an arrangement of $N_{\text{atom}} = 6$ atoms in a domain $0 \le x < L = 12$ that give a constant density of states in the energy range $-2 \times t_{\text{hop}} \le E \le 2 \times t_{\text{hop}}$. Use energy broadening $\gamma = 0.3 \times |t_{\text{hop}}|$ when evaluating the density of states.

(b) Repeat (a) but with $N_{\text{atom}} = 3$ and comment on what you learn.

(c) Explain the difference in average $\mathcal{L}^2$ convergence as a function of iteration number n in (a) and (b). Plot the data using logarithmic scales.

Problem 5.21

N_{atom} atoms with s-orbital atomic states exist in a one-dimensional chain with atom sites at positions x_j with $j = 1, 2, \ldots, N_{\text{atom}}$. Nearest-neighbor electron hopping integral $t_{\text{hop},1} = -1$ and on-site real potential v_j is zero except at the end-points of the chain located at x_1 and $x_{N_{\text{atom}}}$ respectively.

(a) For $N_{\text{atom}} = 2$ find the energy eigenvalues as a function of (i) $v_1 = v_2 = v$ and (ii) $v_1 = -v_2 = v$ with $0 \le v \le 3.5 \times t_{\text{hop},1}$. Explain the difference in behavior between the results for (i) and (ii).

(b) For $N_{\text{atom}} = 7$, plot the real and imaginary parts of the energy eigenvalues as a function of $v_1 = v_{N_{\text{atom}}} = v$ with $0 \le v \le 3.5 \times t_{\text{hop},1}$ in the Hermitian system and explain the emergence and symmetry of the degenerate edge-states.

(c) Compare the density of states for $v = 0$ and $v = 3.5 \times t_{\text{hop},1}$ in (b) when each state is Lorentzian-broadened in energy by $\gamma = 0.1 \times |t_{\text{hop},1}|$. Discuss why you expect the edge-state with $v = 3.5 \times t_{\text{hop},1}$ to have a relatively long lifetime?

(d) Repeat (b) and (c) for the case $v = v_1 = -v_{N_{\text{atom}}}$.

(e) Repeat (d) for a non-Hermitian Hamiltonian that has pure imaginary on-site terms $\nu_1 = -\nu_{N_{\text{atom}}} = \mathrm{i}\nu$ with real $\nu \geq 0$ and explain the exceptional-point behavior you observe.

Problem 5.22

(a) Find the energy eigenvalues of a two-atom ($N_{\text{atom}} = 2$) non-Hermitian system with on-site terms $\nu_1 = -\nu_{N_{\text{atom}}} = \mathrm{i}\nu$, interaction strength $0 \leq v \leq 3.5 \times t_{\text{hop},1}$, and hopping integral $t_{\text{hop},1} = -1$. State the value of the exceptional-point interaction strength, ν_{EP}, and show there is a square-root dependence of energy eigenvalue on v near ν_{EP}.

(b) Find the energy eigenvalues of a three-atom ($N_{\text{atom}} = 3$) non-Hermitian system with on-site terms $\nu_1 = -\nu_{N_{\text{atom}}} = \mathrm{i}\nu$, interaction strength $0 \leq v \leq 3.5 \times t_{\text{hop},1}$, and nearest-neighbor hopping integral $t_{\text{hop},1} = -1$. State the value of ν_{EP} and show there is a cube-root dependence of energy eigenvalue on v near ν_{EP}.

Problem 5.23

Following the work of Haydock and Kelly, [1] in 1998 Bender and Boettcher [2] suggested that the requirement of Hermiticity of a Hamiltonian in quantum mechanics might be unnecessarily strict and could be replaced by a parity-time symmetry such that $\hat{H} = \hat{H}^{\mathcal{PT}}$ in which the parity operator is $\mathcal{P}: \hat{p} \to -\hat{p}, \hat{x} \to -\hat{x}$ and the time-reversal operator is $\mathcal{T}: \hat{p} \to -\hat{p}, i \to -i$, where $\hat{p}$ and $\hat{x}$ are the momentum and position operators respectively and i is the square root of minus one. A class of Hamiltonian with a distinct transition between purely real eigenvalues and real and complex eigenvalues includes

$$\hat{H} = \hat{p}^2 + e^{2ix}$$

and

$$\hat{H} = \hat{p}^2 - (ix)^{\alpha}$$

where α is real and the potential is $V_\alpha(x) = -(ix)^\alpha$. For the latter case, $\mathcal{PT}$ symmetry is *broken* for values of $1 < \alpha < 2$ and there are a finite number of real positive eigenvalues and an infinite number of complex conjugate pairs of eigenvalues. For $\alpha \geq 2$ the eigenvalue spectrum is real and positive. The Hamiltonian reduces to that of a simple harmonic oscillator when $\alpha = 2$.

(a) Show that $\mathcal{P}: \hat{p} \to -\hat{p}, \hat{x} \to -\hat{x}$ and $\mathcal{T}: \hat{p} \to -\hat{p}, i \to -i$.

(b) Show that the potential $V_\alpha(x)$ is $\mathcal{PT}$-symmetric.

Problem 5.24

An electron of eigenenergy E in a one-dimensional potential $V(x)$ has stationary continuous wave function

1. R. Haydock and M. J. Kelly, *J. Phys. C.: Solid State Physics* **8**, L290 (1975)
2. C. M. Bender and S. Boettcher, *Phys. Rev. Lett.* **80**, 5243 (1998)

$$\psi(0 < x < L) = \sum_{n=0}^{N} a_n x^n$$

with the constraint

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

Find the potential $V(x)$ when $N = 2$ and calculate the numerical value of E expressed in eV when $L = 2$ nm.

Problem 5.25

Given a potential $V(x)$ with ground state ψ_0 of eigenenergy E_0, consider the shifted potential $V^{(-)}(x) = V(x) - E_0$ so that

$$\hat{H}^{(-)}\psi_0(x) = \left(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V^{(-)}(x)\right)\psi_0(x) = 0$$

from which it follows that

$$V^{(-)}(x) = \frac{\hbar^2}{2m}\,\frac{1}{\psi_0(x)}\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi_0(x)\right)$$

For any such potential, a corresponding *supersymmetric partner* $V^{(+)}(x)$ exists with Hamiltonian $\hat{H}^{(+)}$ that shares all the excited state ($n = 1, 2, \ldots$) energy eigenvalues (and so is isospectral) with $\hat{H}^{(-)}$ *except* the ground state. It is difficult to distinguish two such potentials simply by measuring their energy eigenvalues. However, introducing a perturbation (such as an external electric field) can change the eigenvalues of $\hat{H}^{(-)}$ relative to $\hat{H}^{(+)}$, thereby making them distinguishable.

(a) Show that $\hat{H}^{(-)} = \hat{A}^\dagger\hat{A}$ if

$$\hat{A} = \frac{\hbar}{\sqrt{2m}}\left(\frac{\mathrm{d}}{\mathrm{d}x} - \left(\frac{1}{\psi_0(x)}\,\frac{\mathrm{d}}{\mathrm{d}x}\psi_0(x)\right)\right)$$

(b) Show that $\hat{H}^{(+)} \equiv \hat{A}\hat{A}^\dagger = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V^{(+)}(x)$ if

$$V^{(+)}(x) = -V^{(-)}(x) + \frac{\hbar^2}{m}\left(\frac{1}{\psi_0(x)}\,\frac{\mathrm{d}}{\mathrm{d}x}\psi_0(x)\right)^2$$

(c) Show that if $\psi_{n>0}(x)$ is an eigenstate of $\hat{H}^{(-)}$ then $\hat{A}\psi_{n>0}$ is an eigenstate of $\hat{H}^{(+)}$ with the same eigenvalue. Show that this fails for $n = 0$. Similarly, show that if $\psi_n(x)$ is an eigenstate of $\hat{H}^{(+)}$ then $\hat{A}^\dagger\psi_n$ is an eigenstate of $\hat{H}^{(-)}$ with the same eigenvalue.

(d) An electron in the conduction band of GaAs has effective mass $m_e^* = 0.07 \times m_0$ and is confined by potential $V^{(-)}(0 < x < L) = 0$ with $L = 10$ nm and $V^{(-)}(0 \geq x \geq L) = \infty$. Find the first four lowest energy eigenvalues and plot the corresponding eigenstates. Numerically determine and plot the supersymmetric partner

potential $V^{(+)}(x)$, check that it agrees with the analytic result, find the first four lowest energy eigenvalues, and plot the corresponding eigenstates.

(e) An applied uniform electric field **E** adds a perturbing potential $W = e|\mathbf{E}|x$. Plot the first four lowest energy eigenvalues of $\hat{H}^{(-)} + W$ and the first three lowest energy eigenvalues of $\hat{H}^{(+)} + W$ as a function of W. Explain the sensitivity of your results to the perturbing potential, W.

Problem 5.26

Consider a one-dimensional lattice with lattice constant L that has integer N unit cells. Each unit-cell contains two atoms labeled A and B respectively with corresponding atomic orbitals ϕ_A and ϕ_B. The tight-binding wave function can be written

$$\psi_k(x) = \frac{1}{\sqrt{N}} \sum_{n=1}^{N} e^{iknL}(c_A\phi_A(x-nL) + c_B\phi_B(x-nL))$$

where k is the Bloch wave vector, c_A and c_B are constants. Multiplying the time-independent Schrödinger equation $\hat{H}|\psi_k\rangle = E|\psi_k\rangle$ from the left by each atomic orbital and integrating over space gives two equations

$$\langle\phi_A|\hat{H}|\psi_k\rangle = E\langle\phi_A|\psi_k\rangle$$

and

$$\langle\phi_B|\hat{H}|\psi_k\rangle = E\langle\phi_B|\psi_k\rangle$$

(a) Keeping only on-site and nearest-neighbor terms on the left hand side of the equations and only the on-site term on the right hand side of the equations, show that

$$E_A c_A - t_{\text{hop},1} c_B(1 + e^{-ikL}) = E c_A$$

and

$$-t_{\text{hop},1} c_A(1 + e^{ikL}) + E_B c_B = E c_B$$

where on-site energies are $E_A = \langle\phi_A|\hat{H}|\phi_A\rangle$ and $E_B = \langle\phi_B|\hat{H}|\phi_B\rangle$, and overlap integral $t_{\text{hop},1} = -\langle\phi_A(x)|\hat{H}|\phi_B(x)\rangle = -\langle\phi_B(x-L)|\hat{H}|\phi_A(x)\rangle$.

(b) Write the two equations in (a) in matrix form and show the characteristic polynomial is $E^2 - (E_A + E_B)E + E_A E_B - 2t_{\text{hop},1}^2(1 + \cos(kL)) = 0$ with solution

$$E = \frac{(E_A + E_B) \pm \sqrt{(E_A - E_B)^2 + 8t_{\text{hop},1}^2(1 + \cos(kL))}}{2}$$

(c) Plot the real and imaginary contributions to the complex band structure in the reduced zone $0 \le k < \pi/L$ when on-site energy for atom A is $E_A = 0$ eV and for atom B is $E_B = 1$ eV and nearest neighbor hoping energy is $t_{\text{hop},1} = 1$ eV.

Problem 5.27

Find an analytic expression for eigenenergies, E_k, of an isolated one-dimensional tight-binding chain of atoms with nearest-neighbor interaction energy $t_{\text{hop},1} = -1$ as a function of number of atoms, $1 \le N_{\text{atom}} \le 20$. Explain the results you obtain.

Problem 5.28

The density matrix operator ρ describes the statistical state of a quantum system and can provide a framework for studying entanglement and dissipation. It is a positive, semi-definite operator on a complex Hilbert space with unit trace. All of its eigenvalues are real and greater than or equal to zero. The state of any quantum system can be characterized by a density matrix $\hat{\rho}$ with a trace equal to unity, $\mathrm{Tr}(\rho) = 1$. For an observable with associated operator $\hat{A}$, the expectation value is

$$\langle A \rangle = \mathrm{Tr}(\hat{A}\rho)$$

For any given normalized pure state $|\psi\rangle$, the density matrix is given as $\rho = |\psi\rangle\langle\psi|$. For pure states it follows that $\rho^2 = |\psi\rangle\langle\psi||\psi\rangle\langle\psi| = |\psi\rangle\langle\psi| = \rho$ since $\langle\psi|\psi\rangle = 1$. The degree of purity of a general density matrix is $\gamma = \mathrm{Tr}(\rho^2)$ and so pure states have $\gamma = \mathrm{Tr}(\rho^2) = \mathrm{Tr}(\rho) = 1$. For a general mixed state, the density matrix is represented by the weighted sum

$$\rho = \sum_{i=1}^{N} p_i |\psi_i\rangle\langle\psi_i|$$

where $p_i \geq 0$ for $i = 1, 2, \ldots, N$, $\sum_i p_i = 1$, and $\langle\psi_i|\psi_j\rangle = \delta_{i,j}$. In the mixed state Hilbert space the expectation value of any Hermitian operator $\hat{A}$ is given by

$$\mathrm{Tr}(\rho\hat{A}) = \sum_{i=1}^{N} p_i \langle\psi_i|\hat{A}|\psi_i\rangle$$

(a) For the following, compute the eigenvalues and check it meets the requirements to be considered a density matrix.

$$\rho = \begin{bmatrix} \frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} \end{bmatrix}$$

Does this matrix represent a pure state or a mixed state, and why? Using the computational basis

$$\left\{ \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \end{bmatrix} \right\}$$

write down a vector state which yields this density matrix (if it is a pure state) or the set of weighted states (if it is a mixed state).

(b) An important operation in the field of quantum information is the tensor product. For example, given two vectors $\upsilon_1 = \begin{bmatrix} a \\ b \end{bmatrix}$ and $\upsilon_2 = \begin{bmatrix} c \\ d \end{bmatrix}$, the tensor product is

$$\upsilon_1 \otimes \upsilon_2 = \begin{bmatrix} a \\ b \end{bmatrix} \otimes \begin{bmatrix} c \\ d \end{bmatrix} = \begin{pmatrix} a \begin{bmatrix} c \\ d \end{bmatrix} \\ b \begin{bmatrix} c \\ d \end{bmatrix} \end{pmatrix} = \begin{pmatrix} ac \\ ad \\ bc \\ bd \end{pmatrix}$$

In general, the tensor product is not commutative so $\upsilon_1 \otimes \upsilon_2 \neq \upsilon_2 \otimes \upsilon_1$. Given $a = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ and $b = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$, compute $|ab\rangle = |a\rangle \otimes |b\rangle$

Explicitly show by hand that $\rho_{ab} = \rho_a \otimes \rho_b$ and from this prove $\langle a| \otimes |b\rangle = |b\rangle\langle a|$. For more complicated systems (e.g., larger matrices) involving the tensor product, it is recommended that you either use MATLAB's "kron" function or construct your own for numerical calculations.

(c) The density matrix is often used to describe many-body systems, and as such one might be interested in the statistical properties of certain subsystems, which would require tracing out all other subsystems (other degrees of freedom). This procedure is called taking the partial trace, and it plays an important role in quantum information and quantum computation. Assume a quantum system S_{AB} described by a density matrix ρ_{AB} existing in the finite-dimensional Hilbert space $H_{AB} = H_A \otimes H_B$ contains two subsystems S_A and S_B (respectively existing in their finite-dimensional Hilbert spaces H_A and H_B). Defining N_A and N_B as the numbers of dimensions in H_A and H_B respectively, the density matrices for each subsystem may be explicitly computed by tracing out the other subsystem. That is,

$$\rho_A = \mathrm{Tr}_B(\rho_{AB}) = \sum_{i=1}^{N_B} (I_A \otimes \langle\phi_i|)\rho_{AB}(I_A \otimes |\phi_i\rangle)$$

and

$$\rho_B = \mathrm{Tr}_A(\rho_{AB}) = \sum_{i=1}^{N_B} (\langle\psi_i| \otimes I_B)\rho_{AB}(|\psi_i\rangle \otimes I_B)$$

where I_A and I_B are identity matrices with respective dimensionality N_A and N_B, $|\psi_i\rangle$ is an orthonormal basis in H_A with $i = 1, 2, \ldots, N_A$, and $|\phi_i\rangle$ is an orthonormal basis in H_B with $i = 1, 2, \ldots, N_B$.

Using the density matrix ρ_{AB} in (b), explicitly compute $\mathrm{Tr}_B(\rho_{AB})$ and $\mathrm{Tr}_A(\rho_{AB})$ by hand, and show that the results agree with the subsystem matrices ρ_A and ρ_B that you generated from the computational basis in part (b).

(d) Given any density operator $\rho = \sum_{i=1}^{N} \lambda_i |\psi_i\rangle\langle\psi_i|$ with $\lambda_i \geq 1$, the von Neumann entropy is defined in units of bits as

$$S(\rho) = -\mathrm{Tr}(\rho \log_2(\rho))$$

with the usual convention that $0\log_2(0) = 0$. In terms of the eigenvalues $\{\lambda_i\}$ of ρ the von Neumann entropy can equivalently be expressed as

$$S(\rho) = -\sum_{i=1}^{N} \lambda_i \log_2(\lambda_i)$$

In this form, the entropy is identical to the Shannon entropy of the density matrix eigenvalues. Purity is $\gamma(\omega) = \mathrm{Tr}(\rho^2(\omega))$.

Given the general 2D density matrix $\rho(\omega) = \frac{1}{2}\begin{pmatrix} 1 & \omega \\ \omega & 1 \end{pmatrix}$ and using the second definition of von Neumann entropy, derive analytic expressions for both the purity, γ, and the entropy, $S(\rho)$, in terms of the mixing parameter ω. Plot the purity and entropy for $-1 \le \omega \le 1$ and comment on any other noteworthy features. For which values of ω is the state a pure state and for which values of ω is it a mixed state?

Problem 5.29

A semiconductor potential well of thickness $L = 15$ nm with uniform substitutional n-type doping density n_0 is modeled such that $V(0 < x < L) = 0$ eV, $V(0 \ge x \ge L) = \infty$ and conduction band effective electron mass is $m_e^* = 0.07 \times m_0$.

(a) Express the discretized Poisson equation using the central-difference approximation and N uniformly-spaced samples in a tridiagonal matrix form.

(b) Using an under-relaxed potential mixing coefficient $\alpha = 0.1$ iteratively solve the time-independent Schrödinger equation and Poisson equation self-consistently to relative error 10^{-4} for electron density $n_0 = 10^{17}$ cm^{-3} at temperature $T = 0$ K.

(c) Plot the first four lowest energy-eigenvalues as a function of voltage difference established across the potential well $0 \le V_{\text{bias}} \le 0.5$ eV. Compare and explain the difference in energy eigenvalues when $n = 10^{18}$ cm^{-3}.

(d) Repeat part (c) with a potential step such that before introduction of electron charge $V(3L/4 < x < L) = 0$ eV and $V(0 < x \le 3L/4) = 0.35$ eV. Explain how you might improve your model.