Chapter 4 problems

Problem 4.1

An electron in a one-dimensional rectangular potential well of thickness L and infinite potential elsewhere 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 4.2

(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 4.3

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 4.4

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 hopping integral between adjacent 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 (b) can, to within a constant, be written $E_k = 2t_{hop,1}\cos(k_x L) + 2t_{hop,2}\cos(2k_x L)$. Write a computer program to plot the dispersion relation. Then calculate and plot the electron

density of states using $\gamma = |t_{\text{hop, 1}}|/10$, $t_{\text{hop, 1}} = -1$, $t_{\text{hop, 2}} = -0.2$ and compare with the result you obtained in (b) 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.

Problem 4.5

(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? If configured as a conducting one-dimensional wire, what is the maximum conductance of the system?

(c) Show that any one-dimensional density of electron states is inversely proportional to electron group velocity, $\upsilon_g = \mathrm{d}\omega/\mathrm{d}k$. Then show that conductance is quantized in an electrically conducting one-dimensional wire, independent of its dispersion relation.

Problem 4.6

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

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

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. In radial coordinates the Hermitian momentum operator is $\hat{p}_r = -i\hbar\frac{1}{r}\frac{\partial}{\partial r}r$.

Problem 4.7
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 4.8
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 $\frac{d}{dx}$ acting on the wave function $\psi(x)$ is anti-Hermitian (i.e., $\left(\frac{d}{dx}\right)^\dagger = -\frac{d}{dx}$).

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

Problem 4.9
A particle mass m is confined to motion in a one-dimensional potential $V(x)$. The Hamiltonian is

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

and the momentum operator is

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

(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 4.10
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 4.11

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 (qubits) is that a qubit 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 qubits 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 qubit gives eigenvalue 0 with probability $|a_{00}|^2 + |a_{01}|^2$. What is the renormalized post-measurement state $|\psi'\rangle$?

(b) The first qubit in a two qubit 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 qubit when initially in state $|\psi\rangle$ and when initially in the state $|\psi'\rangle$?

Problem 4.12

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

(a) Show that the identity operator $\hat{1} \equiv \sum_n |\phi_n\rangle\langle\phi_n|$ 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 4.13

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 4.14

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 the eigenvalue may be written $E_\lambda = \langle\psi_\lambda|\hat{H}_\lambda|\psi_\lambda\rangle$.

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

(b) Starting from the time-independent Schrödinger equation

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

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

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

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

Problem 4.15

(a) Show that

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

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 4.16

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 $\hat{U}(t) = \mathrm{e}^{-\mathrm{i}\hat{H}t/\hbar}$ 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 $\hat{U}(\Delta t) = \hat{1} - \dfrac{\mathrm{i}\hat{H}\Delta t}{\hbar} + O(\Delta t)^2$.

(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 $N \to \infty$ the binomial theorem may be used to write $\mathrm{e}^x = \left(1 + \dfrac{x}{N}\right)^N$, show that $\hat{U}(t) = \mathrm{e}^{-\mathrm{i}\hat{H}t/\hbar}$.

Problem 4.17

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 4.18

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 $\Delta x \Delta p \geq \dfrac{\hbar}{2}$.

(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 units of eV when $L = 1$ nm.

Problem 4.19

(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 results for each of these geometries.

Problem 4.20

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 is learned.

(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 4.21

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 the edge-state with $v = 3.5 \times t_{\text{hop},1}$ is expected 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 observed.

Problem 4.22

(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 find the dependence of energy eigenvalue ν near ν_{EP}.

Problem 4.23

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 $\mathcal{P}\colon \hat{p} \to -\hat{p}, \hat{x} \to -\hat{x}$ and the time-reversal operator is $\mathcal{T}\colon \hat{p} \to -\hat{p}, \mathrm{i} \to -\mathrm{i}$, 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

$$\hat{H} = \hat{p}^2 + \mathrm{e}^{2\mathrm{i}x}$$

and

$$\hat{H} = \hat{p}^2 - (\mathrm{i}x)^{\alpha}$$

where α is real and the potential is $V_\alpha(x) = -(\mathrm{i}x)^{\alpha}$. 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 $\mathcal{P}\colon \hat{p} \to -\hat{p}, \hat{x} \to -\hat{x}$ and $\mathcal{T}\colon \hat{p} \to -\hat{p}, \mathrm{i} \to -\mathrm{i}$.

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

Problem 4.24

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 4.25

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 4.26

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

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

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

$$E_A c_A - t_{\mathrm{hop},1} c_B(1 + \mathrm{e}^{-\mathrm{i}kL}) = E c_A$$

and

$$-t_{\mathrm{hop},1} c_A(1 + \mathrm{e}^{\mathrm{i}kL}) + E_B c_B = E c_B$$

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 $t_{\mathrm{hop},1} = -\langle\phi_A(x)|\hat{H}|\phi_B(x)\rangle = -\langle\phi_B(x-L)|\hat{H}|\phi_A(x)\rangle$.

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

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

(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 $E_B = 1.5$ eV and nearest neighbor hoping energy is $t_{\mathrm{hop},1} = 1$ eV.

Problem 4.27

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

Problem 4.28

Find and plot the complex dispersion of a 1D tight-binding model describing s-orbital atoms with constant lattice constant L and nearest-neighbor hopping energy $t_{\text{hop},1}$ and next nearest-neighbor hopping energy $t_{\text{hop}2}$. Explain the physics of your results for the case when $t_{\text{hop},1} = 1$ eV, and (i) $t_{\text{hop},2} = 0.045 \times t_{\text{hop},1}$, (ii) $t_{\text{hop},2} = 0.2 \times t_{\text{hop},1}$, and (iii) $t_{\text{hop},2} = 0.5 \times t_{\text{hop},1}$.

Problem 4.29

Consider a one-dimensional crystal with lattice constant $L = 0.5$ nm and an s-orbital at each lattice site. The electron dispersion relation of propagating states in a tight-binding approximation is $E(k) = 2t_{\text{hop},1}(1 - \cos(kL))$, where the nearest-neighbor interaction energy is $t_{\text{hop},1}$ and Bloch wave vector is k.

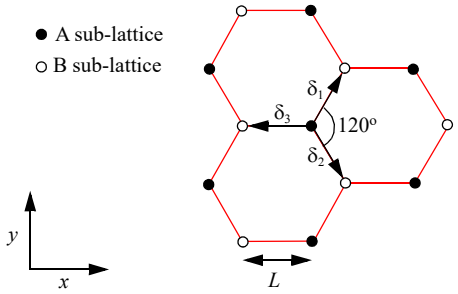
(a) Find the value of the energy $t_{\text{hop},1}$ in units of eV that gives an effective electron mass of $m_e^* = 0.07 \times m_0$ at $k = 0$, where m_0 is the bare electron mass.

(b) What is the electron dispersion relation for propagating states if both the nearest-neighbor interaction, $t_{\text{hop},1}$, and next nearest-neighbor interaction, $t_{\text{hop},2}$, is included?

(c) Find an expression for the effective electron mass in (b) when $k = 0$. What is the value of $t_{\text{hop},1}$ in units of eV that gives an effective electron mass of $m_e^* = 0.07 \times m_0$ if $t_{\text{hop},2} = 0.5 \times t_{\text{hop},1}$?

Problem 4.30

As illustrated in the following figure, the crystal structure of graphene can be described using two sub-lattices. The three nearest neighbors of type-A atoms in the honeycomb lattice of graphene are type-B atoms.



(a) Find expressions for the vectors δ_1, δ_2, and δ_3.

(b) Keeping *only* nearest neighbors, the **k**-space Hamiltonian is pure off-diagonal

$$H_{\mathbf{k}} = \begin{bmatrix} 0 & H_{\text{AB}} \\ H_{\text{AB}}^* & 0 \end{bmatrix}$$

If the matrix element coupling nearest neighbors is $t_{\text{hop},1}$ and using the values for the vectors δ_1, δ_2, and δ_3, find an analytic expression for

$$H_{\mathrm{AB}} = t_{\mathrm{hop},\,1} \sum_{j=1}^{3} \mathrm{e}^{\mathrm{i}(\mathbf{k}\cdot\delta_j)}$$

(c) The eigenvalues of $H_{\mathbf{k}}|\mathbf{k}\rangle = E_{\mathbf{k}}|\mathbf{k}\rangle$ are such that

$$\begin{vmatrix} -E_{\mathbf{k}} & H_{\mathrm{AB}} \\ H_{\mathrm{AB}}^{*} & -E_{\mathbf{k}} \end{vmatrix} = E_{\mathbf{k}}^2 - |H_{\mathrm{AB}}|^2 = 0$$

Show that the solution is

$$E_{\mathbf{k}} = \pm t_{\mathrm{hop},\,1} \sqrt{1 + 4\cos\left(3k_x\frac{L}{2}\right)\cos\left(\sqrt{3}k_y\frac{L}{2}\right) + 4\cos^2\left(\sqrt{3}k_y\frac{L}{2}\right)}$$

(d) Find the values of $\mathbf{k}$ for which $E_{\mathbf{k}} = 0$.

Problem 4.31

The nearest-neighbor tight-binding Schrödinger equation for a one-dimensional array of integer N_{at} sites, lattice spacing L, on-site potential V_n, and hopping energy $-t_{\mathrm{hop},1}$ is

$$\hat{H}_n\psi_n = V_n\psi_n - t_{\mathrm{hop},1}\psi_{n+1} - t_{\mathrm{hop},1}\psi_{n-1} = E_n\psi_n$$

The Hamiltonian is modified to include an impulse source at far left site position $x_{n=1}$ so that $\hat{H}' = \hat{H} - \hat{B}$ where the boundary matrix is $\hat{B}$.

(a) Show that if source vector $\mathbf{s}$ is $\mathbf{s} = (\hat{H}' - E\mathbf{1})\psi = \tilde{H}\psi$ and Green's function $G = \tilde{H}^{-1}$, then $\psi = G\mathbf{s}$.

(b) Consider a source vector that has one entry $s_1 = -2t_{\mathrm{hop},1}\mathrm{i}\sin(kL)\mathrm{e}^{\mathrm{i}kx_1}$ corresponding to a particle incident from the left and that $\hat{B}$ is null except for $B_{11} = B_{N_{\mathrm{at}}N_{\mathrm{at}}} = t_{\mathrm{hop},1}\mathrm{e}^{\mathrm{i}kL}$. Calculate transmission $|\psi(x_{N_{\mathrm{at}}})|^2$ of an electron mass m_0 incident on a rectangular potential barrier of energy $V_0 = 1$ eV and thickness $L_{\mathrm{b}} = 1$ nm as a function of energy $0 \le E \le 4$ eV when $L = 0.25$ nm and $t_{\mathrm{hop},1} = 0.6096$ eV. Repeat the calculation for $L = 0.1$ nm and $t_{\mathrm{hop},1} = 3.8100$ eV. Explain your results.