1. Multi-channel scattering and Feshbach resonances
Here we will generalize HW2 by adding one more close channel to model Feshbach resonance in nuclear and in atomic physics.

A. Given the Hamiltonian $H = \frac{p^2}{2\mu} - V(r)$ with $V(r > r_0) = \begin{pmatrix} \infty & 0 \\ 0 & 0 \end{pmatrix}$ and $V(r < r_0) = -\frac{\hbar^2}{2\mu} \begin{pmatrix} q_c^2 & \epsilon \\ \epsilon & q_o^2 \end{pmatrix}$, where $\epsilon$ couples the open and closed channels with wavenumber $q_o$ and $q_c$. Assume an open channel scattering state with energy $E = \frac{\hbar^2 k^2}{2\mu} > 0$ is phase shifted as $r\psi(r > r_0) = \begin{pmatrix} 0 \\ \sin(kr + \delta) \end{pmatrix}$. Show that

$$k \cot(k r_0 + \delta) = q_c \cos^2 \alpha \cot q_c r_0 + q_o \sin^2 \alpha \cot q_o r_0,$$

where $\tan 2\alpha = \frac{2\epsilon}{q_c^2 - q_o^2}$ and $q_\pm$ is the eigen-wavenumber and approaches $q_o$ and $q_c$ in the limit of weak coupling $\epsilon \to 0$ and low scattering energy $k \to 0$.

Hint: Use the boundary conditions to relate the wavefunctions: $\psi(r_0^+) = \psi(r_0^-)$ and $\psi'(r_0^+) = \psi'(r_0^-)$.

B. In most atoms, we can assume that $\epsilon < |q_c^2 - q_o^2|$ because spin coupling is typically weaker than the molecular potential. We further assume that the closed channel supports a bound state at energy $E_c$ very close to the open channel threshold $E = 0$. Show that the existence of the bound state gives $\sin \sqrt{\epsilon^2 + \frac{2\mu E_c}{\hbar^2} r_0} = 0$, and thus we can rewrite the last term in Eq. (1) as $q_o \sin^2 \alpha \cot q_o r_0 \approx -\frac{\Gamma/2}{r_0 E_c}$, where Feshbach coupling strength is defined as $\Gamma \approx 4\alpha^2 \frac{\hbar^2 q_c^2}{2\mu}$. We thus have

$$k \cot(k r_0 + \delta) = q_c \cos^2 \alpha \cot q_c r_0 - \frac{\Gamma/2}{r_0 E_c}$$
C. Show that scattering length can be defined as \( \lim_{k \to 0} k \cot(k r_0 + \delta) = -\frac{1}{a - r_0} \) and thus
\[
q_s \cos^2 \alpha \cot q_s r_0 = -\frac{1}{a_{bg} - r_0},
\]
where \( a_{bg} \) is the background scattering length in the absence of closed channel bound state.

D. Finally we assume the bound state energy can be magnetically tuned as 
\( E_c = \mu(B - B_c) \), where \( \mu \) is the magnetic moment and \( B_c \) is field values that the state crosses the continuum. Show that the scattering length can be rewritten as
\[
a = a_{bg} \left(1 - \frac{\Delta B}{B - B_0}\right).
\]
Determine the resonance width \( \Delta B \) and resonance position \( B_0 \) in terms of \( a_{bg} \), \( \Gamma \), \( \mu \) and \( B_c \).

E. One might naively expect that Feshbach resonance occurs when scattering atoms resonantly couple to the bound state \( E_c = 0 \). Show that this is false. What is the scattering length when \( E_c = 0 \), and what is the energy of the bound state when the scattering length diverges \( a \to \pm \infty \)?

Hint: You may look at Eq.(2) and see the conditions for \( a \to \pm \infty \) and for \( E_c = 0 \).

2. Bare molecules vs Feshbach molecules

A. Use the same Hamiltonian in the previous question and show that for a bound state with energy \( E = -E_b = -\frac{\hbar^2}{2\mu} k_m^2 < 0 \), the wavefunction outside the potential is given by
\[
r \psi(r > r_0) \propto \begin{cases} 0 \\ \exp(-k_m r) \end{cases},
\]
where \( E_b \) is called the molecular binding energy.

B. Matching the boundary condition like what you did in 1A with \( E = -E_b < 0 \) slightly below the continuum, show that you get
\[
k_m = \frac{1}{a_{bg} - r_0} + \frac{\Gamma/2}{r_0(E_b + E_c)}.
\]
C. Show that a molecular bound state with vanishing energy \( k_m \to 0 \) exists when the scattering length approaches positive infinity \( a \to +\infty \). The molecule, also called Feshbach molecule, is the eigen-state of the system and is different from the bare molecule in problem 1D.

D. Show that the Feshbach bound state has a binding energy of
\[
E_b = \frac{\hbar^2}{2\mu(a - a_0 + R)^2} + O(a^{-2}).
\]
Determine the resonance length scale \( R \).
3. Band structure in 1D lattice
For a single particle in a 1D lattice with $N \gg 1$ sites $\hat{E}_k = -t \sum_j \hat{a}_{j+1}^\dagger \hat{a}_j + h.c.$, we showed in
the class that $\frac{1}{\sqrt{N}} \sum_j (\pm 1)^j a_j^\dagger |0> \text{ has the lowest/highest energy of } E_k \equiv \langle E_k \rangle = \mp 2t$.

A. The above 2 states are special cases of the more general state $|k> = \frac{1}{\sqrt{N}} \sum_j e^{i j k} a_j^\dagger |0>$. Evaluate its energy $E_k$.

B. Show that for small $k$, we can write $E_k \approx \frac{\hbar^2 k^2}{2m} + \text{const.}$, what is the effective mass $m$ of the particle?

C. Argue that $|k>$ is the same as the plane wave state in the continuum $\psi(x) = e^{iKx}$ of a free particle with wavenumber $K$ if you assume the spacing between two sites is small $a \to 0$. How would you choose the tunneling $t$ if the mass of the particle is $m$?

4. 3-site Bose-Hubbard model

Three Bosons are loaded into three optical tweezers forming an equilateral triangle. The Hamiltonian is

$H = \hat{E}_k + \hat{E}_{int}$, where $\hat{E}_k = -t (\hat{a}_1^\dagger \hat{a}_2 + \hat{a}_2^\dagger \hat{a}_3 + \hat{a}_3^\dagger \hat{a}_1) + h.c.$ and $\hat{E}_{int} = \frac{U}{2} \sum_{i=1}^{3} \hat{n}_i (\hat{n}_i - 1)$.

A. Write down the ground state in the limit of $U = 0$ and $t = 0$. If the system can only occupy either of the two states, at what value of $U/t$ does the ground state switches from one to the other?

B. If we wish to solve the problem analytically, what is the dimension of the Hilbert space (how many possible configurations can you distribute 3 atoms)?
Hint: a general state can be written as the superposition of the states $|n_1, n_2, n_3>$, where $n_1 + n_2 + n_3 = 3$.

C. Repeat B if you assume the state must respect the symmetry of the system.