1.) VARIATIONAL METHOD FOR 1d OSCILLATOR

To get a feel for how well the variational approximation works, it is useful to try it out on a simple soluble model - here the 1d Harmonic oscillator with Hamiltonian,

\[ H = \frac{\hat{\mathbf{p}}^2}{2m} + \frac{1}{2} m \omega^2 \hat{x}^2. \]  (1)

Using the following variational wave functions:

a.) \[ \psi_\alpha(x) = e^{-\alpha|x|}, \]

b.) \[ \psi_\alpha(x) = e^{-\alpha x^2}, \]

c.) \[ \psi_\alpha(x) = \alpha - |x| \text{ for } |x| \leq \alpha \text{ and } \psi = 0 \text{ otherwise}, \]

estimate the ground state energy of the harmonic oscillator, and discuss how your estimate compares with the exact result, \( E_0 = \hbar \omega / 2 \).

A variational bound on the energy of the first excited state, \( E_1 \), can be obtained by using an odd parity variational wave function (why?). Estimate \( E_1 \) using

d.) \[ \psi_\alpha(x) = xe^{-\alpha |x|}, \]

e.) \[ \psi_\alpha(x) = xe^{-\alpha x^2}, \]

and compare to the exact result.

The quality of your variational estimate for the ground state wavefunction can be determined by evaluating the overlap between the (normalized) variational state \( |\psi_{\text{var}}\rangle \) and the exact (normalized) ground state \( |0\rangle \) as

\[ O = \sqrt{|\langle \psi_{\text{var}} | 0 \rangle|^2}. \]  (2)

Bonus: Evaluate \( O \) for the three variational states (a), (b) and (c) and discuss.

2.) PERTURBATION THEORY FOR A NON-LINEAR OSCILLATOR

Consider the Hamiltonian \( \hat{H} = \hat{H}_0 + \hat{H}_1 \), where \( \hat{H}_0 \) is the (beloved!) Harmonic oscillator Hamiltonian,

\[ \hat{H}_0 = \frac{1}{2m} \hat{\mathbf{p}}^2 + \frac{1}{2} m \omega^2 \hat{x}^2; \]  (3)

and \( \hat{H}_1 \) is a perturbation produced by additional cubic and quartic terms, which can be expressed in the dimensionally transparent form as

\[ \hat{H}_1 = \frac{1}{2} m \omega^2 \hat{x}^2 [g_3(\hat{x}/x_0) + g_4(\hat{x}/x_0)^2], \]  (4)

where \( x_0 = (\hbar/2m \omega)^{1/2} \) is a characteristic length and \( g_3 \) and \( g_4 \) are dimensionless coupling constants. (If \( \hat{H}_0 \) is regarded as an approximate Hamiltonian for a particle near the minimum of a general potential well, \( V(x) \), then \( \hat{H} \) can be regarded as a more accurate representation, obtained by taking terms through \( \hat{x}^4 \) in the expansion of \( V(x) \) about its minimum at \( x = 0 \).

A.) Calculate the change in the ground state energy and wave function to linear order in \( g_3 \) and \( g_4 \).

B.) Calculate the change in the ground state energy to second order in \( g_3 \) and \( g_4 \).

Hint: It will be useful to express \( \hat{x} \) in terms of oscillator raising and lowering operators as \( \hat{x}/x_0 = \hat{a} + \hat{a}^\dagger \).
3.) TWO-LEVEL SYSTEM

Physical systems that can be modeled in terms of a simple 2-level quantum mechanical system are common, a classic example being two nearby tunneling states for an impurity atom in a solid. More generally, the two states can often represent two adjacent energy levels in the spectrum of a more complicated system.

The Hamiltonian for a two-state system can be represented as a $2 \times 2$ Hermitian matrix, $H_{ij} = H_{ji}^*$ with $i, j = 1, 2$. In the absence of time reversal symmetry breaking terms the Hamiltonian is real, and hence symmetric, and in general is given by,

$$H_{11} = E_1^{(0)}, \quad H_{22} = E_2^{(0)}, \quad H_{12} = H_{21} = \Delta,$$

where $E_1^{(0)}$ and $E_2^{(0)}$ are the “unperturbed” energies, and $\Delta$ is a (real) tunneling matrix element. For $\Delta = 0$, the energy eigenfunctions are given by, $\phi_1^{(0)} = (1, 0)^T$ and $\phi_2^{(0)} = (0, 1)^T$.

A.) Solve this problem exactly to find the energy eigenfunctions $\psi_1$ and $\psi_2$, and associated eigenvalues, $E_1$ and $E_2$.

B.) Assuming that $\Delta << |E_1^{(0)} - E_2^{(0)}|$, use time independent perturbation theory to solve for the eigenfunctions $\psi_1, \psi_2$ up to first order in $\Delta$, and the eigenvalues up to second order. Compare with the exact expressions.

C.) Show that, up to an additive constant, $H_{ij}$ is equivalent to the Hamiltonian of a spin-$1/2$ particle (with gyromagnetic ration $\gamma$) in a magnetic field,

$$H = -\gamma \vec{S} \cdot \vec{B},$$

with $\vec{B} = B_x \hat{x} + B_z \hat{z}$, and express $B_x$ and $B_z$ in terms of $E_i^{(0)}$ and $\Delta$.

Energy Level repulsion: When $E_i^{(0)}$ correspond to the adjacent energy levels in a very complicated quantum system (eg. a high Z-nucleus, or electron states in a disordered solid) with mixing $\Delta$, it is often useful to presume that these parameters are essentially random. In this case, the (exact) energy level spacing $E = |E_1 - E_2|$ will also be random. To be concrete, assume that the (“fictitious”) magnetic field $\vec{B}$ is uniformly distributed in the $B_x - B_z$ plane, with $|\vec{B}| \leq B_0$.

D.) Under this assumption, compute the energy level spacing distribution $P(E)$ (where $P(E)dE$ = probability that energy spacing is in the interval $E$ to $E + dE$), and show that it vanishes as $E \to 0$, varying as $P(E) \sim E^n$. Determine the exponent $n$. The vanishing probability for degenerate energy levels is referred to as “level repulsion” - an extremely useful concept in complicated quantum systems.

4.) VAN DER WAALS INTERACTION

The van der Waals interaction is a weak interaction between two neutral atoms, which are separated by a distance much larger than their size. It arises from the interaction between fluctuating electric dipoles on the two atoms.

Here, consider the van der Waals interaction between two Hydrogen atoms, with their protons fixed in space, at a distance $r$ along the $z-$ axis from one another. In terms of $\vec{r}_1$ (a vector from the first proton to its electron) and $\vec{r}_2$ (from the 2nd proton to its electron) the Hamiltonian can be written as $\hat{H} = \hat{H}_0 + \hat{H}_1$ with

$$\hat{H}_0 = \frac{1}{2m} \vec{P}_1^2 + \frac{1}{2m} \vec{P}_2^2 - \frac{e^2}{r_1} - \frac{e^2}{r_2},$$

$$\hat{H}_1 = \frac{e^2}{r} + \frac{e^2}{|\vec{r} + \vec{r}_2 - \vec{r}_1|} - \frac{e^2}{|\vec{r} + \vec{r}_2|} - \frac{e^2}{|\vec{r} - \vec{r}_1|},$$

with $\vec{r} = r\hat{z}$. In the ground state of $H_0$, the two electrons are confined within a Bohr radius of their protons, so that $r_i \sim a_0$.

A.) For large separation, $r >> a_0$, show that $H_1$ can be approximated as,

$$H_1 = \frac{e^2}{r^2}(\vec{r}_1 \cdot \vec{r}_2 - 3z_1 z_2) + O(1/r^4),$$

which corresponds to the interaction between two electric dipoles, $e\vec{r}_i$, separated by $\vec{r}$. 


B.) Treating this approximate form of $H_1$ as a perturbation, show that the first order correction to the ground state energy of $H_0$ vanishes.

C.) Show that the 2nd order correction is non-vanishing and corresponds to an attractive van der Waal interaction between the two Hydrogen atoms, which varies as $1/r^6$.

5.) DEGENERATE PERTURBATION THEORY FOR 2D OSCILLATOR  
(Sakurai Problem 5.4)

Consider an isotropic harmonic oscillator in two dimensions, with Hamiltonian

$$H_0 = \frac{P_x^2}{2m} + \frac{P_y^2}{2m} + \frac{m \omega^2}{2} (X^2 + Y^2). \quad (10)$$

A.) What are the energies and degeneracies of the states with the three lowest-lying energies?

B.) Consider a small perturbation,

$$H_1 = \epsilon m \omega^2 XY, \quad (11)$$

where $\epsilon$ is a small dimensionless real number. Find the zeroth-order energy eigenket(s) and the first order eigen-energy shift(s), for each of the three lowest-lying multiplets.

C.) Solve the full problem, $H_0 + H_1$, exactly, and compare with your perturbation theory results.

6.) TWO-SITE QUANTUM ISING MODEL

One of the simplest many-body Hamiltonians is the so-called Quantum Ising Model which consists of a lattice of $s = 1/2$ spins coupled thru an exchange interaction, $J$, in an applied magnetic field, $h$. Here we consider a baby-version of this model with just 2-sites with Hamiltonian, $\hat{H} = \hat{H}_0 + \hat{H}_1$, where,

$$\hat{H}_0 = J \hat{\sigma}_1^z \hat{\sigma}_2^z, \quad (12)$$

$$\hat{H}_1 = h (\hat{\sigma}_1^x + \hat{\sigma}_2^x + \hat{\sigma}_1^z + \hat{\sigma}_2^z). \quad (13)$$

Here, $\hat{\sigma}_j^\mu$ with $(\mu = x, y, z)$ are Pauli spin operators for the 2-sites, $j = 1, 2$. A convenient basis of states can be constructed from the eigenstates of $\hat{\sigma}_j^z$, i.e. four kets denoted by $|\sigma_1^z, \sigma_2^z\rangle$ with $\sigma_j^z = \pm 1 = \uparrow, \downarrow$.

$$|\uparrow\uparrow\rangle, |\downarrow\downarrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle. \quad (14)$$

A.) Using degenerate perturbation theory compute the energies of the four eigenstates perturbatively for $h \ll J$ up to order $h^2$.

B.) Obtain the four corresponding eigenfunctions to leading non-trivial order (up to order $h$).