Homework 1

1. [10 pt] Consider a simple two-state system where a particle is either absent $|0\rangle$ or present $|1\rangle$. The first has energy E_0, while the second has energy E_1. This is a simple model for fermions, where a state can only be occupied by one particle at a time. Define the *annihilation operator* $\hat{a}$ by $\hat{a}|1\rangle = |0\rangle$ and $\hat{a}|0\rangle = 0$, and the *creation operator* as the Hermitian conjugate, $\hat{a}^\dagger$.

   a. Write the matrix forms for $\hat{a}$, $\hat{a}^\dagger$, $\hat{a}^\dagger\hat{a}$ and $\hat{a}\hat{a}^\dagger$.
   b. What is the anticommutator $\{\hat{a}, \hat{a}^\dagger\}$?
   c. Write the Hamiltonian operator $\hat{H}$ in terms of creation and annihilation operators.

2. [15 pt] Prove that if an operator $\hat{A}$ is Hermitian, then the operator $\hat{U} = \exp(i\theta\hat{A})$ is unitary for real values of θ. (*Hint:* write $\hat{A}$ and $\hat{U}$ in terms of an eigenfunction expansion).

3. [15 pt] Consider the 1D problem of particles in a box of length a. In this case, the energy is purely due to kinetic energy. If we have identical, non-interacting fermions, then the ground state energy of N particles is the sum of the lowest N single particle energies. Determine the large N limit of the kinetic energy per particle E/N in terms of the density $n = N/a$ as

$$\frac{E}{N} = A \cdot n^\alpha$$

   and find the values of A and α.

4. [10 pt] Consider a set of functions $r(\theta) \geq 0$ in polar coordinates. The area and perimeter are:

$$A[r] = \int_0^{2\pi} \frac{1}{2}(r(\theta))^2 \, d\theta$$

$$P[r] = \int_0^{2\pi} \sqrt{(r(\theta))^2 + \left(\frac{dr}{d\theta}\right)^2} \, d\theta$$

   Use the Euler-Lagrange equations to write the expression that would minimize $P[r]$ for a given $A[r] = A_0$. This should be a differential equation. Identify a solution to this equation.

5. [25 pt] The harmonic oscillator Hamiltonian,

$$\hat{H}^0 = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2$$

   has solutions in terms of Hermite polynomials with $\alpha = \sqrt{\hbar/m\omega}$,

$$\psi_n^0(x) = \sqrt{\frac{1}{\alpha 2^n n! \sqrt{\pi}}} e^{-\frac{1}{2}(x/\alpha)^2} H_n(x/\alpha)$$

   with energy $E_n = (n + \frac{1}{2})\hbar\omega$. There is a creation operator $\hat{a}^\dagger$ where $\hat{a}^\dagger|\psi_n^0\rangle = \sqrt{n+1}|\psi_{n+1}^0\rangle$ and an annihilation operator $\hat{a}$ where $\hat{a}|\psi_n^0\rangle = \sqrt{n}|\psi_{n-1}^0\rangle$. You can show that $[\hat{a}, \hat{a}^\dagger] = 1$ and $\hat{H}^0 = \hbar\omega(\hat{a}^\dagger\hat{a} + \frac{1}{2})$. Moreover, the position operator $\hat{x}$ is

$$\hat{x} = \frac{\alpha}{\sqrt{2}}(\hat{a} + \hat{a}^\dagger)$$

Consider adding a quartic term to the potential,

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2 + \gamma\left(\frac{x}{\alpha}\right)^4$$

for $\gamma > 0$.

a. Write out the new Hamiltonian in terms of the operators $\hat{a}$ and $\hat{a}^\dagger$.
b. Using $|\psi_n^0\rangle$ as orthonormal basis functions, what is the matrix form of the Hamiltonian H_{mn}? (*Hint:* you can evaluate $\langle\psi_m^0|(\hat{x}/\alpha)^4|\psi_n^0\rangle$ as the inner product of $(\hat{x}/\alpha)^2|\psi_m^0\rangle$ and $(\hat{x}/\alpha)^2|\psi_n^0\rangle$).
c. Using your favorite language for solving numerical problems, estimate the ground state energy for $\hbar\omega = \gamma = 1$, using a finite number of basis functions. How does your estimate change with the number of basis functions that you use?

6. [25 pt] The He singlet state can be approximately solved using the variational principle. Take the two electron Hamiltonian (in atomic units),

$$\hat{H} = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{|\vec{r}_1 - \vec{r}_2|}$$

The spin singlet state is

$$|\Psi\rangle = \frac{1}{\sqrt{2}}\left[|\psi(r_1)\rangle|\uparrow_1\rangle \otimes |\psi(r_2)\rangle|\downarrow_2\rangle - |\psi(r_1)\rangle|\downarrow_1\rangle \otimes |\psi(r_2)\rangle|\uparrow_2\rangle\right]$$

with the same spatial orbital $\psi(r)$ for both electrons. Taking inspiration from the H atom, let's use the normalized orbital

$$\psi(r) = \frac{1}{\sqrt{\pi}}a^{-3/2}e^{-r/a}$$

where a is a variable to be determined. If we considered the He^+ ion, then a would be $1/Z = 1/2$, and the energy would be $-Z^2/2 = -2$, so if there were *no interaction*, the energy of He would be -4 Hartree. We'll use the variational principle to find the optimal a value and estimate the energy.

a. First, determine $\langle\Psi|\hat{H}^0|\Psi\rangle$, where $\hat{H}^0$ is the *non-interacting* part of the Hamiltonian.
b. To evaluate the electron-electron interaction term, show that it can be written as

$$\int d^3r_1|\psi(r_1)|^2 \int d^3r_2 \frac{|\psi(r_2)|^2}{|\vec{r}_1 - \vec{r}_2|}$$

c. Next, recall that the inner integral is the electrostatic potential at $\vec{r}_1$ from the density $|\psi(r)|^2$, and that for a spherical density $\rho(r)$, the potential is

$$V(r) = \frac{4\pi}{r}\int_0^r u^2\rho(u)\,du + 4\pi\int_r^\infty u\rho(u)\,du$$

Use this to evaluate the electron-electron interaction energy.
d. Finally, write the total energy $E(a)$, and find the minimizer. What is the ground state energy? How does it compare with the known value of -2.903724377 Hartree?
e. Recall that for a single electron, $a = 1/Z$. What does your optimal value of a tell you about the nuclear charge that each electron "sees"?