1. In the previous assignment you developed Python code to solve Schrödinger's equation for a pair of interacting oscillators with Hamiltonian

$$\mathcal{H} = h(x) + h(y) + ax^4y^4, \tag{1}$$

where

$$h(x) = -\frac{1}{2}\frac{\partial^2}{\partial x^2} + \frac{1}{2}x^2 \qquad \text{and} \qquad h(y) = -\frac{1}{2}\frac{\partial^2}{\partial y^2} + \frac{1}{2}y^2.$$

The method you used, expanding the wavefunction $\psi(x, y)$ in a basis set of 2-d Gaussians spanning the xy-plane, is limited in accuracy only by the number of basis functions included. With a few hundred functions, the result is essentially exact.

Here you will study the same problem using the more approximate mean field theory we developed in class. Based on the variation principle, we found that the optimal *uncorrelated* wavefunction

$$\tilde{\psi}(x, y) = \chi_1(x)\chi_2(y)$$

satisfies the self-consistent mean-field equations,

$$h_{\text{eff}}(x)\chi_1(x) = \epsilon_1\chi_1(x), \qquad h_{\text{eff}}(y)\chi_2(y) = \epsilon_2\chi_2(y), \tag{2}$$

with

$$h_{\text{eff}}(x) = h(x) + a\left(\int dy\, \chi_2^2(y)y^4\right)x^4 \quad \text{and} \quad h_{\text{eff}}(y) = h(y) + a\left(\int dx\, \chi_1^2(x)x^4\right)y^4.$$

(i) Add a thorough set of comments to the code `interacting_oscillators_scf.py` we wrote to solve Eq. 2 (also see the Lecture 9 Notebook).

(ii) Use the code to calculate the mean-field ground state energy $\tilde{E}_0$ for many a values between $a = 0$ and $a = 0.01$. Set the spacing between basis functions at $\Delta x = 0.5$, the Gaussian width parameter at $\alpha = 2$, and the number of basis functions at $K = (2 \times 10 + 1)$. In solving the mean field equations, perform at least 100 iterations.

Plot $\tilde{E}_0$ as a function of a, together with the estimate from perturbation theory

$$E_0^{(\text{PT})}(a) = 1 + 9a/16 \tag{3}$$

Does our mean field approach accurately capture the response of these oscillators to a weak interaction?

(iii) Use the mean field code to calculate $\tilde{E}_0$ over a larger range of a. Report results for $a = 0.001, 0.01, 0.05, 0.1, 0.5, 1$, and 10 in a table.

(iv) Describe in a few sentences how your results in part (iii) compare with the more exact results from direct basis set expansion in Problem Set 4. (If you are feeling ambitious, you could plot both sets of results in the same graph.)

(v) For the case $a = 10$, make a contour plot of the mean field ground state wavefunction over a range of x and y values spanning -2.5 to 2.5. How does your result differ from the more exact result you obtained in in Problem Set 4? Can you explain the difference in terms of correlations that are neglected in mean field theory?

The two oscillators studied in problem 1 (and in previous assignments) are *distinguishable*, since the probability

$$P(x, y) = |\psi(x, y)|^2$$

can differ from the probability $P(y, x)$ in which the particles' labels have been exchanged.

The rest of this assignment focuses on oscillators that are instead *indistinguishable*. More specifically, we will take them to be indistinguishable in the same way as electrons: Their wavefunction $\psi(x, y)$ must be *antisymmetric* with respect to exchange of x and y:

$$\psi(x, y) = -\psi(y, x).$$

Here you will solve for energies and wavefunctions of antisymmetric oscillators using a direct basis set expansion,

$$\psi(x, y) = \sum_A c_A \phi_A(x, y),$$

with basis functions $\phi_A(x, y)$ that are centered at various points in the xy-plane.

2. This problem considers a *noninteracting* ($a = 0$ in Eq. 1) pair of indistinguishable oscillators.

   (i) To respect the constraint of indistinguishability, the basis functions $\phi_A(x, y)$ must themselves be antisymmetric.

   The basis states $|x_A, y_A\rangle$ we have used in the past, representing the function

   $$\exp[-\alpha(x - x_A)^2 - \alpha(y - y_A)^2]$$

   are not antisymmetric. Show that this is true.

   (ii) Acceptable basis functions for the antisymmetric system cannot distinguish between x and y, and therefore cannot be centered on a specific point (x_A, y_A) in the xy-plane. Instead, a function centered at the point (u_A, v_A) could be paired with another function centered at the exchanged point (v_A, u_A):

   $$\phi_A(x, y) = \exp[-\alpha(x - u_A)^2 - \alpha(y - v_A)^2] - \exp[-\alpha(x - v_A)^2 - \alpha(y - u_A)^2] \qquad (4)$$

   (We have switched the notation from (x_A, y_A) to (u_A, v_A) because these parameters can no longer be associated exclusively with x or y.) Show that the basis function in Eq. 4 is in fact antisymmetric, and make a contour plot of $\phi_A(x, y)$ in the xy-plane for the case $u_A = 2$ and $v_A = 1$.

   (iii) Let us denote the basis function of Eq. 4 as

   $$|\phi_A\rangle = |u_A, v_A\rangle - |v_A, u_A\rangle$$

   Show that the overlap between two such functions is

   $$\begin{aligned} S_{AB} &= \langle \phi_A | \phi_B \rangle \\ &= 2s(u_A, u_B)s(v_A, v_B) - 2s(v_A, u_B)s(u_A, v_B), \end{aligned}$$

   where

   $$s(x_A, x_B) = \int dx\, e^{-\alpha(x-x_A)^2} e^{-\alpha(x-x_B)^2} = \sqrt{\frac{\pi}{2\alpha}}\, \exp\left[-\frac{\alpha}{2}(x_A - x_B)^2\right].$$

   as in the previous assignment. (The result of the integral is included here as a reminder – you do not need to show it.)

(iv) Similarly, show that the single-particle matrix elements $\langle\phi_A|h(x)|\phi_B\rangle$ and $\langle\phi_A|h(y)|\phi_B\rangle$ evaluate to

$$\begin{aligned} h_{AB} &= \langle\phi_A|h(x)|\phi_B\rangle = \langle\phi_A|h(y)|\phi_B\rangle \\ &= f(u_A,u_B)s(v_A,v_B) + f(v_A,v_B)s(u_A,u_B) \\ &\quad -f(u_A,v_B)s(v_A,u_B) - f(v_A,u_B)s(u_A,v_B), \end{aligned}$$

where

$$\begin{aligned} f(x_A,x_B) &= \int dx\, e^{-\alpha(x-x_A)^2} h(x) e^{-\alpha(x-x_B)^2} \\ &= \frac{s(x_A,x_B)}{2}\left[\alpha + \frac{1}{4\alpha} + \frac{1}{4}(x_A+x_B)^2 - \alpha^2(x_A-x_B)^2\right] \end{aligned}$$

(The result of the integral is included here as a reminder – you do not need to show it.)

(vi) To implement this approach in Python, we need to set up a list of basis function centers (u_A, v_A) in the xy-plane. For the antisymmetrized basis, the centers (u_A, v_A) and (v_A, u_A) correspond to the same basis state, so we should restrict our choices to $u_A < v_A$. Noting as well that $u_A = v_A$ is not a viable choice, we would like the collection of centers to be arranged as in Fig. 2.

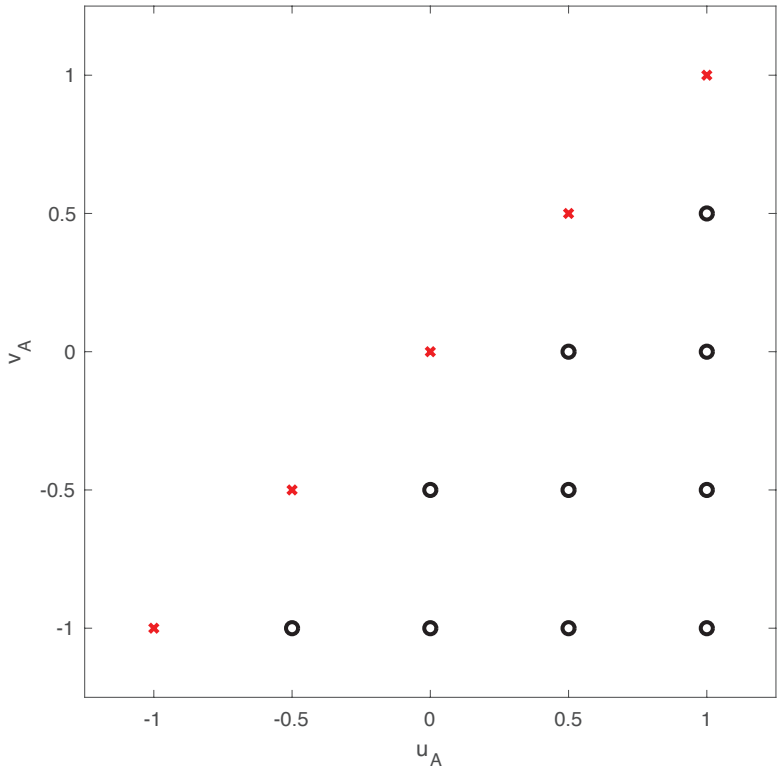

Figure 1: Circles indicate a possible set of non-redundant choices for basis function parameters u_A and v_A. Red x's are a reminder that points with $u_A = v_A$ must be excluded.

The following code generates an appropriate list of $K = n(2n+1)$ centers:

```
center = zeros((K,2))
count=0
for i in range(-(n-1),n+1):
    uA = i*deltax
    for j in range(-n,i):
        vA = j*deltax
        center[count,:]  = [uA, vA]
        count=count+1
```

(5)

Using Python, together with our linear algebra formulation of the Schrödinger equation and previous results of this problem, calculate the 9 lowest energies of the noninteracting pair of indistinguishable oscillators. With a sufficient number of basis functions you should be able to closely reproduce your expectations for these energy levels and their corresponding degeneracy. Python functions that calculate the quantities $s(x_A, x_B)$ and $f(x_A, x_B)$ are provided on bcourses (in a file `oscillator_functions.py`) for your convenience.

Set the spacing between basis functions at $\Delta x = 0.5$ (in both x and y directions), and the Gaussian width parameter at $\alpha = 2$.

3. In this problem we will add interactions ($a > 0$ in Eq. 1) to the antisymmetric oscillators.

   (i) For the interacting system we need matrix elements of the operator x^4y^4. Show that

$$\begin{aligned} G_{AB} &= \langle \phi_A | x^4 y^4 | \phi_B \rangle \\ &= 2g(u_A, u_B)g(v_A, v_B) - 2g(v_A, u_B)g(u_A, v_B), \end{aligned}$$

   where

$$\begin{aligned} g(x_A, x_B) &= \int_{-\infty}^{\infty} dx\, e^{-\alpha(x-x_A)^2}\, x^4\, e^{-\alpha(x-x_B)^2} \\ &= s(x_A, x_B)\left[\frac{3}{16\alpha^2} + \frac{3}{8\alpha}(x_A + x_B)^2 + \frac{1}{16}(x_A + x_B)^4\right]. \end{aligned}$$

   (The result of the integral is included here as a reminder – you do not need to show it.)

   (ii) Extending your code from problem 2 to the interacting case, calculate the ground state energy E_0 for several values of the interaction strength: $a = 0.001$, $a = 0.01$, $a = 0.1$, $a = 1$, and $a = 10$. Use the same parameters as in the previous problem.

   A Python function that calculates the quantity $g(x_A, x_B)$ is provided on bcourses (in the file `oscillator_functions.py`) for your convenience.

   (iii) Make a contour plot of the ground state wavefunction for each of the a values of part (ii), as well as for $a = 0$.

   (iv) Your results for small a should be consistent with perturbation theory:

$$E_0(a) \approx E_0(0) + a\langle \psi_0 | x^4 y^4 | \psi_0 \rangle = 2 + \frac{45}{16}a, \tag{6}$$

where $E_0(a)$ denotes the ground state energy for a given value of a, and $|\psi_0\rangle$ denotes the unperturbed ground state wavefunction at $a = 0$.

Plot the perturbation theory estimate of Eq. 6 as a function of a over the range $a = 0$ to $a = 0.01$. Include your basis set expansion results for comparison.