Project 3: Non-interacting 2D Electrons in a planar trap

Roi Baer
Fritz Haber Center for Molecular Dynamics, Institute of Chemistry, The Hebrew University of Jerusalem 91904

In this project you will learn to compute the number of electrons in a potential trap at given temperature and chemical potential. Please submit a short report according to the following instructions.

In this project you will compute the number of electrons in a potential trap at low temperature and chemical potential. For a specific case we consider two-dimensional electrons placed on the X-Y plane between 4 negative charges, each of charge –Q, fixed at points $a((-1)^n,(-1)^m)$, $m,\, n = 0, 1$. Please study this system using a harmonic approximation (this is a semi-analytical approach) where the calculations can be done using the known eigenvalues of the harmonic potential and then using a general program that you will write.

You will use the semi-analytical results to check the general numerical code.

I. THE POTENTIAL AND THE HARMONIC APPROXIMATION

1. Write down the potential $V(x,y)$ of an electron due to the charges.
2. Show that this potential has a (local) minimum in the origin.
3. Write down the harmonic approximation to the potential $V_H(x,y)$. What is the harmonic frequency as a function of the electron mass, the trap size a and the trap charge Q.
4. A Semi-analytical calculation:
   (a) Assuming the electrons within the harmonic trap are non-interacting give an expression (can be an infinite sum) for the number of electrons $N_e(\beta,\mu)$ and their entropy $S(\beta,\mu)$ as a function of inverse temperature $\beta = (k_B T)^{-1}$ and chemical potential μ and the trap frequency ω.
   (b) Write a short computer code to perform numerically the sums in expressions you derived for the number of electrons $N_e(\beta,\mu)$ and their entropy $S(\beta,\mu)$. Plot the two functions as functions of β and μ and explain the behavior of N_e in terms of the energy levels of the 2D harmonic potential as temperature is lowered.
   Note: you can plot the functions for $\hbar\omega = 1$ and then argue that these plots as functions of $\beta\hbar\omega$ and $\mu/\hbar\omega$ instead of β and μ cover all isotropic harmonic traps.

II. THERMODYNAMICS OF NON-INTERACTING ELECTRONS IN A HARMONIC TRAP

1. Suppose $Q = 2e$ and $a = 600a_0$.
2. Define a 2D mesh starting at $x_0 = y_0 = -\frac{L}{2}$ and $x_N = y_N = \frac{L}{2}$ where L is the grid size. If there are $N+1$ grid points in each direction then $h = \frac{L}{N}$ is the grid spacing. You will need to figure out a good value of L.
3. Every wave function is represented as $\psi(x_i, y_j) \equiv \psi_{i,j}$. We assume $\psi = 0$ on grid boundaries. The overlap integral is $\langle\phi|\psi\rangle = h^2 \sum_{ij} \phi^*_{ij}\psi_{ij}$.
4. The Hamiltonian is $\hat{H} = \hat{T} + \hat{V}$ where the kinetic energy is $\hat{T} = -\frac{\hbar^2}{2m}L^h$ where L^h is the 2D finite difference Laplacian defined in the previous project and the potential energy operator is: $\left(\hat{V}\psi\right)_{ij} = V_{ij}\psi_{ij}$.

5. First take the Harmonic potential $V(x,y) = \frac{1}{2}m\omega^2\left(x^2+y^2\right)$. In all calculations work using work with atomic units ($\hbar = 1$, $m = 1$,$e^2/4\pi\epsilon_0 = 1$, the length unit is the Bohr a_0 and energy is the Hartree E_h).

6. Check your Hamiltonian by operating with it on the function $\psi_{ij} = e^{-\frac{\left(x^2+y^2\right)}{2\sigma^2}}$ where σ is chosen so that ψ is on the ground state of the Harmonic oscillator. If you chose correctly then $|r|$ is a small number, where $r_{ij} \equiv \left(\hat{H}\psi - \hbar\omega\psi\right)_{ij}$. As you add grid points by increasing N r should reduce in proportion to h^2. When this works, you have a grid representation of quantum mechanics.

III. STOCHASTIC TRACE CALCULATION OF THE NUMBER OF ELECTRONS AND ENTROPY

1. Use the document on the Chebyshev calculation in the theory section of the course web-page explaining how to calculate numerically traces of functions of the Hamiltonian to write a program implementing the algorithm. You need to identify the function of the Hamiltonian (see what you did in section 4b).

2. Run the program for the same harmonic potential as you used in the semi-analytical calculation section 4b. Compare the results. If you choose a certain β then you have to make sure that your grid is large enough to support the eigenstates with energy $\hbar\omega + n\beta^{-1}$ (let's assume that n is less than 10).

3. Apply your program for the potential you calculated in section 1.

4. Apply your program to a slightly modified non-harmonic potential:

$$V(x,y) = V_H(x,y) + V_0 e^{-\frac{1}{2}\left(\frac{x^2}{\sigma_x^2}+\frac{y^2}{\sigma_y^2}\right)} \tag{1}$$

   Choose "interesting" values of V_0, and the σ's so as to create a double well system (plot the potential using a contour plot program). Calculate the number of electrons $N_e(\beta,\mu)$ and their entropy $S(\beta,\mu)$. Plot the two functions as functions of β and μ and explain.