Computational Physics - Exercise 4

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Variational Monte Carlo for a 2D semiconductor Quantum Dot

A quantum dot is in general a device that displays the behavior of a "zero dimensional" system, i.e. it presents spectra that are similar to those, for instance, of an atom as opposed to that of a "wire", a "sheet" or a bulk system. Two-dimensional quantum dots are a special class of such devices that are normally obtained by etching a so-called "quantum well", an interface between two differently doped sempicondctor layers (such as, for instance, GaAs and $Al_xGa_{1-x}As$). At the interface a potential well is formed, such that the effective trabsverse confinement energy $\hbar\omega_\perp >> E$, where E are the typical energy scales in the longitudinal direction. In this regime a 2D quantum dot containing N electrons can be described by an effective Hamiltonian of the form:

$$\hat{H} = \sum_{i=1}^{N} \left(-\frac{\hbar^2}{2m_e m^*} \nabla_i^2 + \frac{1}{2} m_e m^* \omega^2 r_i^2 \right) + \frac{e^2}{\epsilon} \sum_{i<j} \frac{1}{|\vec{r}_i - \vec{r}_j|}, \tag{1}$$

with $\vec{r}_i = (x_i, y_i)$, where m^* is the electron effective mass and ϵ an effective dielctric constant partly accounting for the reduced dimensionality effects. For example, in typical GaAs quantum wells m^*=0.067 and ϵ=12.4. When considering units $\hbar$=$m_e m^*$=e^2/ϵ=1, this corresponds to measuring energies in effective Hartrees H^*=11.86 meV and distances in effective Bohr radii a_0^*=9.793 nm.

The aim of this exercise is to find an estimate of the ground state solution for the Schroedinger equation corresponding to the Hamiltonian in Eq. (1) by means of the Variational Monte Carlo (VMC) method, and for a set of small N.

As discussed in class the general form of the variational wavefunction can be assumed to be:

$$\Psi(\vec{r}_1 \dots \vec{r}_N) = \left[\prod_{i<j}^{N} f_{ij}(r_{ij})\right] \det_{\uparrow}[\phi_\alpha(r_{\beta_\uparrow})]\det_{\downarrow}[\phi_\alpha(r_{\beta_\downarrow})], \tag{2}$$

where $\beta_\uparrow = 1 \dots N_\uparrow$ and $\beta_\downarrow = N_\uparrow + 1 \dots N$, and $N_\uparrow$ is the number of electrons with spin $+1/2$. The orbitals $\phi_\alpha(r)$ can be taken as the solutions of the non-interacting problem:

$$-\frac{1}{2}\nabla\phi_\alpha(r) + \frac{1}{2}\omega^2 r^2 \phi(r)_\alpha = \lambda_\alpha \phi_\alpha(r), \tag{3}$$

with $\alpha = \{n, m\}$, where n is the principal quantum number $n = 1, 2, 3, \dots$, and $m = 0, \pm 1, \pm 2, \pm 3, \dots$ is the z component of the angular momentum. By symmetry we must have $l = |m|$.

The Jastrow function $f_{ij}(r_{ij})$ has the form:

$$f_{ij}(r_{ij}) = \exp\left[\frac{a_{ij} r_{ij}}{1 + b_{ij} r_{ij}}\right], \tag{4}$$

1. Find the values of $\alpha_{\uparrow\uparrow}$ (corresponding to particles i and j having parallel spin), and $\alpha_{\uparrow\downarrow}$ (for antiparallel spins) that satisfy the cusp condition for this 2D system, i.e. for which:

   $$\lim_{r_{ij}\to 0} \frac{H\Psi}{\Psi} < \infty \tag{5}$$

   Remember that for a pair of electrons with antiparallel spin the relative wavefunction is simply $f_{ij}(r_{ij})$, while for parallel spins one needs to consider the effect of the determinant that ampunts to multiply the Jastrow factor by r.

2. Write down the explicit expressions for the local kinetic energy both written as (shorthand notation) $-\hbar^2/2m \int \Psi_T \nabla^2 \Psi_T dR$ and $-\hbar^2/4m[\int \Psi_T \nabla^2 \Psi_T dR - \int \nabla\Psi_T \nabla \Psi_T dR]$ for the wavefunctions ψ in Eq.(2). Draw a flux diagram evidencing the different blocks and the different routines you intend to write for implementing this computation. Pay particular attention to all the blocks that are needed to reconstruct the Laplacian.

3. Solve analytically Eq.(3), and verify that the spectrum is given by $\lambda_\alpha = \omega(2n + l + 1)$. Map the solutions, including the angular parts, from polar coordinates to cartesian coordinates. Construct a set of

real orbitals by taking instead of the $m = \pm l$ solutions the corresponding real and imaginary parts. These will be the orbitals to be used in the construction of the Slater determinants.

4. By using a set of library routines to compute the Slater determinant and the inverse of the Slater matrix (for example

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   gsl_linalg_LU_det
   gsl_linalg_LU_invert
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   in GSL), construct a code that performs by a VMC-like procedure the evaluation of the expectation of an N electrons system described by the Hamiltonian

   $$\hat{H}_0 = \sum_{i=1}^{N} \left(-\frac{1}{2}\nabla_i + \frac{1}{2}\omega^2 r_i^2 \right)$$

   for $\omega = 1$ and $N = 2, \ldots, 6$. Verify that the energy obtained corresponds to that predicted on the basis of the single particle spectrum given above.

5. Include the Coulomb interaction in the Hamiltonian and the Jastrow factor in the wavefunction, and compute the VMC energies for the equantum dots with $N = 2, 3, 5, 6$, and for $\omega = 1$ and $\omega = 0.5$. Minimize the energy with respect to the two variational parameters $b_{\uparrow\uparrow}$ and $b_{\uparrow\downarrow}$ only. If possible, use the reweighting technique for the optimization. As a reference, for $\omega = 1$ and $N = 2$ there is a nice analytic solution due to Taut[1], which gives as ground state eigenvalue $E_0 = 3.0$. Some other reference values can be found for instance in the work of M. Pedersen Lohne et al.[2]

6. For the $N = 4$ case it is necessary to consider different possible total spin S and total angular momentum L configurations. In particular, you might have the states with $L = 0, S = 0$ (spin singlet), $L = 0, S = 1$ (spin triplet), each one needing **two** products of $\uparrow$ and $\downarrow$ determinants to be described (be careful with the total antisymmetry request, as discussed in class!), and $L = 2, S = 0$, which needs a single product of determinants. Try to determine which of these states is the ground state, and try to explain the answer.

[1] see M. Taut, J. Phys. A: Math. Gen. **27** 1045 (1994)
[2] see https://arxiv.org/pdf/1009.4833.pdf