QMC school at S.B.Bose Centre: QMC exam

February 22, 2013, 74 minutes

Instructions: *do as many questions as you can. Feel free to find the answers on books/manuals/papers etc. Hartree atomic units are used throughout.*

Grading: *each of the questions 1–5 is worth 10 points, divided as indicated. Extra points are awarded for being funny, inventive or otherwise amusing in the opinion of the person correcting the exam. The maximum score is 50 points.*

1.

The imaginary-time Schrödinger equation for a many-electron system is

$$\left(\hat{H} - E_T\right) \Phi(\mathbf{R}, t) = -\frac{\partial \Phi\left(\mathbf{R}, t\right)}{\partial t} \,, \tag{1}$$

where the wave function $\Phi(\mathbf{R}, t)$ is a function of point $\mathbf{R}$ in configuration space and imaginary time t, E_T is the reference energy and

$$\hat{H} = -\frac{1}{2}\nabla^2 + U(\mathbf{R}) \tag{2}$$

is the Hamiltonian operator, where U is the potential energy.

(i) *(3 points)* By expanding Φ in terms of eigenfunctions of the Hamiltonian, prove that the excited-state components of Φ die away exponentially relative to the ground state.

(ii) Let $f(\mathbf{R}, t) = \Phi(\mathbf{R}, t)\Psi(\mathbf{R})$, where $\Psi(\mathbf{R})$ is an approximation to the ground-state wave function.

(ii.1) *(4 points)* Prove that f satisfies the importance sampled imaginary-time Schrödinger equation

$$-\frac{1}{2}\nabla^2 f(\mathbf{R}, t) + \nabla \cdot (\mathbf{V}(\mathbf{R}) f(\mathbf{R}, t)) + \left(E_L(\mathbf{R}) - E_T\right) f(\mathbf{R}, t) = -\frac{\partial f\left(\mathbf{R}, t\right)}{\partial t} \,, \tag{3}$$

where $\mathbf{V}(\mathbf{R}) = \Psi^{-1}(\mathbf{R})\nabla\Psi(\mathbf{R})$, and $E_L(\mathbf{R}) = \Psi^{-1}(\mathbf{R})\hat{H}\Psi(\mathbf{R})$. This can be done by substituting the expression for $f(\mathbf{R}, t)$ in the equation.

(ii.2) *(3 points)* Explain the consequences of the importance-sampling transformation for the DMC algorithm.

2.

(i) *(3 points)* Why are the nodes of the trial wave function of particular relevance in QMC?

(ii) *(3 points)* Enumerate at least two possible ways in which one can modify a given wave function in order to improve its nodes.

(iii) *(2 points)* There exists a theorem related to wave function nodes which is called: (a) the Nodal Theorem, (b) the Jigsaw Theorem, (c) the Tiling Theorem, (d) the Fur Bikini Theorem, or (e) the Puzzle Theorem.

(iv) *(2 points)* The HF wave function for a beryllium atom is the product of an up-spin and a down-spin determinant,

$$\Psi_{\mathrm{HF}}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_4) = \begin{vmatrix} \phi_1(r_1) & \phi_2(r_1) \\ \phi_1(r_2) & \phi_2(r_2) \end{vmatrix} \begin{vmatrix} \phi_1(r_3) & \phi_2(r_3) \\ \phi_1(r_4) & \phi_2(r_4) \end{vmatrix} \,, \tag{4}$$

where r_i is the distance from the i-th electron to the nucleus. What is the shape of the nodes of Ψ_{HF} as seen by electron number 1? Explain why a multi-determinant expansion can radically change the shape of the nodes, whereas backflow cannot.

3.

(i) *(5 points)* What are "cusp conditions"? Why is it important to impose them on any given wave function? What happens if they are not?

(ii) Consider a Slater-Jastrow wave function for an N-electron system ($N_\uparrow$ spin-up electrons and $N_\downarrow$ spin-down electrons),

$$\Psi(\mathbf{R}) = \exp\left[J(\mathbf{R})\right] \begin{vmatrix} \psi_1^\uparrow(\mathbf{r}_1) & \cdots & \psi_{N_\uparrow}^\uparrow(\mathbf{r}_1) \\ \vdots & \ddots & \vdots \\ \psi_1^\uparrow(\mathbf{r}_{N_\uparrow}) & \cdots & \psi_{N_\uparrow}^\uparrow(\mathbf{r}_{N_\uparrow}) \end{vmatrix} \begin{vmatrix} \psi_1^\downarrow(\mathbf{r}_{N_\uparrow+1}) & \cdots & \psi_{N_\downarrow}^\downarrow(\mathbf{r}_{N_\uparrow+1}) \\ \vdots & \ddots & \vdots \\ \psi_1^\downarrow(\mathbf{r}_N) & \cdots & \psi_{N_\downarrow}^\downarrow(\mathbf{r}_N) \end{vmatrix}. \tag{5}$$

(ii.1) *(3 points)* Why is it not possible to impose the electron-electron cusp conditions on the Slater determinants?

(ii.2) *(2 points)* The backflow displacement of the i-th particle of a system, $\boldsymbol{\xi}_i(\mathbf{R})$, must be constrained to be zero when $\mathbf{r}_i$ coincides with the position of an all-electron nucleus. Why is this so?

4.

(i) *(4 points)* Explain why the variance of the local energy distribution is a valid objective function to minimize in order to optimize a wave function.

(ii) *(2 points)* Explain why it is relatively difficult to optimize parameters that affect the nodal surface of the trial wave function by unreweighted variance minimization.

(iii) *(4 points)* List and briefly describe other approaches for optimizing parameters in QMC.

5.

(i)

(i.1) *(3 points)* How is the variance of the local energy distribution $\sigma_{E_L}^2$ related to the standard error in the mean energy $\sigma_{\bar{E}}$?

(i.2) *(2 points)* How can $\sigma_{E_L}^2$ be reduced for a given system?

(i.3) *(2 points)* If you run a VMC calculation and afterwards you realize that you need to reduce the standard error in the mean energy by a factor of 2, how long does the continuation run need to be?

(ii) *(3 points)* What is serial correlation? Describe the reblocking algorithm, and explain why it works. Draw a picture of what a typical reblocking plot looks like to aid your answer.