Some Mathematical Puzzles in QMC

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Self-Consistent Unreweighted Varmin

How many graduate students' lives have been lost optimising wave functions?

D. M. Ceperley

- Tests show that SC unreweighted varmin gives lower energies than reweighted varmin.
- For many model systems, SC unreweighted varmin gives the same result as energy minimisation.
- Will see an example of this in my talk on varmin tomorrow.

The first challenge: *Can anyone* **prove** *that SC unreweighted varmin gives a lower energy than reweighted varmin? Or give a counterexample? Alternatively, can anyone find necessary or sufficient conditions for this to occur?*

Varmin for Linear Jastrow Parameters

- Tests show that the unreweighted variance generally has only a single minimum as a function of parameters that occur linearly in the exponent of a Jastrow factor.

- The only exceptions are when the sampling of configuration space is very poor.

- One can show that the unreweighted variance is a quartic function of linear parameters. See my talk on varmin.

- One would still expect multiple minima to exist in general.

The second challenge: *Can anyone determine the conditions under which the unreweighted variance has just a single minimum in the space of linear Jastrow parameters?*

A General Algorithm for Calculating Minimum-Image Distances

The obsession returns. Aaaaaarghghgh!

W. M. C. Foulkes

- We often need to calculate the distance between the **closest images** of a pair of particles in periodic systems.

- If the separation of the pair of particles is $\mathbf{r}$, we need to add integer multiples of the lattice vectors to $\mathbf{r}$ so as to minimise the length of the resulting vector.

- Equivalent problem: given a point $\mathbf{r}$ in a periodic lattice, what is the closest lattice point to $\mathbf{r}$?

- CASINO's general purpose minimum-image algorithm does the following:

    1. The parallelepiped-shaped unit cell in which $\mathbf{r}$ occurs is determined using the reciprocal lattice vectors;

    2. The closest lattice point to $\mathbf{r}$ is *assumed* to be one of the vertices of this parallelepiped. The distances from $\mathbf{r}$ to the vertices of the parallelepiped are calculated, and the shortest of these is taken to be the minimum-image distance.

- It is easy to draw sets of lattice vectors for which this procedure fails.

- Zoltan pointed out that choosing the **shortest possible** pair of lattice vectors is important. He proved that the vertex-checking algorithm is then valid in 2D.

- A program was written to test whether vertex-checking is valid in 3D. It seems to be valid about 99.99% of the time. . .

- We have explicit counterexamples proving that the method is not general.

- A very ugly scheme was devised for determining a set of lattice points to be checked, thus making the extended vertex-checking algorithm completely general.

The third challenge: *Can anyone come up with a* **rapid**, **elegant** *and* **completely general** *method for computing minimum-image distances?*