Three Mathematical Puzzles (of Little or No Practical Consequence) 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.

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.
- 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?*

Real Orbitals for Spiral Spin-Density-Wave Calculations

[Suggested by Zoltan; see his talk yesterday.]

- Noncollinear-spin calculations: use orbitals with up- and down-spin components.
- Spiral spin-density wave in HEG:
  - Up-like orbitals: $\psi^+_{\mathbf{k}}(\mathbf{r},\sigma) = \exp(i\mathbf{k}\cdot\mathbf{r})\left[\alpha(\sigma) + c\exp(i\mathbf{q}\cdot\mathbf{r})\beta(\sigma)\right].$
  - Down-like orbitals: $\psi^-_{\mathbf{k}}(\mathbf{r},\sigma) = \exp(i\mathbf{k}\cdot\mathbf{r})\left[\beta(\sigma) - c\exp(-i\mathbf{q}\cdot\mathbf{r})\alpha(\sigma)\right].$
- Would be nice if components of $\alpha(\sigma)$ and $\beta(\sigma)$ were real.
- Make linear combination of occupied orbitals? Conditions on $\mathbf{k}$ and $\mathbf{q}$?

The third challenge: *Can anyone work out how to construct real orbitals for use in spin-density-wave calculations?*

Other problems. . .

Of course there are plenty of other problems to think about once you have solved these:

- *Solve the fermion sign problem.*
- *Work out how to calculate the entire spectrum of excited-state energies.*
- *Modify DMC algorithm so that simulation of particles with very different masses is feasible.*
- *Work out how to perform DMC calculations for noncollinear-spin systems.*
- . . .