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: \( \psi_+^k(r, \sigma) = \exp(i k \cdot r) \left[ \alpha(\sigma) + c \exp(i q \cdot r) \beta(\sigma) \right] \).
  - Down-like orbitals: \( \psi_-^k(r, \sigma) = \exp(i k \cdot r) \left[ \beta(\sigma) - c \exp(-i q \cdot r) \alpha(\sigma) \right] \).

- Would be nice if components of \( \alpha(\sigma) \) and \( \beta(\sigma) \) were real.

- Make linear combination of occupied orbitals? Conditions on \( k \) and \( q \)?

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.*

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