How does "linear scaling" QMC scale with system size?

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December 10, 2003

"Standard" QMC

- The rate-determining step in QMC is the evaluation of Slater determinants in the trial wavefunction after each electron move.

- In "standard" QMC this scales as $O(N^2)$, where N is the number of electrons. (Must update N orbitals expanded in $O(N)$ basis functions.)

- Hence the time taken for a configuration move scales as $O(N^3)$.

Localised functions

- Nonsingular linear transformations of the orbitals leave Slater determinants unchanged.

- Carry out such a transformation to a highly localised set of functions, truncate the functions so they are zero outside a certain radius and smoothly interpolate them to zero at the truncation radius.

- Now, when an electron is moved, only a few functions need to be evaluated; the others are zero because the electron is outside their truncation radii. So the number of orbitals to be updated is $O(1)$.

Numerical bases

- Represent the functions numerically using splines on a grid. Hence there are no basis functions to recalculate when an electron is moved.

- So the time taken for the Slater determinant to be updated after a single electron move is $O(1)$. Hence the CPU time for a configuration move scales as $O(N)$.

Scaling of the energy variance

- If the energies of the electrons were uncorrelated then the variance of the energy σ_E^2 would scale as $O(N)$.

- If the energies of the electrons were completely correlated then σ_E^2 would scale as $O(N^2)$.

- The truth lies somewhere in between, but, ultimately, the energies of widely separated electrons must be uncorrelated. So we assume the variance scales as $O(N)$.

How many configuration moves?

- The standard error in the mean QMC energy is proportional to σ_E and hence to $N^{1/2}$. It is inversely proportional to the square root of the number of configuration moves.

- Therefore, if we choose a desired error bar and fix it, the required number of configuration moves scales as $O(N)$.

- Hence, to achieve a given error bar, the amount of CPU time for "linear scaling" QMC scales as $O(N^2)$.

Energy per electron

- The energy per electron has a variance that falls off as $O(N^{-1})$.

- Therefore, the number of moves required to achieve a given error bar on the energy per electron scales as $O(N^{-1})$.

- So, if one is interested in the energy per electron, the CPU time for "linear scaling" QMC to achieve a given error bar scales as $O(1)$.