Slicing a system for optimization in QMC

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Extended systems and target accuracy

QMC studies of extended systems require calculations at multiple system sizes.

Let $M \equiv$ (# steps), $N \equiv$ (# electrons), assume Slater-Jastrow wfn:

- Cost of QMC run is $\sim MN^3$
- Statistical error in total energy is $\sigma \sim \sqrt{N/M}$
  $\rightarrow$ for fixed error in total energy σ, cost of run is $\sim N^4$
- Statistical error in energy per electron is $\sigma \sim 1/\sqrt{NM}$
  $\rightarrow$ for fixed error per electron σ, cost of run is $\sim N^2$

Wave function optimization and system size

Wave function optimization in QMC:

- Generate $\{\mathbf{R}_m(\boldsymbol{\alpha}_0)\}_{m=1}^{M}$ distributed according to $|\Psi(\boldsymbol{\alpha}_0)|^2$
- Minimize target function evaluated at $\{\mathbf{R}_m(\boldsymbol{\alpha}_0)\}$, giving $\boldsymbol{\alpha}_1$
- Repeat until converged

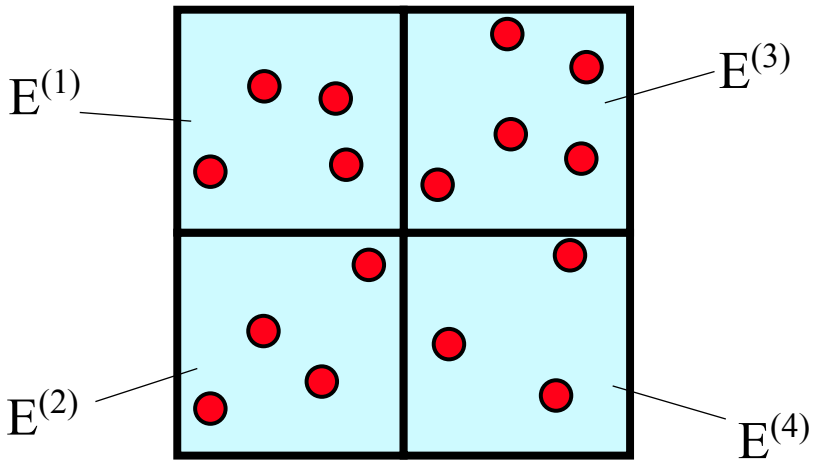
How to scale M with N in optimization?

- Local energy relatively smoother for larger $N \rightarrow$ **reduce** M?
- Each $\mathbf{R}_m$ represents **one** data point for target function;
  Some methods have a hard lower limit on M;
  $\rightarrow$ **keep** M **constant**?

Slicing the system

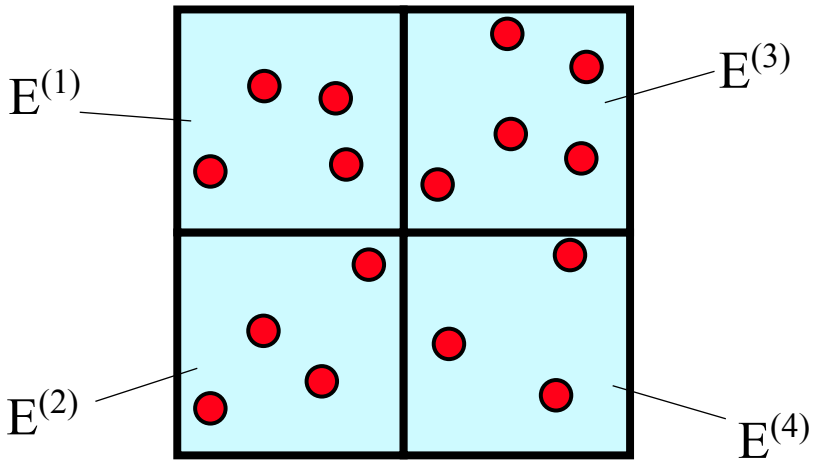
Divide, conquer?

What if we divide the system into n pieces (e.g., primitive cells) to make n times more data points available to the optimizer?



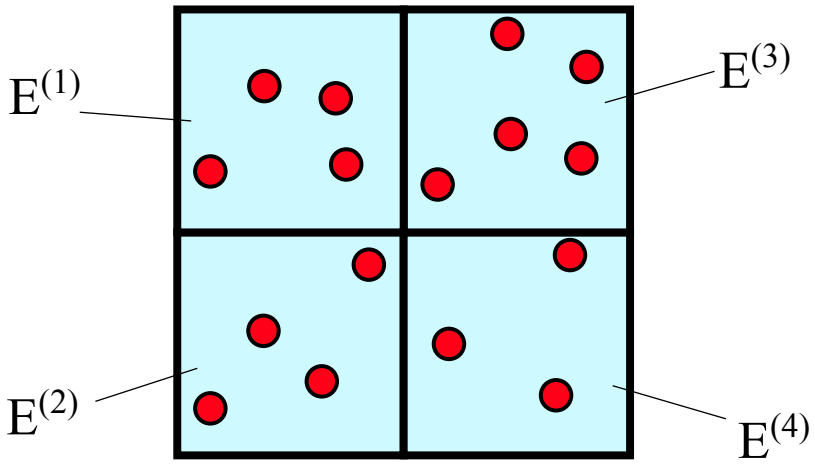
The slicing idea

- Divide the system into n slices
- Compute the energy of each slice
- Pass nM data points to the optimizer



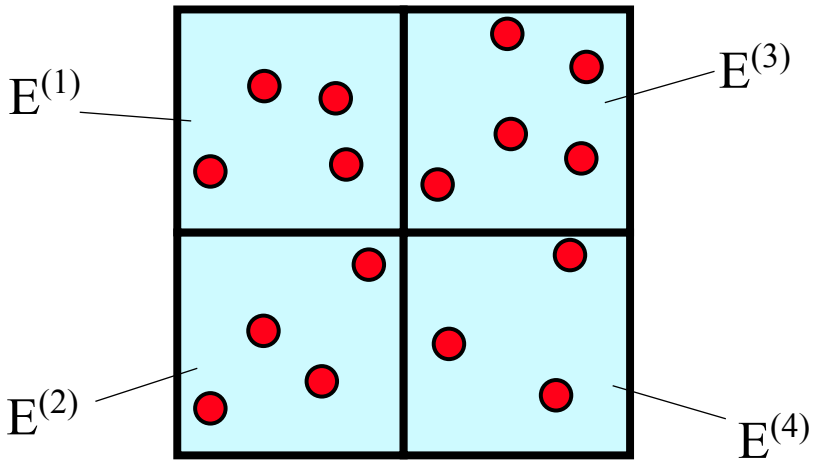
The slicing idea: options

- How to divide the system?
- What is "the energy" of a slice of the system?
- Slices with different $N \rightarrow$ fluctuations. What do we do?



The slicing idea: tentative choices

- Divide geometrically.
- $E^{(k)} = \sum_{i \in \Omega_k} \left(-\frac{1}{2} \nabla_i^2 \Psi + v_{ii} + \frac{1}{2} \sum_{j \neq i} v_{ij} \right)$ such that $E = \sum_k E^{(k)}$
- Pass energies per electron to the optimizer.

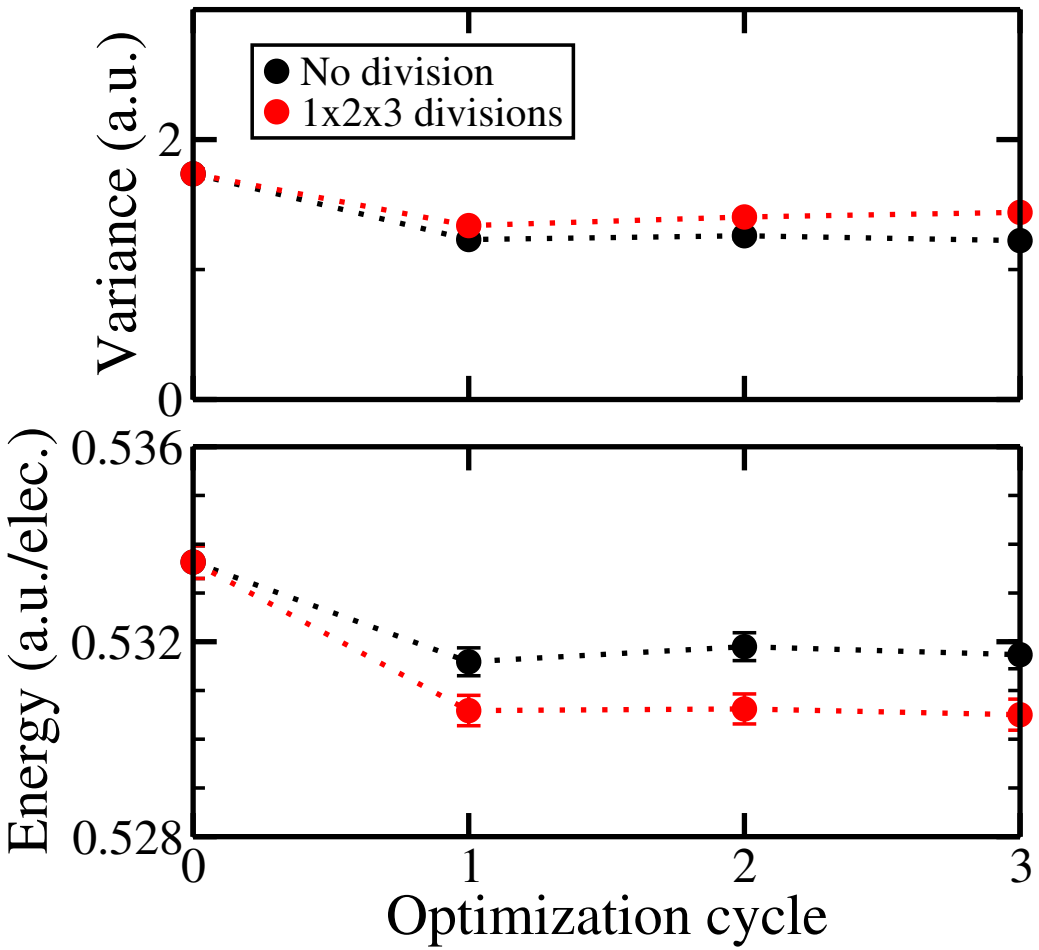


Test system

- Paramagnetic 38-electron gas at $r_s = 1$ a.u.
- Simple cubic cell
- Slater-Jastrow wave function with 16 parameters
- Optimize by minimizing median absolute deviation of local energies from median (MADmin)

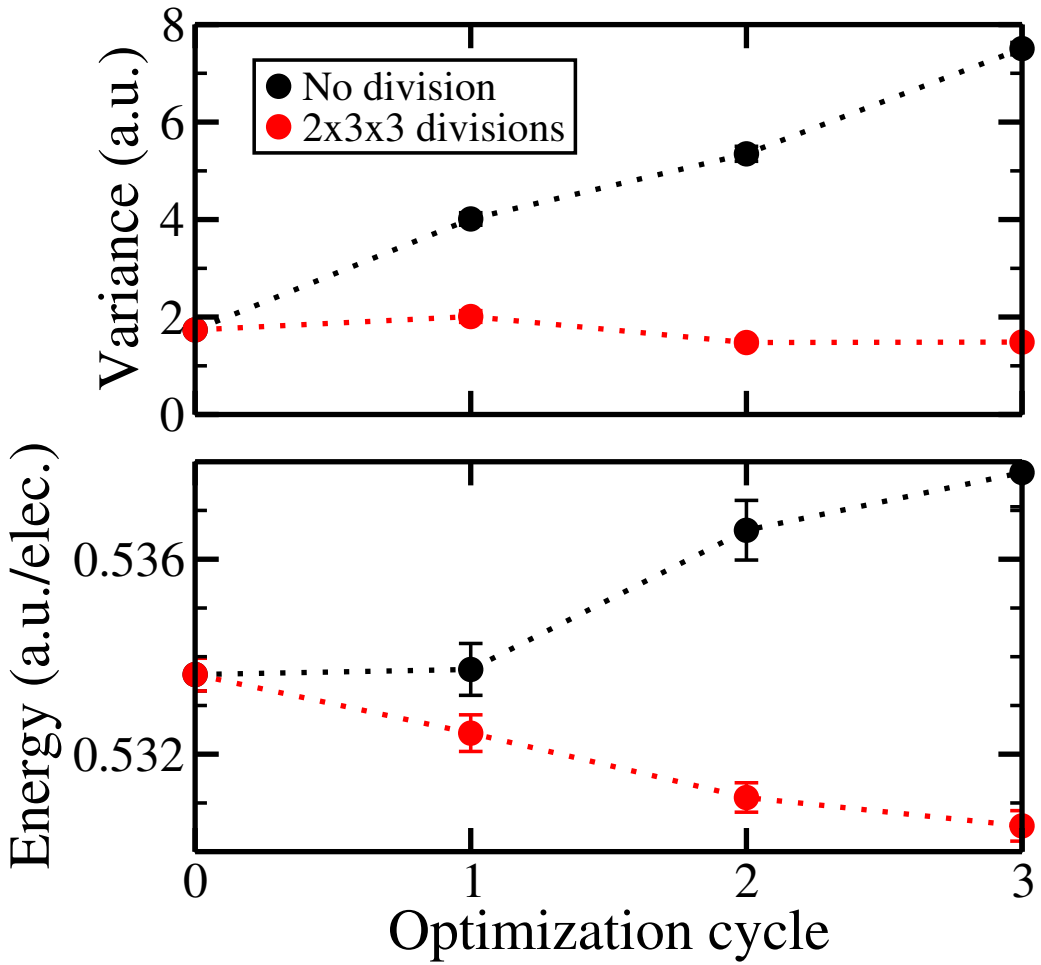
Results

Running with $M = 2500$ configurations:



Results

Running with $M = 20$ configurations:



Summary

- Slices seem to work OK for the HEG
- Slices seem advantageous at (very) small M
- Slices not expected to be terribly useful, however might be an idea to keep in mind

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