Targeting Real chemical accuracy at the EXascale

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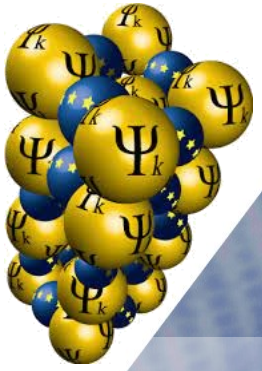

TREX e-School on Quantum Monte Carlo with TurboRVB

Diffusion Monte Carlo

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Outline

- Diffusion Monte Carlo
- Power method
- Lattice-regularized diffusion Monte Carlo

- Looking for the **ground state** of a Hamiltonian H

  by minimizing the variational energy of a **trial state**

  $E_{GS} = \min_{\Psi} \langle \Psi | H | \Psi \rangle$ with Ψ belonging to the Hilbert space

- **Variational freedom** in choosing Ψ (in general a complex many-body state)

- Variational principle:

$$\forall \Psi, E = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} \geq E_{GS}$$

- **Optimization** of the parameters in the variational form of the wave function (it requires the computation of forces and the minimization of a noisy functional)

many body forces: $\frac{\partial E}{\partial c_i} = \frac{\partial}{\partial c_i}\frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle}$ → QMC molecular dynamics possible!

- **Stochastic projection** of the initial trial state which follows the imaginary time dynamics

$$(H - E_T)G(\mathbf{R},\mathbf{R}_0,t) = -\frac{\partial G(\mathbf{R},\mathbf{R}_0,t)}{\partial t}$$

iterative application of the Green's function equation:

$$\Psi^{(n)}(\mathbf{R}',t+\tau) = \int d\mathbf{R}\; G(\mathbf{R}',\mathbf{R},\tau)\Psi^{(n-1)}(\mathbf{R},t)$$

Construct an operator which inverts spectrum of H
Use it to stochastically project the ground state of H

- Diffusion Monte Carlo (DMC) $\exp\{-\tau(H-E_T)\}$
- Power method $\Lambda - H$

Diffusion Monte Carlo projection

$$\Psi^{(n)} = e^{-n\tau(H-E_T)}\Psi^{(0)} = \sum_i \Psi_i \left\langle \Psi^{(0)} \middle| \Psi_i \right\rangle e^{-n\tau(E_i-E_T)}$$

In the limit of large projection time, the initial state is projected to the ground state, provided the initial guess is non orthogonal

$$\lim_{n\to\infty} \Psi^{(n)} = \Psi_0 \left\langle \Psi^{(0)} \middle| \Psi_0 \right\rangle e^{-n\tau(E_0-E_T)} \propto \Psi_0$$

Rewrite the projection equation in an integral form:

$$\Psi^{(n)}(\mathbf{R}',t+\tau) = \int d\mathbf{R}\, G(\mathbf{R}',\mathbf{R},\tau)\Psi^{(n-1)}(\mathbf{R},t)$$

$$G(\mathbf{R}',\mathbf{R},\tau) = \left\langle \mathbf{R}' \middle| e^{-\tau(H-E_T)} \middle| \mathbf{R} \right\rangle$$

where *G* is the **Green's function**, solution of the imaginary time Schrödinger equation:

$$(H-E_T)G(\mathbf{R},\mathbf{R}_0,t) = -\frac{\partial G(\mathbf{R},\mathbf{R}_0,t)}{\partial t}$$

with the initial condition $G(\mathbf{R}',\mathbf{R},0) = \delta(\mathbf{R}'-\mathbf{R})$

Can we interpret *G* as a transition probability?

If yes, we can solve the projection equation stochastically.

- ***H=K (V=0)***

$$-\frac{1}{2}\nabla^2 G(\mathbf{R},\mathbf{R}_0,t) = -\frac{\partial G(\mathbf{R},\mathbf{R}_0,t)}{\partial t}$$

The Green's function is given by a Gaussian

$$G(\mathbf{R}',\mathbf{R},\tau) = (2\pi\,\tau)^{-3N/2}\exp\left[-\frac{(\mathbf{R}'-\mathbf{R})^2}{2\tau}\right]$$

Diffusion process!

- ***H=V (K=0)***

$$(V(\mathbf{R}) - E_T)G(\mathbf{R},\mathbf{R}_0,t) = -\frac{\partial G(\mathbf{R},\mathbf{R}_0,t)}{\partial t}$$

The Green's function is given by an exponential

$$G(\mathbf{R}',\mathbf{R},\tau) = \exp\left[-\tau(V(\mathbf{R}) - E_T)\right]\delta(\mathbf{R}'-\mathbf{R})$$

Weighting factor!

$$e^{-\tau(K+V)} = e^{-\tau K} e^{-\tau V} + O(\tau^2)$$

Short time approximation valid up to the second order in time step, merging the diffusion and weighting process

$$G(\mathbf{R}', \mathbf{R}, \tau) = (2\pi\,\tau)^{-3N/2} \exp\left[-\frac{(\mathbf{R}' - \mathbf{R})^2}{2\tau}\right] \exp\left[-\tau(V(\mathbf{R}) - E_T)\right]$$

DMC results must be extrapolated in the limit of zero time step

Problem with the above Green's function: *V(R)* diverges when two electrons get close, explosion of the weights, algorithm unstable

Start from the integral equation:

$$\Psi^{(n)}(\mathbf{R}', t+\tau) = \int d\mathbf{R}\, G(\mathbf{R}', \mathbf{R}, \tau)\Psi^{(n-1)}(\mathbf{R}, t)$$

Multiply each side by the trial wave function $\Psi_T(\mathbf{R})$ and define $f^{(n)}(\mathbf{R}, t) = \Psi^{(n)}(\mathbf{R}, t)\Psi_T(\mathbf{R})$

$$f^{(n)}(\mathbf{R}', t+\tau) = \int d\mathbf{R}\, \tilde{G}(\mathbf{R}', \mathbf{R}, \tau)\, f^{(n-1)}(\mathbf{R}, t)$$

where the **importance sampled Green's function** is

$$\tilde{G}(\mathbf{R}', \mathbf{R}, \tau) = \frac{\Psi_T(\mathbf{R}')}{\Psi_T(\mathbf{R})}\left\langle \mathbf{R}' \middle| e^{-\tau(H-E_T)} \middle| \mathbf{R} \right\rangle$$

and in the large projection time limit we sample the **mixed distribution**

$$\lim_{n\to\infty} f^{(n)} = \Psi_0 \Psi_T$$

$$G(\mathbf{R}',\mathbf{R},\tau) = (2\pi\,\tau)^{-3N/2} \exp\left[-\frac{(\mathbf{R}'-\mathbf{R}-\tau\mathbf{V}(\mathbf{R}))^2}{2\tau}\right] \exp\left[-\tau(E_L(\mathbf{R})-E_T)\right]$$

Two important new features

Drift velocity $\mathbf{V}(\mathbf{R}) = \dfrac{\nabla\Psi_T(\mathbf{R})}{\Psi_T(\mathbf{R})}$

Pushes the walkers away from the nodes, by enforcing the importance sampling according to the trial wave function

Weighting factor with the local energy $E_L(\mathbf{R}) = \dfrac{H\Psi_T(\mathbf{R})}{\Psi_T(\mathbf{R})}$

The divergencies of the bare potential are cured by the fulfillment of the cusp conditions. The algorithm is now stable at least for bosons.

For **fermions**, the mixed distribution $\Psi_0\Psi_T$ will not be positive definite: the nodes of the ground state can be different from the nodes of the trial wave function.

Nodes: 3N-1 surfaces with $\mathbf{R}$ s.t. $\Psi(\mathbf{R})=0$

Fixed node approximation: constrain the projected state to have the same nodes as the trial wave function

$$\Psi_0(\mathbf{R})\Psi_T(\mathbf{R}) \square 0 \qquad \forall \mathbf{R}$$

the mixed distribution can be interpreted as a probability distribution.

Solve the Schrödinger equation with different boundaries conditions, set by the nodes of the initial trial wavefunction.

- **If the nodes are exact, no approximation**
- **The fixed node approximation gives an upper bound of the true ground state energy**

E_L and **V** still diverge at the nodes of the trial wavefunction!

Regularization:

$$\mathbf{V} = (\mathbf{v}_1, \ldots, \mathbf{v}_N) \longrightarrow \bar{\mathbf{V}} = (\bar{\mathbf{v}}_1, \ldots, \bar{\mathbf{v}}_N)$$

Velocity

$$\bar{\mathbf{v}}_i = \frac{-1 + \sqrt{1 + 2av_i^2\tau}}{av_i^2\tau}\mathbf{v}_i; \quad \mathbf{v}_i = \nabla_i \log|\psi_G(\mathbf{R})|$$

Branching factor

$$\bar{S}(\mathbf{R}) = [E_T - E_{\text{best}}] + [E_{\text{best}} - E_L(\mathbf{R})]\frac{\bar{V}}{V}$$

Global cutoff → we lost the size-consistency

$$\bar{S}(\mathbf{R}) = E_T - \bar{E}_L(\mathbf{R});$$

$$\bar{E}_L(\mathbf{R}) = E_{\text{best}} + \text{sign}[E_L(\mathbf{R}) - E_{\text{best}}] \times \min\{E_{\text{cut}}, |E_L(\mathbf{R}) - E_{\text{best}}|\}$$

$$E_{\text{cut}} = \alpha\sqrt{N/\tau}$$

Andrea Zen, Sandro Sorella, Michael J. Gillan, Angelos Michaelides, and Dario Alfè, Physical Review B **93**, 241118(R) (2016)

$$w_M = \Pi_{j=1}^{M} \exp[-\tau(E_L(\mathbf{R}_j) - E_T)]$$

large fluctuation for the weight (product of M random variables)

Solution: multi-walkers (N_w) algorithm!

Variance reduced by a factor $\mathbf{N_w}$

Branching step

Reconfiguration of the walkers before the variance becomes too large:
Choose new configurations among the old ones with a probability

$$p_i = \frac{w_i}{\sum_j w_j}$$

N_w correlated random numbers: $z_\alpha = (\alpha + \chi - 1)/N_w$ with $\alpha = 1, \ldots, N_w$

χ homogeneously distributed in $[0, 1[$

Count how many z_α fall into a p_i interval

1. Sample initial walkers from $|\Psi_T(\mathbf{R})|^2$
2. Propose a new move from the distribution $T(\mathbf{R}',\mathbf{R},\tau) = \exp\left[-\frac{(\mathbf{R}'-\mathbf{R}-\tau\mathbf{V}(\mathbf{R}))^2}{2\tau}\right]$

   Drift and diffusion $\mathbf{R}' = \mathbf{R} + \xi + \tau\mathbf{V}(\mathbf{R})$ with ξ sampled from

   $g(\xi) = (2\pi\tau)^{-3N/2}\exp\left(-\xi^2/2\tau\right)$

   Fixed node approximation: reject the move if $sign(\Psi_T(\mathbf{R}')) \neq sign(\Psi_T(\mathbf{R}))$

   Rejection scheme, accept the new move with probability

   $p = \min\left[1, \frac{|\Psi_T(\mathbf{R}')|^2 T(\mathbf{R},\mathbf{R}',\tau)}{|\Psi_T(\mathbf{R})|^2 T(\mathbf{R}',\mathbf{R},\tau)}\right]$
3. **Branching step** according to the weighting factor
4. Iterate 2. And 3. over walkers and for many generations in order to accumulate statistics.

VMC **distribution function is given** $\Pi(\mathbf{R}) = \frac{|\Psi(\mathbf{R})|^2}{\int d\mathbf{R}\, |\Psi(\mathbf{R})|^2}$

Construct M which satisfies stationarity condition $M\Pi(\mathbf{R}) = \Pi(\mathbf{R})$

Π is eigenvector of M with eigenvalue 1
Π is the dominant eigenvector

DMC different procedure!

The matrix M is given $\frac{\Psi_T(\mathbf{R}')}{\Psi_T(\mathbf{R})} \langle \mathbf{R}' | e^{-\tau(H-E_T)} | \mathbf{R} \rangle$

We want to find the dominant eigenvector $\Pi = \Psi_0 \Psi_T$

Construct an operator which inverts spectrum of H
Use it to stochastically project the ground state of H

- Diffusion Monte Carlo (DMC) $\exp\{-\tau(H - E_T)\}$
- Power method $\Lambda - H$

Power method projection

$$\lim_{n\to\infty} (\Lambda - H)^n |\Psi^{(0)}\rangle \propto |\Psi_0\rangle$$

In the limit of large powers, the initial state is projected to the ground state, provided the initial guess is non orthogonal

$$(\Lambda - H)^n |\Psi^{(0)}\rangle = \sum_i a_i (\Lambda - E_i)^n |\Psi_i\rangle$$

$$(\Lambda - E_0)^n \left[a_0 |\Psi_0\rangle + \sum_{i \neq 0} a_i \left(\frac{\Lambda - E_i}{\Lambda - E_0} \right)^n |\Psi_i\rangle \right]$$

If λ such that $\max_i |\Lambda - E_i| = |\Lambda - E_0|$

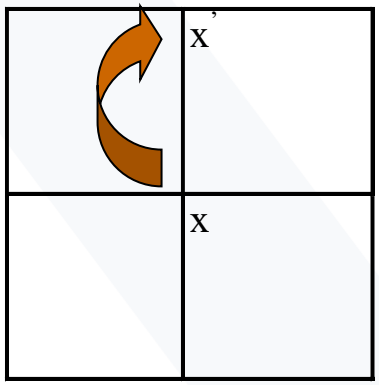
verified by $\lambda > (E_{max} + E_0)/2$

$$\lim_{n \to \infty} (\Lambda - H)^n |\Psi^{(0)}\rangle \propto |\Psi_0\rangle$$

Lattice Hamiltonian: $$H = -t\sum_{i,a}(c^{\dagger}_{i+a}c_i + h.c.) + \frac{1}{2}\sum_{i,j}V_{ij}n_i n_j$$

Propagator: $$G_{x,x'} = (\Lambda\delta_{x,x'} - H_{x,x'})\frac{\Psi_G(x')}{\Psi_G(x)}$$ $\Rightarrow$ importance sampling

Hopping:



transition probability

$$p_{x,x'} = \frac{G_{x,x'}}{\sum_{x'}G_{x,x'}} = \frac{G_{x,x'}}{\Lambda - e_L(x)}$$

weight $$w^{i+1} = w^i(\Lambda - e_L(x))$$

For **fermions**, **lattice fixed node approximation**
to have a well defined transition probability

$$G_{x\,y} = \Lambda\delta_{x\,y} - H_{x\,y}\Psi_G(x)/\Psi_G(y) \quad \text{Green function}$$

$$\hat{H}^{eff}_{x\,y} = \hat{H}_{x\,y} \quad \text{if} \quad G_{x\,y} > 0 \qquad \text{OFF DIAGONAL TERMS}$$

$$\hat{H}^{eff}_{x\,y} = 0 \qquad \text{otherwise}$$

$$\hat{H}^{eff}_{x\,x} = V(x) + v_{sf}(x) \qquad \text{DIAGONAL TERM}$$

$$v_{sf}(x) = -\sum_y G_{x\,y} \quad \text{with } G_{x\,y} < 0 \quad \text{SIGN FLIP TERM}$$

Hopping with sign change replaced by a positive diagonal potential

LATTICE UPPER BOUND THEOREM !

D.F.B. ten Haaf et al. PRB **51**, 13039 (1995)

$$\left\langle \Psi_0^{eff} \middle| H \middle| \Psi_0^{eff} \right\rangle \leq \left\langle \Psi_0^{eff} \middle| H^{eff} \middle| \Psi_0^{eff} \right\rangle \quad \Psi_0^{eff} \text{ GS of } H^{eff}$$

On the continuum, usually H not bounded from above!

$$G_{x,x} = \Lambda - H_{x,x} \geq 0 \quad \Rightarrow \quad \Lambda \to \infty$$

$$G \approx \Lambda \exp\left(-\delta\tau H\right) \qquad \delta\tau = \frac{1}{\Lambda}$$

Probability of leaving x

$$q = \frac{\sum_{x'(\neq x)} G_{x',x}}{\Lambda - E_L(x)} \approx \delta\tau \sum_{x'(\neq x)} G_{x',x}$$

Probabilty of leaving x after k time slices

$$f(k) = q\left(1-q\right)^{k-1}$$

$\tau_x = k\ \delta\tau$ *k* distributed according to *f*

$$\tau_x = \frac{-\log(r)}{\sum_{x'(\neq x)} G_{x',x}} \qquad r \in]0,1] \ \text{ random}$$

Advantages of the power method

- ✓ ***No instabilities in the effective fixed-node Hamiltonian***

  (no nodal divergencies)

- ✓ ***No time step error***

  (exact continuous-time limit formulation)

- ✓ ***Possibility of including non-local potentials***

- For heavy atoms pseudopotentials are **necessary**

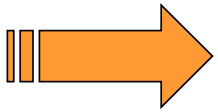
to reduce the computational time

- Usually they are **non local**

$$V_P(x_i) = \sum_l v_l(x_i) \sum_m |lm\rangle\langle lm|$$

In QMC angular momentum projection is calculated by using a **quadrature rule** for the integration

S. Fahy, X. W. Wang and Steven G. Louie, PRB 42, 3503 (1990)



Natural discretization of the projection

Can a lattice scheme be applied?

Kinetic term: discretization of the Laplacian

One dimension:

$$\frac{d^2}{dx^2} f(x) = \frac{f(x+a) + f(x-a) - 2f(x)}{a^2} + O(a^2)$$

General case:

$$\Delta \to \Delta_a = \sum_{i=1}^{d} \frac{T_{a_i} + T_{-a_i} - 2I}{a_i^{\,2}} + O(a^2)$$

where $T_{\hat{a}} \Psi_T(\bar{x}) = \Psi_T(\bar{x} + \hat{a})$

hopping term $t \to 1/a^2$

Possible choice: double mesh for the discretized Laplacian

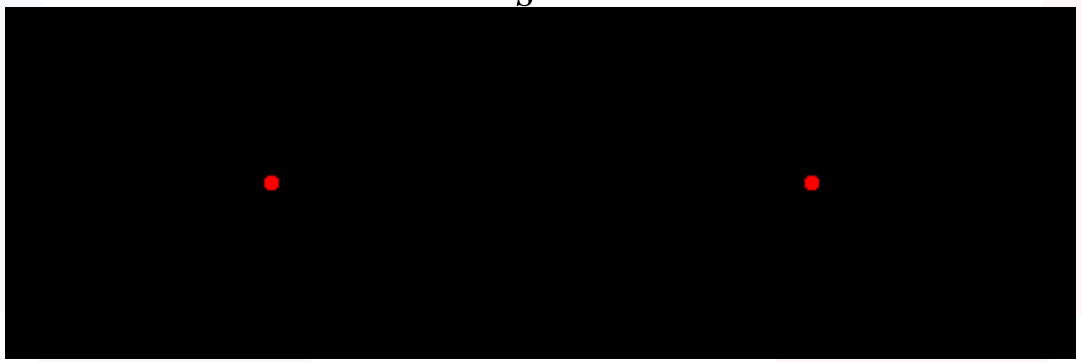
$$\Delta\Psi(x) \approx p\Delta_a\Psi(x) + (1-p)\Delta_b\Psi(x) + O(a^2)$$

If *a* and *b* are incommensurate, the random walk can sample all the space!

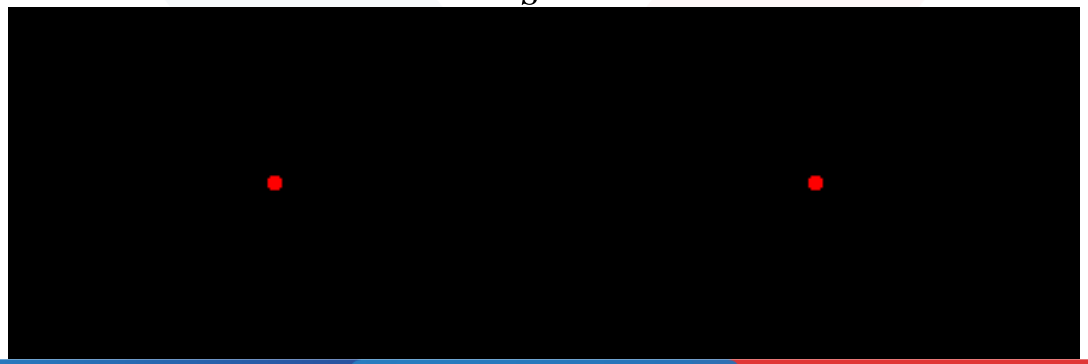
$$b/a = \sqrt{Z^2+1}$$

Example: 1D system electrons: 1 up, 1 down, PBC

$a = 0.25\ r_s \qquad b = 2a$



$a = 0.25\ r_s \qquad b = \sqrt{5}a$



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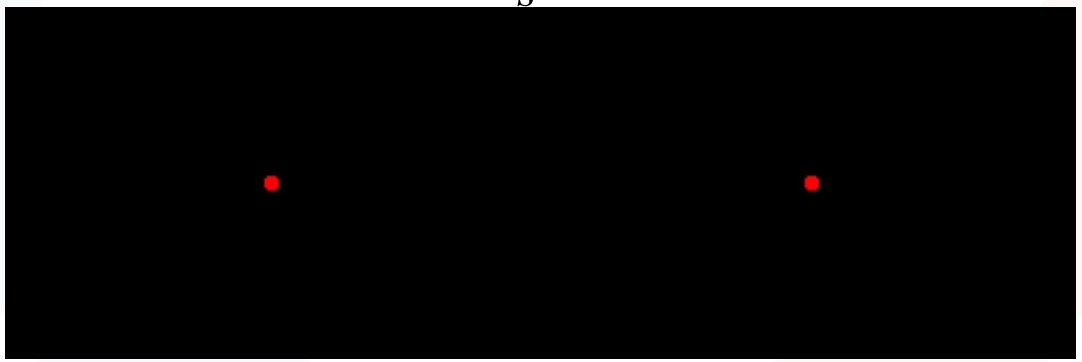

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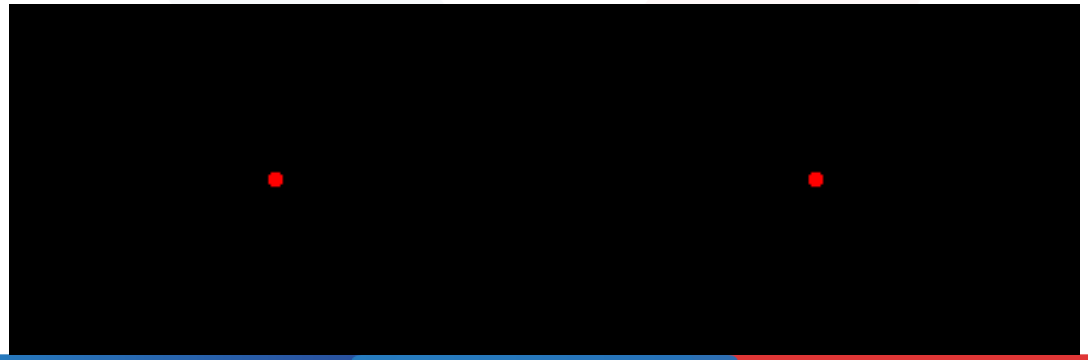


Double mesh optimized

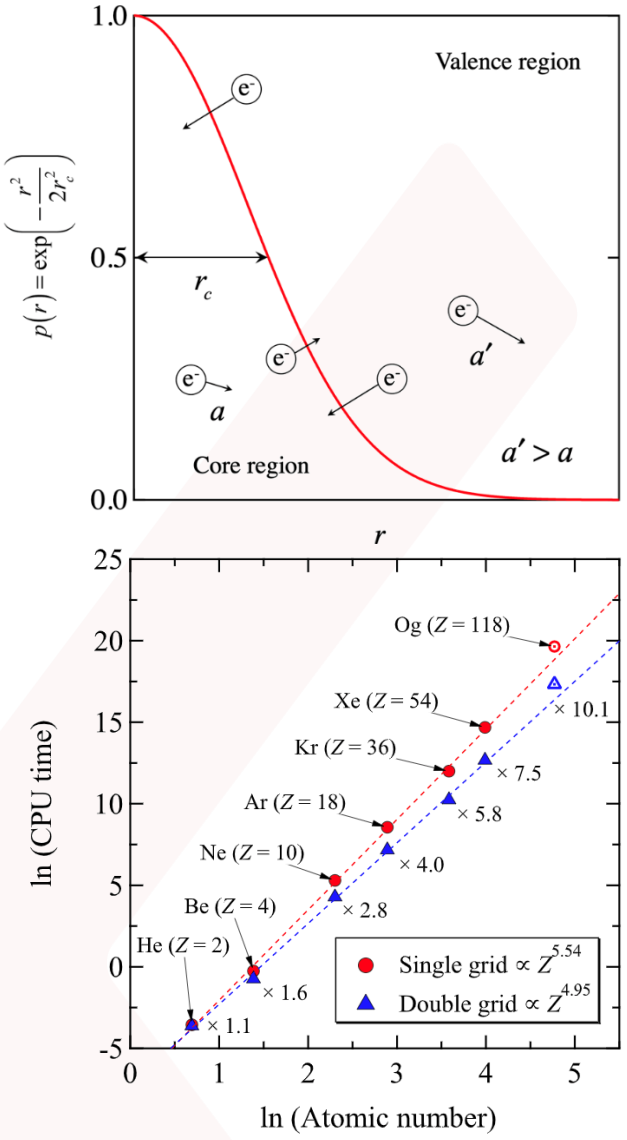
Most efficient choice $p(\vec{r}) = \exp\left(-\frac{|\vec{r} - \vec{R}_c|^2}{2{r_c}^2}\right)$

with $r_c(Z) = \beta Z^{-5/7}$ and $\beta = 0.75$

$N_{\text{core}}(r_c) \propto (Zr_c)^{3/2}$ from Thomas-Fermi model

$$\frac{a'}{a} = \sqrt{\frac{lN_{\text{valence}}(r_c)}{N_{\text{core}}(r_c)}} \equiv \sqrt{\frac{l[Z - N_{\text{core}}(r_c)]}{N_{\text{core}}(r_c)}}$$

K. Nakano, R. Maezono, and S. Sorella,
Phys. Rev. B **101**, 155106 (2020)



Definition of lattice regularized Hamiltonian

$$H_a = \Delta_a + V_a$$

- Continuous limit: **for a→0, H_a→H**
- Local energy of H_a = local energy of H

$$e_L(x) = \sum_{x'} G_{x,x'} = \frac{H\Psi_G(x)}{\Psi_G(x)} = E_L(x)$$

$$\Rightarrow \quad V(x) \to V^a(x) = V(x) + \left(\frac{\Delta_a \Psi_G(x)}{\Psi_G(x)} - \frac{\Delta \Psi_G(x)}{\Psi_G(x)} \right)$$

Faster convergence in a!

Near the nodes **and** near the nuclei,
the modified potential V^a can **diverge negatively**

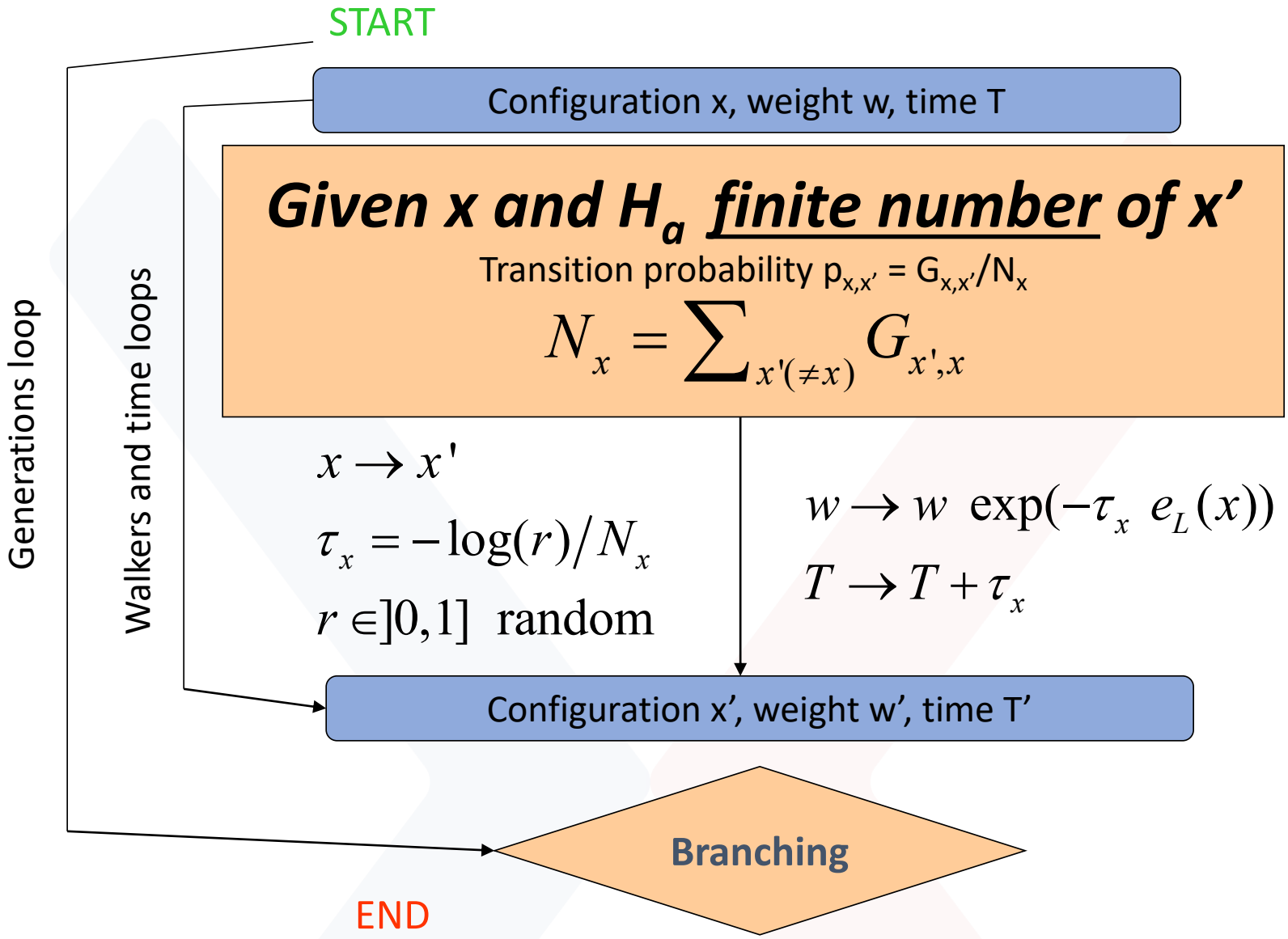
$$v_{el-ion}(\mathbf{r}_i) \longrightarrow v_i^a(\mathbf{R})$$

$$v_i^a(\mathbf{R}) = v_{el-ion}^a(\mathbf{r}_i) + \frac{(\nabla_{i,a}^2 - \nabla_i^2)\Psi_G(\mathbf{R})}{2\Psi_G(\mathbf{R})}$$ **far from the nodes**

$$v_i^a(\mathbf{R}) = v_{el-ion}^a(\mathbf{r}_i)$$ **close to the nodes**

where $$v_{el-ion}^a(\mathbf{r}_i) = -\sum_{I=ions} \frac{Z_I}{Max[|\mathbf{r}_i - \mathbf{R}_I|, a]}$$

Lattice regularized DMC: the algorithm

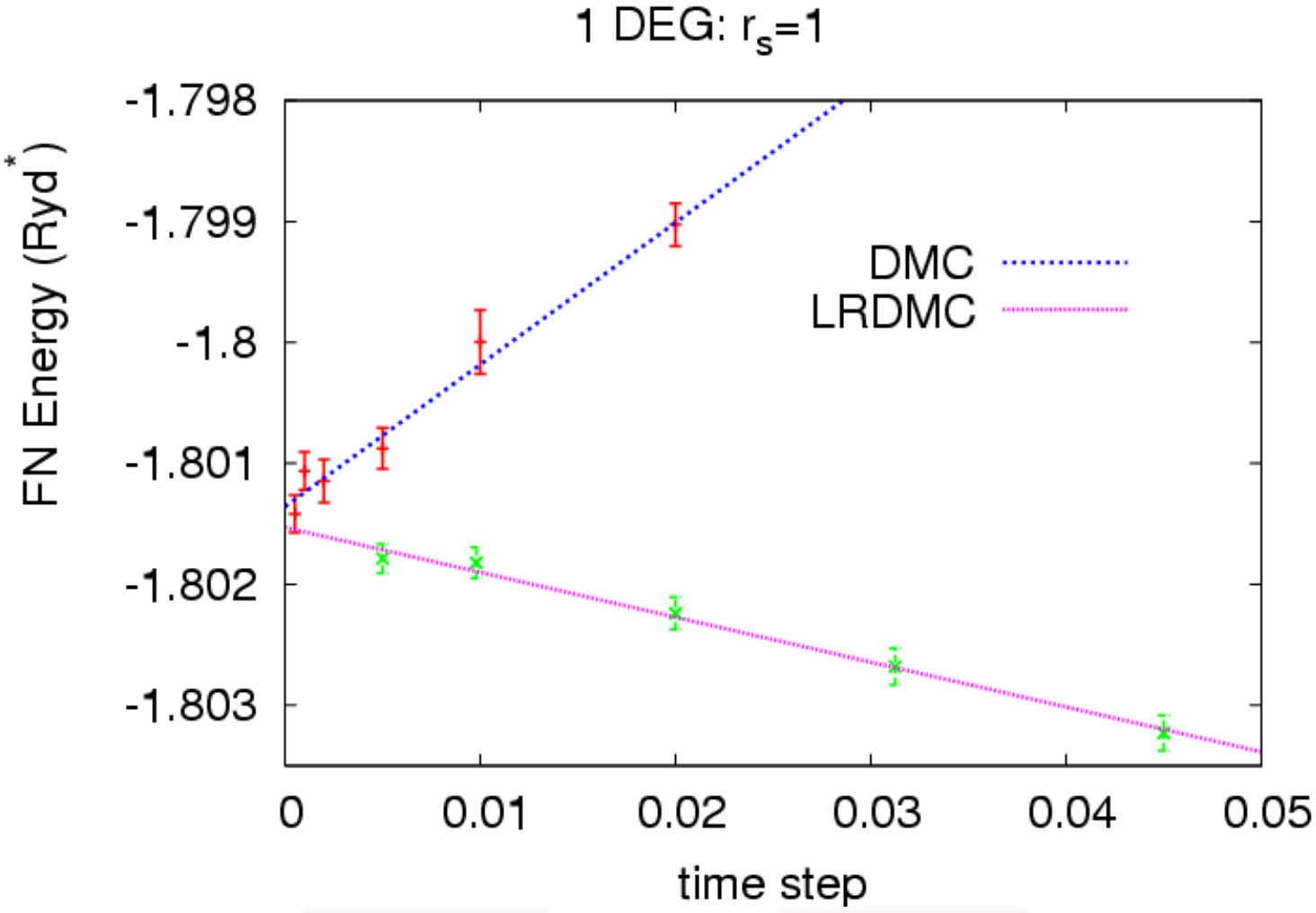


extrapolation properties

DMC	LRDMC
Trotter approximation	**For each *a* well defined effective H**
τ extrapolation	***a* extrapolation**
τ^2 behaviour	**a^4 behaviour**

$\sqrt{\tau} = a$ ⟹ same diffusion constant

CPU time $\propto \tau^{-1}(a^{-2})$


1 DEG: r_s=1
FN Energy (Ryd*)
-1.798
-1.799
-1.8
-1.801
-1.802
-1.803
0
0.01
0.02
0.03
0.04
0.05
time step
DMC
LRDMC

Possibility of including pseudopotentials

Off diagonal matrix elements

$$G_{x\,y} = \Lambda\delta_{x\,y} - H_{x\,y}\Psi_G(x)/\Psi_G(y) \quad \text{propagator}$$

From the discretized Laplacian:

$$G_{x\,y} = \frac{p}{a^2}\frac{\Psi_G(\bar{x})}{\Psi_G(\bar{y})} \qquad \bar{x} = \bar{y} \pm \bar{a}$$

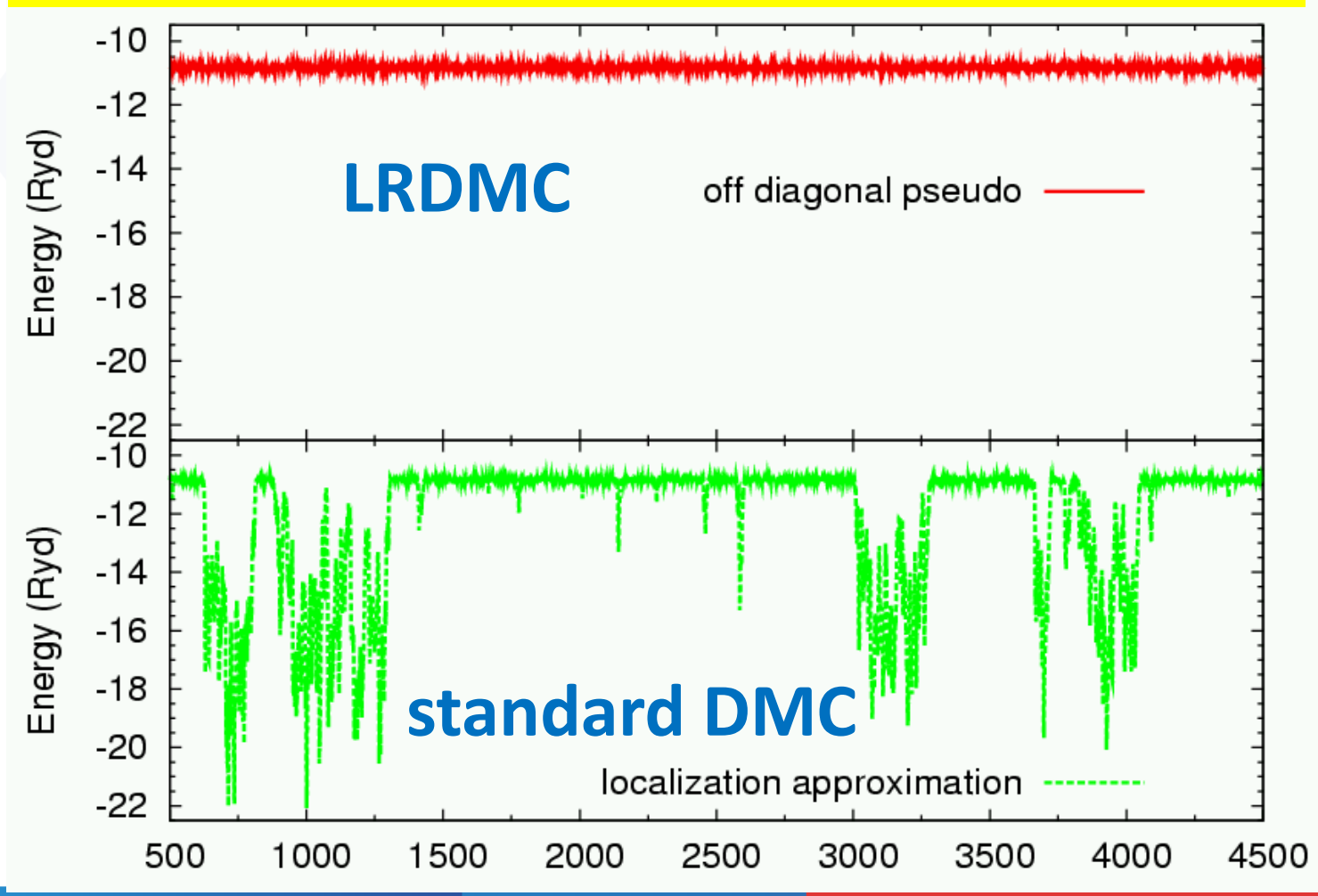
a: translational vectors

From the non local pseudopotential:

$$G_{x\,y} = -\left(\sum_l \frac{2l+1}{4\pi} \mathrm{v}_l(\bar{y}) P_l\left[\cos\vartheta_{x\,y}\right]\right)\frac{\Psi_G(\bar{x})}{\Psi_G(\bar{y})} \qquad \bar{x} = \bar{y} + \bar{c}$$

c: quadrature mesh (rotation around a nucleus)

Carbon pseudoatom: 4 electrons (SBK pseudo)



LRDMC properties

- ✓ LRDMC is a projection technique
- ✓ It is as an alternative variational approach for dealing with non local potentials
- ✓ Very stable simulation also for poor wave functions
- ✓ Smooth extrapolation as a function of the lattice space
- ✓ LRDMC is size consistent

DFT part

Solve Kohn-Sham equations

gaussian orbitals $\varphi_I(\mathbf{r})$

Interfacing

Slater determinant from DFT orbitals

QMC part (I)

Wave function optimization:

$J(\mathbf{r}_1,\ldots,\mathbf{r}_N)\, D^{\uparrow}_{DFT}(\mathbf{r}_1,\ldots,\mathbf{r}_N) D^{\downarrow}_{DFT}(\mathbf{r}_1,\ldots,\mathbf{r}_N)$

QMC part (II)

Wave function projection

(diffusion Monte Carlo):

$e^{-tH}\ \Psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)$

Casula, Moroni, Sorella, Filippi, JCP **131**, 154116 (2010)

S. Sorella, M. Casula, D. Rocca, J. Chem. Phys. **127**, 014105 (2007)

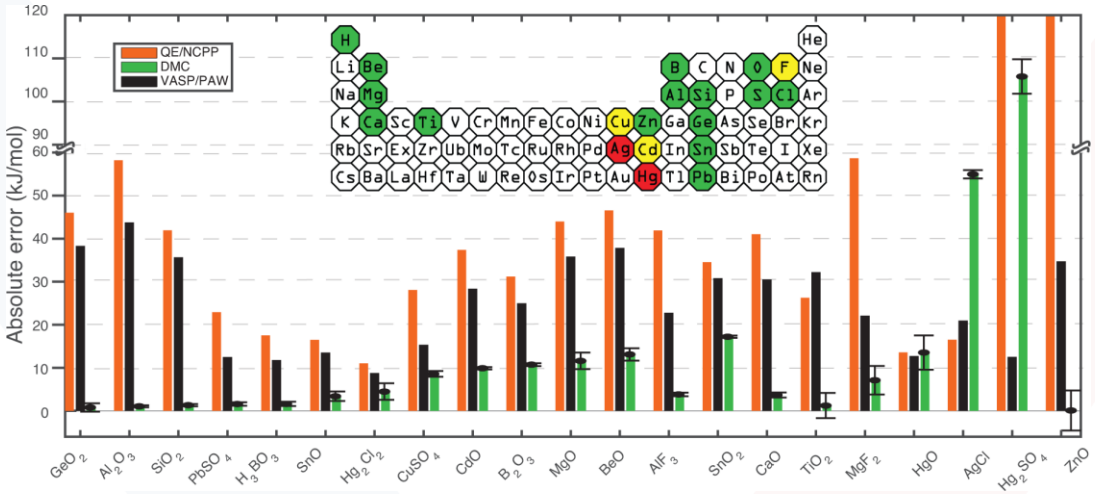
• The Bloch theorem does not apply in a many-body framework:
the k-point integration is ill-defined in the QMC real-space approach
Need of an explicit finite size scaling in QMC!
(some improvements along these lines but still not enough to afford large unit cell crystals)

• Sign problem in the stochastic projection
Fixed-node error in diffusion Monte Carlo
(alleviated by the wave function optimization but the residual error is sometime hard to estimate)

• Use of pseudopotentials necessary to reduce the computational cost
Lack of a consistent way to determine pseudopotentials in QMC
(usually determined by Hartree-Fock or DFT but the error can be significant in calculations under pressure)

- DMC is **one of the most accurate *ab initio* methods** for both molecular and extended systems

Formation energies



JCTC **13** (2017)

- It is **variational** (namely, one can check the convergence to the true ground state energy by variance extrapolation)
- It is a ”local” theory (**locality can be exploited** to speed up the calculation)
- It **scales well** with the number of particles
- It is an **embarrassingly parallel** technique

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