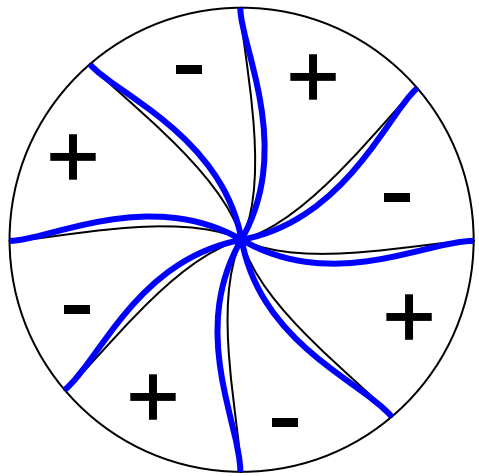
The search for the nodes of the fermionic ground state

$$\psi(R) = 0$$



Some believe that unicorns are just shy and difficult to find.
However, most people believe blue ones do not exist.
We all believe that the nodes of a many body fermionic wave-functions exist.
However, many think they are as hard to find as blue unicorns.

DMC for poets

The node

$$\psi_T(R) = 0$$

“Nothing really matters
Anyone can see
Nothing really matters, nothing really matters - to me”

Freddie Mercury

A self-healing DMC algorithm

(a systematic correction of nodal surfaces in small systems)

Fernando A. Reboredo (ORNL)

Paul R. C. Kent (ORNL) R. Q. Hood (LLNL)

Research performed at the Materials Science and Technology Division and the Center of Nanophase Material Sciences at Oak Ridge National Laboratory sponsored the Division of Materials Sciences and the Division of Scientific User Facilities U.S.

OAK RIDGE National Laboratory

Office of Basic Energy Sciences • Serving the Present. Shaping the Future •

DMC run

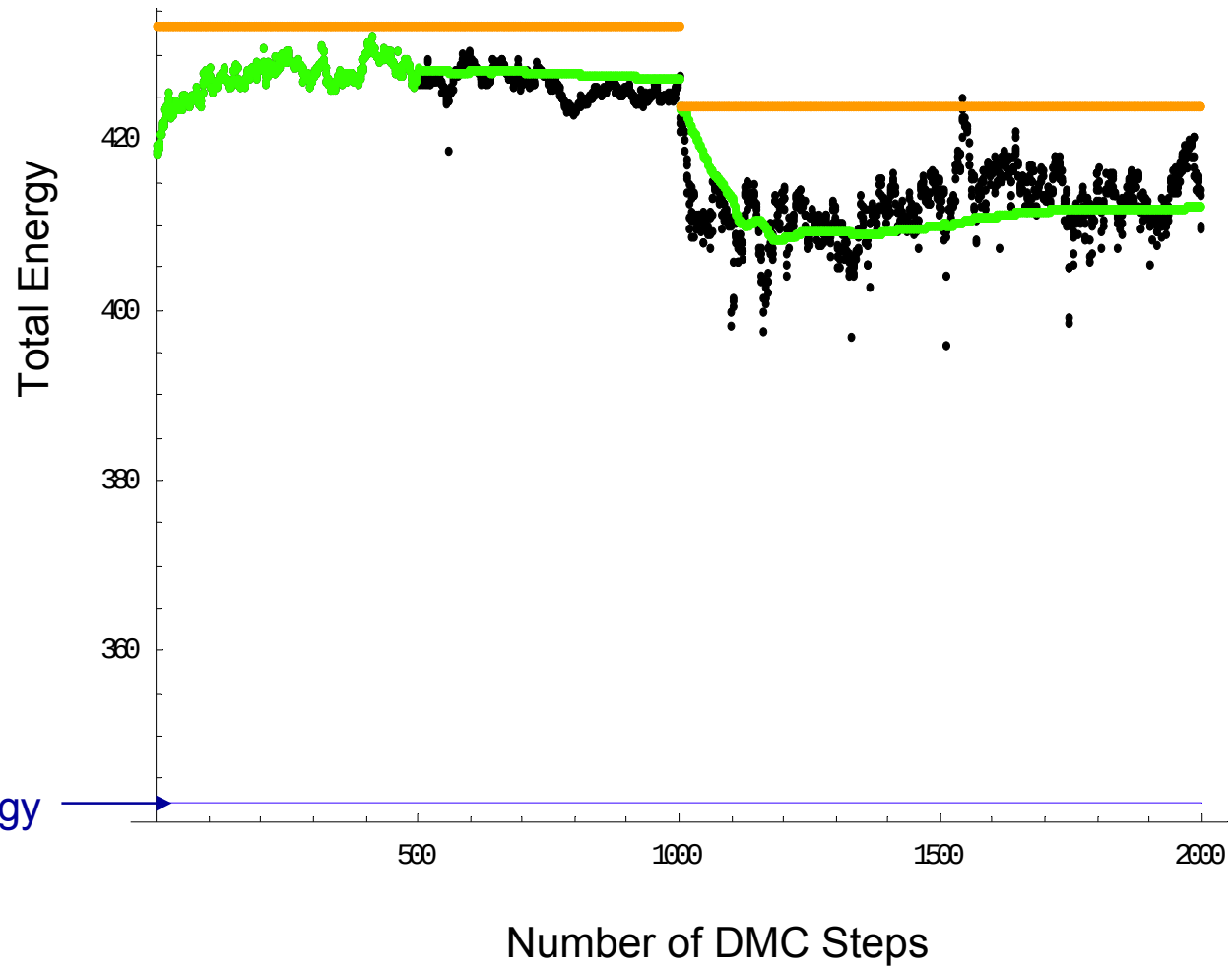
E best
E Local
Total Energy
420
400
380
360
200
400
600
800
1000
Number of DMC Steps
Exact (Full CI) energy

DMC run

E_{best}
E_{Local}
Total Energy
420
400
380
360
500
1000
1500
2000
Number of DMC Steps
Exact (Full CI) energy

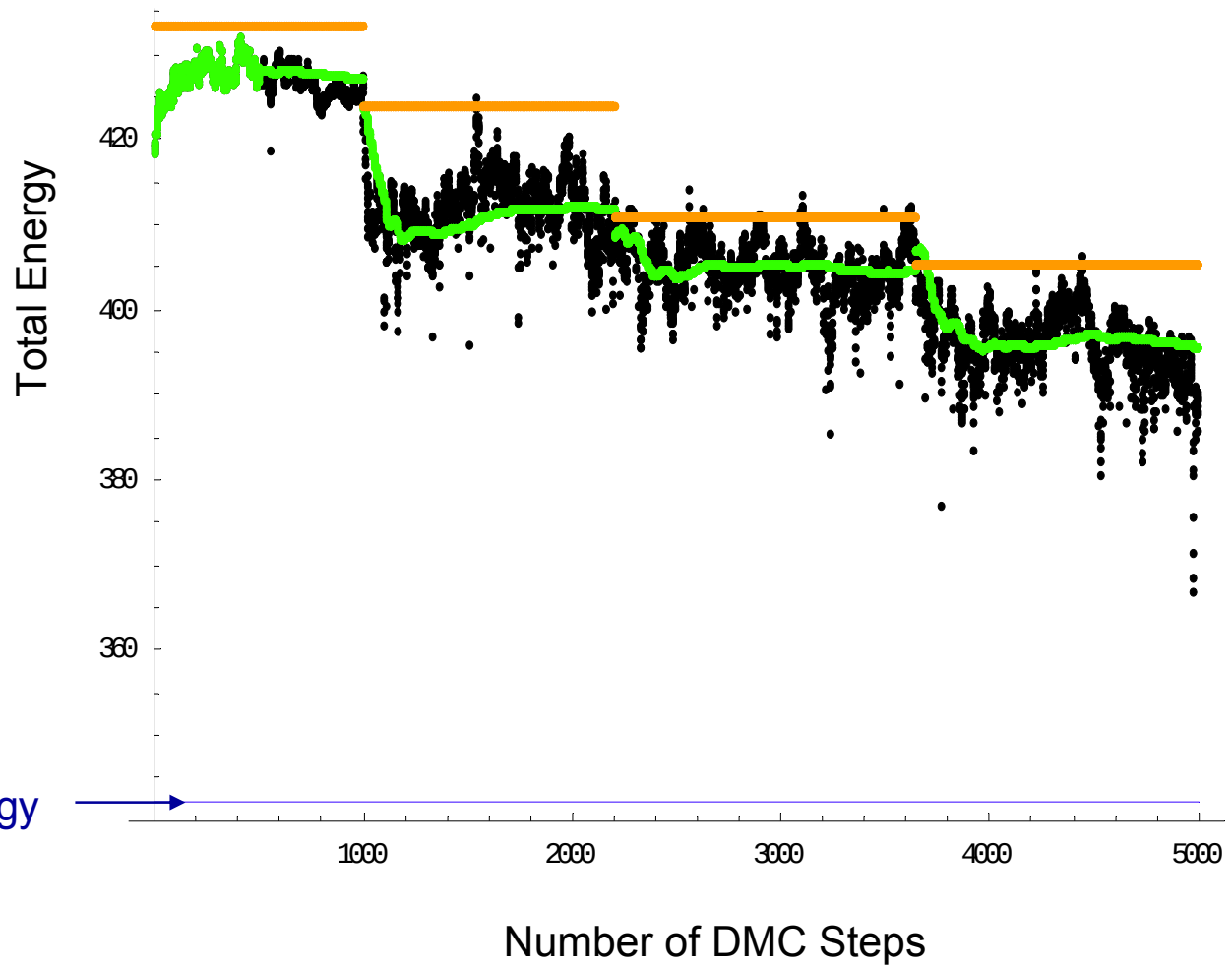
DMC run

Exact (Full CI) energy



DMC run

Exact (Full CI) energy



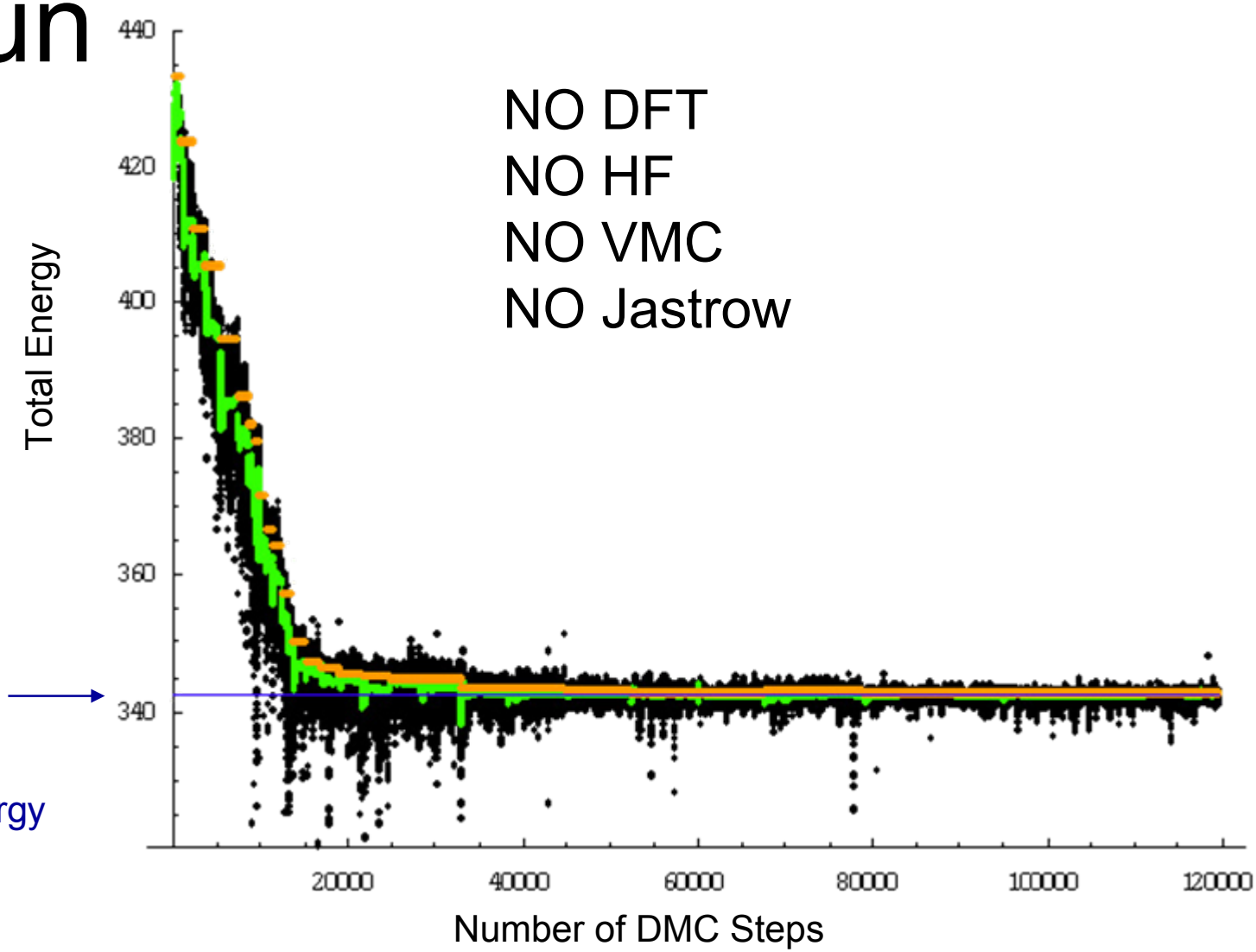
A Theoretical Blue Unicorn : finding the blue nodes

DMC run

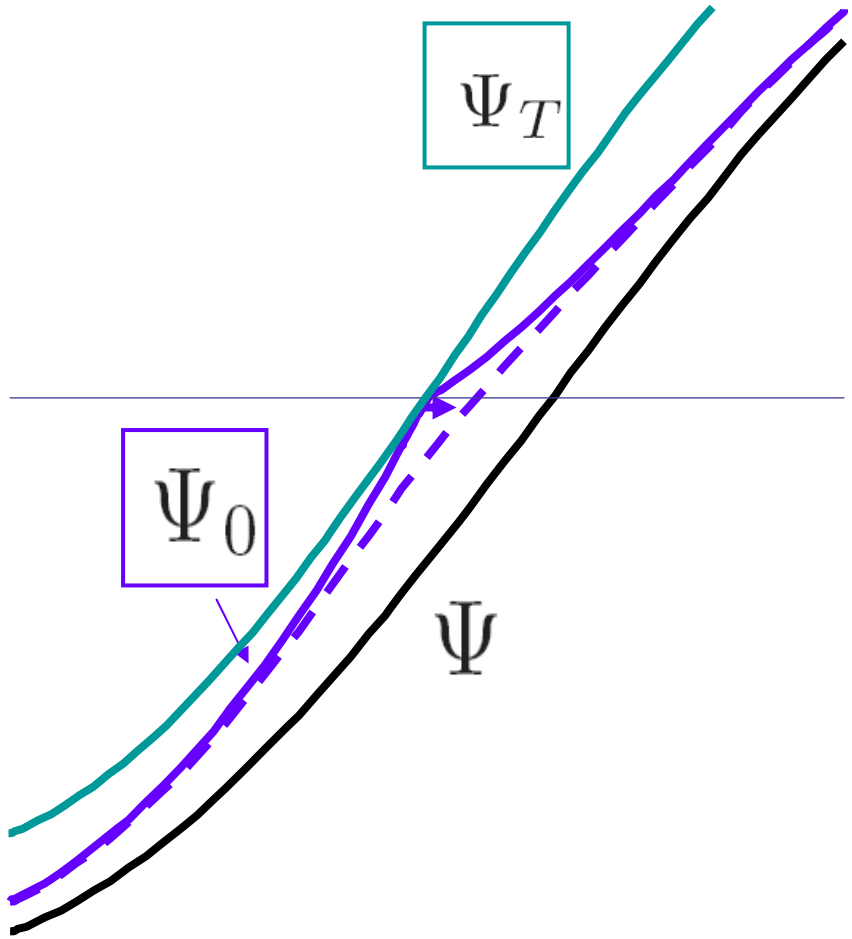
E_{best} E_{Local} $E= \langle \psi_T|H|\psi_T \rangle_I$

NO DFT
NO HF
NO VMC
NO Jastrow

Exact (Full CI) energy



What could we do if we new the Fixed Node wave function?



Removing the kink in Ψ_T moves the node in the right direction

Standard **Importance Sampling** Diffusion Monte Carlo Algorithm

D. M. Ceperley and B. J. Alder, Phys. Rev. Lett. **45**, 566 (1980)

Number of configurations

$$f(\mathbf{R}) = \frac{N_c}{\nu_T}\Psi_0(\mathbf{R})\Psi_T(\mathbf{R})$$

Trial Wave-Function

Fixed-Node Ground State Wave-Function

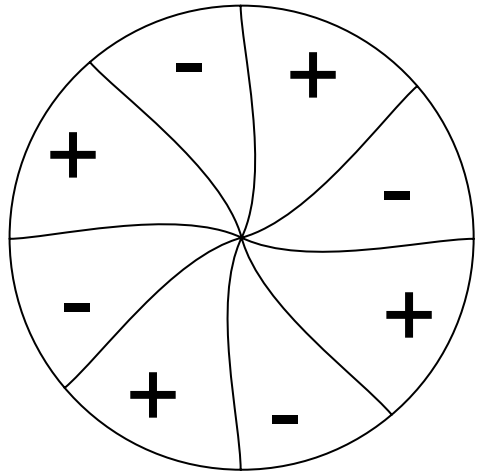
Distribution of walkers

We know $\Psi_T(\mathbf{R})$, N_c and $f(\mathbf{R})$

We want to know $\Psi_0(\mathbf{R})$ and ν_T

One equation with three known quantities and two unknowns could be soluble

Expansion of the Fixed-Node Ground-State Wave-Function



$$f(\mathbf{R}) = \frac{N_c}{\nu_T}\Psi_0(\mathbf{R})\Psi_T(\mathbf{R})$$

$$\begin{aligned}
\Psi_0(\mathbf{R}) &= e^{-J(\mathbf{R})}e^{J(\mathbf{R})}\Psi_0(\mathbf{R}) \\
&= e^{-\hat{J}}\sum_n \lambda_n\left(\prod c^\dagger \prod c\right)|\Phi_T> \\
&= e^{-J(\mathbf{R})}\sum_n \lambda_n \Phi_n(\mathbf{R})
\end{aligned}$$

Multi-Determinant Expansion

Every **anti-symmetric function** can be written as a **product of** a **symmetric function** (Jastrow) and a **complete sum of anti-symmetric functions**.

Expansion of the Fixed-Node Ground-State Wave-Function

$$f(\mathbf{R}) = \frac{N_c}{\nu_T}\Psi_0(\mathbf{R})\Psi_T(\mathbf{R})$$

$$\Psi_0(\mathbf{R}) = e^{-J(\mathbf{R})}\sum_n \lambda_n \Phi_n(\mathbf{R})$$

$$\boxed{\int \mathbf{dR}\Phi_n(\mathbf{R})\Phi_m(\mathbf{R}) = \delta_{n,m}}$$

Every **anti-symmetric function** can be written as a **product of** a **symmetric function** (Jastrow) and a **complete sum of anti-symmetric functions**.

Expansion of the Fixed-Node Walker Distribution Function

$$f(\mathbf{R}) = \frac{N_c}{\nu_T}\Psi_0(\mathbf{R})\Psi_T(\mathbf{R})$$

$$\Psi_0(\mathbf{R}) = e^{-J(\mathbf{R})}\sum_n \lambda_n \Phi_n(\mathbf{R})$$

$$\int \mathbf{dR}\Phi_n(\mathbf{R})\Phi_m(\mathbf{R}) = \delta_{n,m}$$

$$f(\mathbf{R}) = \frac{N_c}{\nu}e^{-2J(\mathbf{R})}\Phi_T(\mathbf{R})\sum_n \lambda_n \Phi_n(\mathbf{R})$$

Any expression of the trial wave-function
- Single determinant
- Multi determinant
- Back flow
- Pfaffian
- etc

Expansion of the Fixed-Node Walker Distribution Function

$$f(\mathbf{R}) = \frac{N_c}{\nu_T}\Psi_0(\mathbf{R})\Psi_T(\mathbf{R})$$

$$\Psi_0(\mathbf{R}) = e^{-J(\mathbf{R})}\sum_n \lambda_n \Phi_n(\mathbf{R})$$

$$\int \mathbf{dR}\Phi_n(\mathbf{R})\Phi_m(\mathbf{R}) = \delta_{n,m}$$

$$f(\mathbf{R}) = \frac{N_c}{\nu}e^{-2J(\mathbf{R})}\Phi_T(\mathbf{R})\sum_n \lambda_n \Phi_n(\mathbf{R})$$

The Wave-Functions Projectors

$$f(\mathbf{R}) = \frac{N_c}{\nu_T}\Psi_0(\mathbf{R})\Psi_T(\mathbf{R})$$

$$\Psi_0(\mathbf{R}) = e^{-J(\mathbf{R})}\sum_n \lambda_n \Phi_n(\mathbf{R})$$

$$\int \mathbf{dR}\Phi_n(\mathbf{R})\Phi_m(\mathbf{R}) = \delta_{n,m}$$

$$f(\mathbf{R}) = \frac{N_c}{\nu} e^{-2J(\mathbf{R})}\Phi_T(\mathbf{R})\sum_n \lambda_n \Phi_n(\mathbf{R})$$

$$\xi_n(\mathbf{R}) = e^{2J(\mathbf{R})}\frac{\Phi_n(\mathbf{R})}{\Phi_T(\mathbf{R})}$$

Reboredo & Proetto
PRB **67**, 115325 (2003).

$$\tilde{\lambda}_n = \lambda_n \frac{N_c}{\nu} = \int \mathbf{dR} f(\mathbf{R})\xi_n(\mathbf{R})$$

The Wave-Functions Coefficients

$$\Psi_0(\mathbf{R}) = e^{-J(\mathbf{R})} \sum_n \lambda_n \Phi_n(\mathbf{R})$$

$$f(\mathbf{R}) = \frac{N_c}{\nu} e^{-2J(\mathbf{R})} \Phi_T(\mathbf{R}) \sum_n \lambda_n \Phi_n(\mathbf{R})$$

$$\xi_n(\mathbf{R}) = e^{2J(\mathbf{R})} \frac{\Phi_n(\mathbf{R})}{\Phi_T(\mathbf{R})}$$

$$\int \mathbf{dR} f(\mathbf{R}) \longrightarrow \sum_{\text{DMC}}$$

$$\tilde{\lambda}_n = \lambda_n \frac{N_c}{\nu} = \int \mathbf{dR} f(\mathbf{R}) \xi_n(\mathbf{R})$$

$$< \tilde{\lambda}_n > = \sum_i \xi_n(\mathbf{R_i}) \quad \gamma(\mathbf{R_i})$$

Umrigar, Nightingale &Runge J.CP **99**, 2865-2890 (1993).

The Wave-Functions Coefficients

$$\Psi_0(\mathbf{R}) = e^{-J(\mathbf{R})} \sum_n \lambda_m \Phi_n(\mathbf{R})$$

$$\xi_n(\mathbf{R}) = e^{2J(\mathbf{R})} \frac{\Phi_n(\mathbf{R})}{\Phi_T(\mathbf{R})}$$

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The Wave-Functions Coefficients

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$$\xi_n(\mathbf{R}) = e^{2J(\mathbf{R})} \frac{\Phi_n(\mathbf{R})}{\Phi_T(\mathbf{R})}$$

$$< \tilde{\lambda}_n >= \sum \xi_n(\mathbf{R_i}) \quad \gamma(\mathbf{R_i})$$

$$\gamma(\mathbf{R_i}) = \frac{-1 + \sqrt{1 + 2|\mathbf{v}|^2 \tau}}{|\mathbf{v}|^2 \tau} \text{ with } \mathbf{v} = \frac{\nabla \Psi_T(\mathbf{R_i})}{\Psi_T(\mathbf{R_i})}$$

Umrigar, Nightingale &Runge
J.CP **99**, 2865-2890 (1993).

Errors in the Wave-Functions Coefficients

$$\Psi_0(\mathbf{R}) = e^{-J(\mathbf{R})} \sum_n \lambda_m \Phi_n(\mathbf{R})$$

$$\xi_n(\mathbf{R}) = e^{2J(\mathbf{R})} \frac{\Phi_n(\mathbf{R})}{\Phi_T(\mathbf{R})}$$

$$< \tilde{\lambda}_n > = \sum \xi_n(\mathbf{R_i}) \quad \gamma(\mathbf{R_i})$$

$$< \tilde{\lambda}_n^2 > = \sum \xi_n(\mathbf{R_i})^2 \gamma(\mathbf{R_i})^2$$

$$< \tilde{\sigma_n} > = \sqrt{\frac{< \tilde{\lambda}_n >^2 - < \tilde{\lambda}_n^2 >}{N_c}}$$

$$\tilde{\lambda}_n \simeq < \tilde{\lambda}_n > \pm \frac{< \tilde{\sigma_n} >}{\sqrt{N_c - 1}}$$

The Fixed Node Wave-Function…

$$\Psi_0(\mathbf{R}) = e^{-J(\mathbf{R})} \sum_n \lambda_m \Phi_n(\mathbf{R})$$

Fixed-Node Ground State

$$\xi_n(\mathbf{R}) = e^{2J(\mathbf{R})} \frac{\Phi_n(\mathbf{R})}{\Phi_T(\mathbf{R})}$$

Wave-Function Projectors

$$< \tilde{\lambda}_n >= \sum \xi_n(\mathbf{R_i}) \quad \gamma(\mathbf{R_i})$$

$$< \tilde{\lambda}_n^2 > = \sum \xi_n(\mathbf{R_i})^2 \gamma(\mathbf{R_i})^2$$

DMC sampling

$$\int \mathrm{dR} f(\mathrm{R}) \rightarrow \sum$$

….can be obtained directly by sampling over the walker distribution.

Errors in the Wave-Functions Coefficients

$$\Psi_0(\mathbf{R}) = e^{-J(\mathbf{R})} \sum_n \lambda_m \Phi_n(\mathbf{R})$$

Fixed-Node Ground State

$$\xi_n(\mathbf{R}) = e^{2J(\mathbf{R})} \frac{\Phi_n(\mathbf{R})}{\Phi_T(\mathbf{R})}$$

$$\tilde{\lambda}_n \simeq < \tilde{\lambda}_n > \pm \frac{< \tilde{\sigma_n} >}{\sqrt{N_c - 1}}$$

- The nodes move because of errors.

A Self-Healing DMC Algorithm

$$\Psi_0(\mathbf{R}) = e^{-J(\mathbf{R})} \sum_n \lambda_m \Phi_n(\mathbf{R})$$

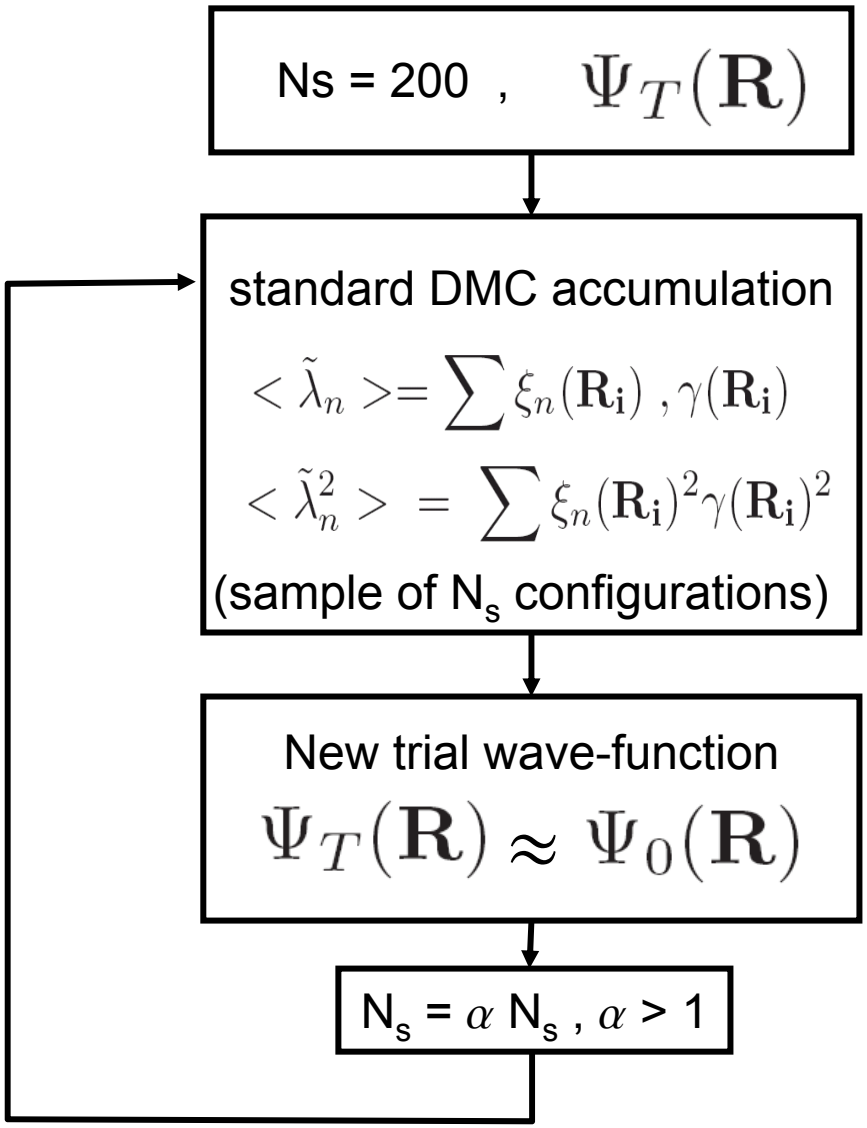
Fixed-Node Ground State

$$\xi_n(\mathbf{R}) = e^{2J(\mathbf{R})} \frac{\Phi_n(\mathbf{R})}{\Phi_T(\mathbf{R})}$$

$$\tilde{\lambda}_n \simeq <\tilde{\lambda}_n> \pm \frac{<\tilde{\sigma_n}>}{\sqrt{N_c - 1}}$$

- The nodes can move because of errors
- How do we take advantage of errors?

A Simple Self-Healing DMC Algorithm



starting trial wave function: **anything**

A Simple Self-Healing DMC Algorithm

1)

$$\Psi_0(\mathbf{R}) = e^{-J(\mathbf{R})} \sum_n \lambda_m \Phi_n(\mathbf{R}) \qquad \boxed{\int d\mathbf{R} \Phi_n(\mathbf{R}) \Phi_m(\mathbf{R}) = \delta_{n,m}}$$

$\Phi_n(\mathbf{R})$ Are non-interacting eigen-functions:
$\Longrightarrow$ increasing kinetic energy

2)

$\lambda_n = 0$ if $\left| < \tilde{\lambda}_n > \right| < \dfrac{< \tilde{\sigma}_n >}{\sqrt{N_c - 1}}$ x 4

else $\lambda_n = < \tilde{\lambda}_n >$

3)

We set $\Psi_T(\mathbf{R}) = \Psi_0(\mathbf{R})$

A Simple Self-Healing DMC Algorithm: **Model**

The model test system: two interacting spinless fermions in a box

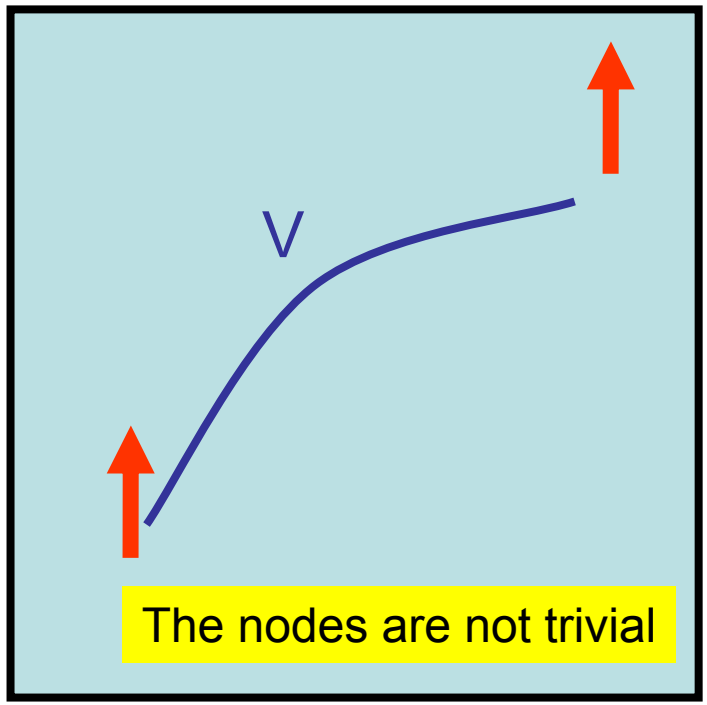
Case (1) Model interaction

$V = 8\gamma\,\pi^2 \cos[\alpha\pi(x-x')] \cos[\alpha\pi(y-y')]$

α and γ control the shape and strength of V

V is repulsive for $|\alpha| < 1/2$ and $\gamma > 0$

Full CI: H expanded in the first 300 non-interacting eigenfunctions with the symmetry of the ground state. **All integrals done analytically**. Converged results

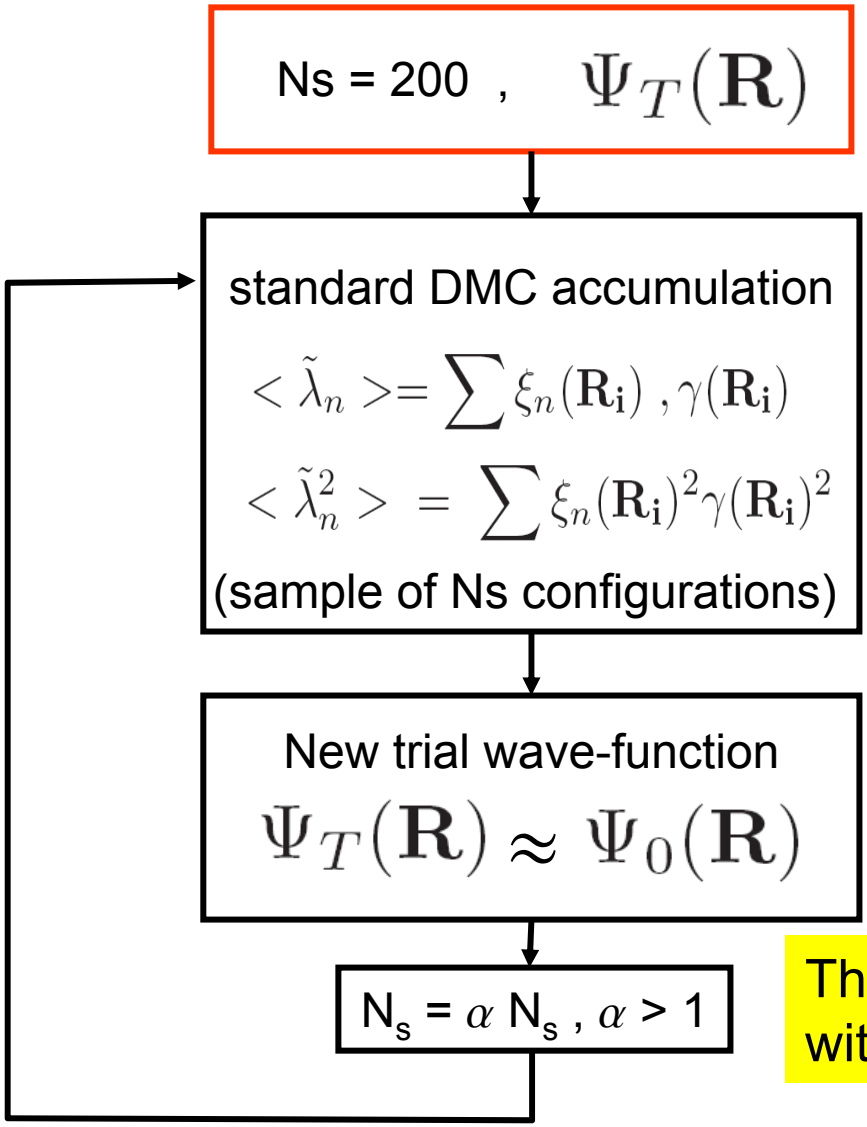


Case (2) Coulomb interaction

$V = 20\,\pi^2\, 1/\mathrm{sqrt}[(x-x')^2+(y-y')^2]$

We will compare the algorithm against almost-analytical results

A Simple Self-Healing DMC Algorithm: **Initial Ψ_T**



starting trial wave function: **anything**

$\lambda_1 = - a_3$

$\lambda_3 = a_1$

$\lambda_n = 0$ (for any other λ_n)

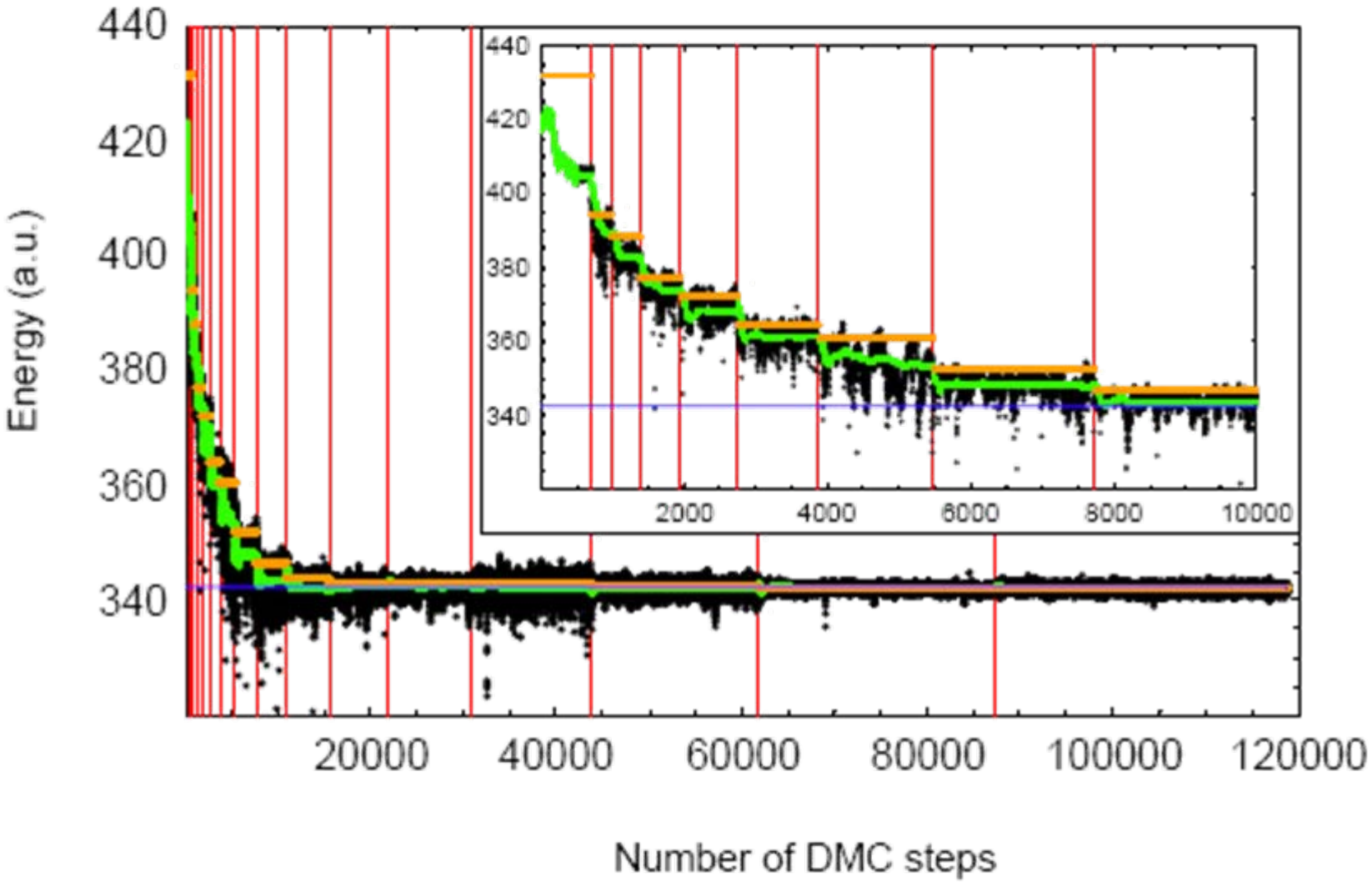
a_n (full CI coefficients)

The starting trial wave function: is orthogonal to the "exact" CI ground state

The standard DMC algorithm must fail with this trial wave-function choice

$$e^{-J(\mathbf{R})} = 1$$

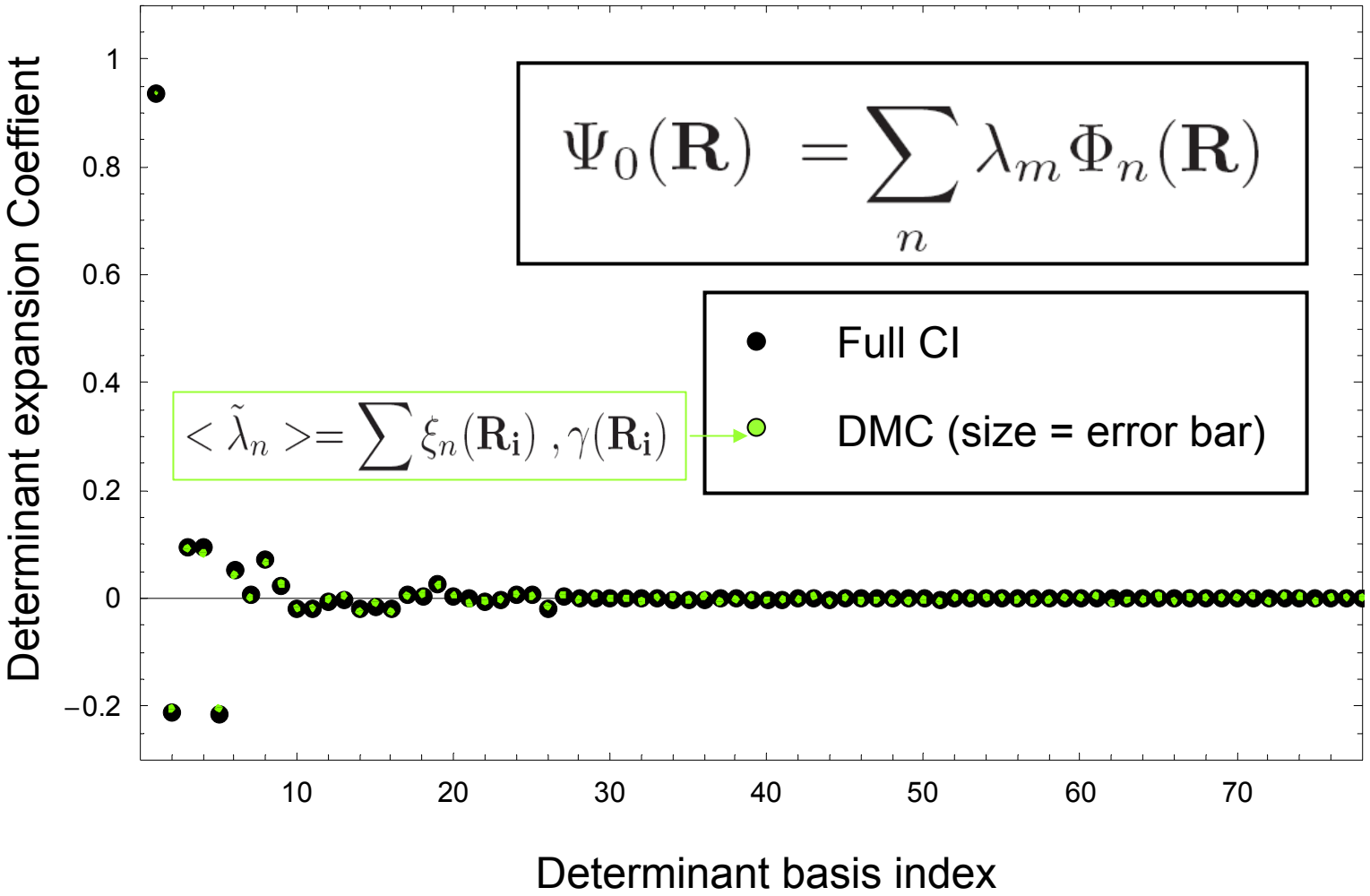
A Simple Self-Healing DMC Algorithm: **Results**



The DMC energy converges to the full CI even starting from the worst trial wavefunction

A Simple Self-Healing DMC Algorithm: **Results**

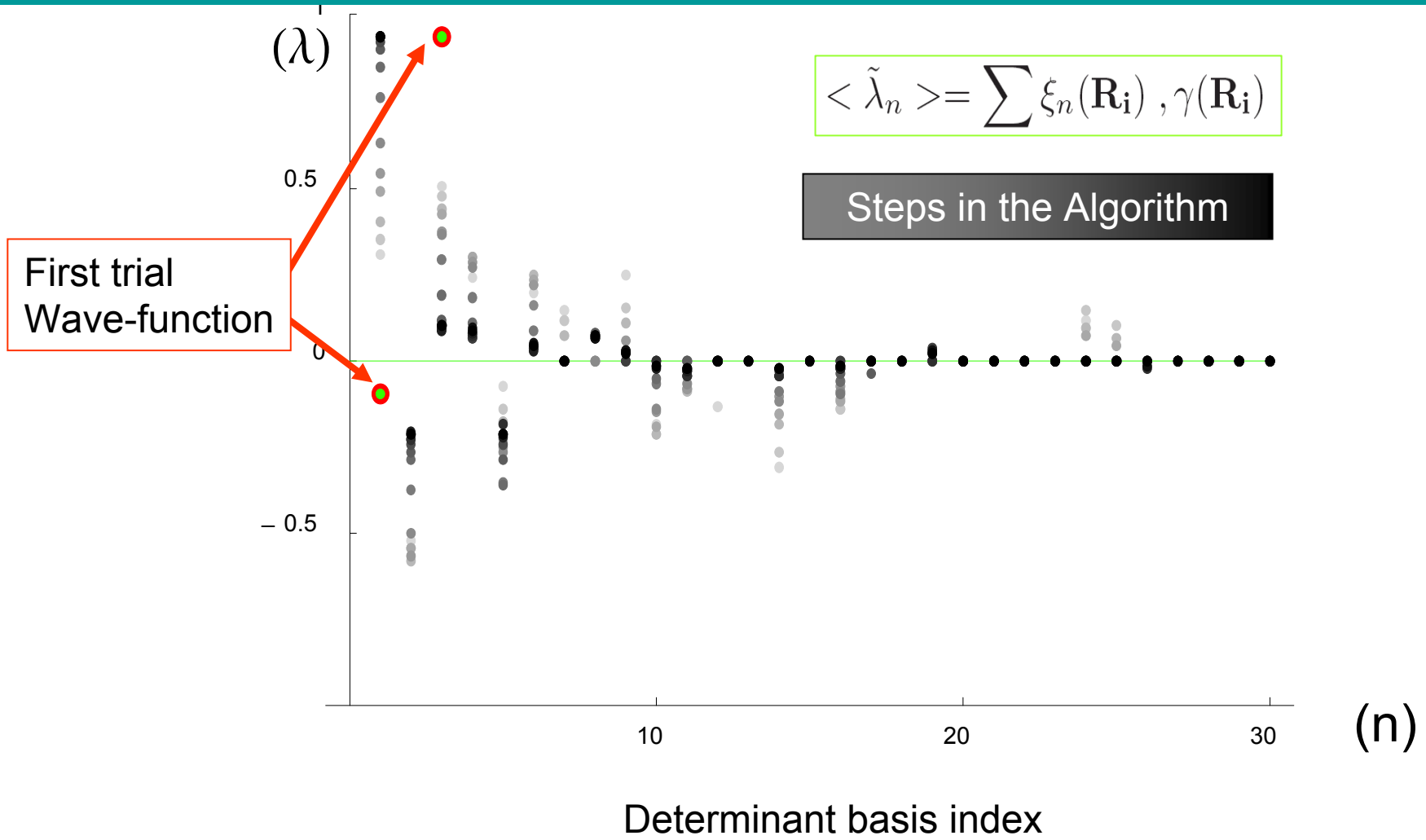
Expansion of the Ground-State Wave-Function



An expansion of the Ground-State Wave-Function can be obtained from DMC with full CI quality

A Simple Self-Healing DMC Algorithm: **Results**

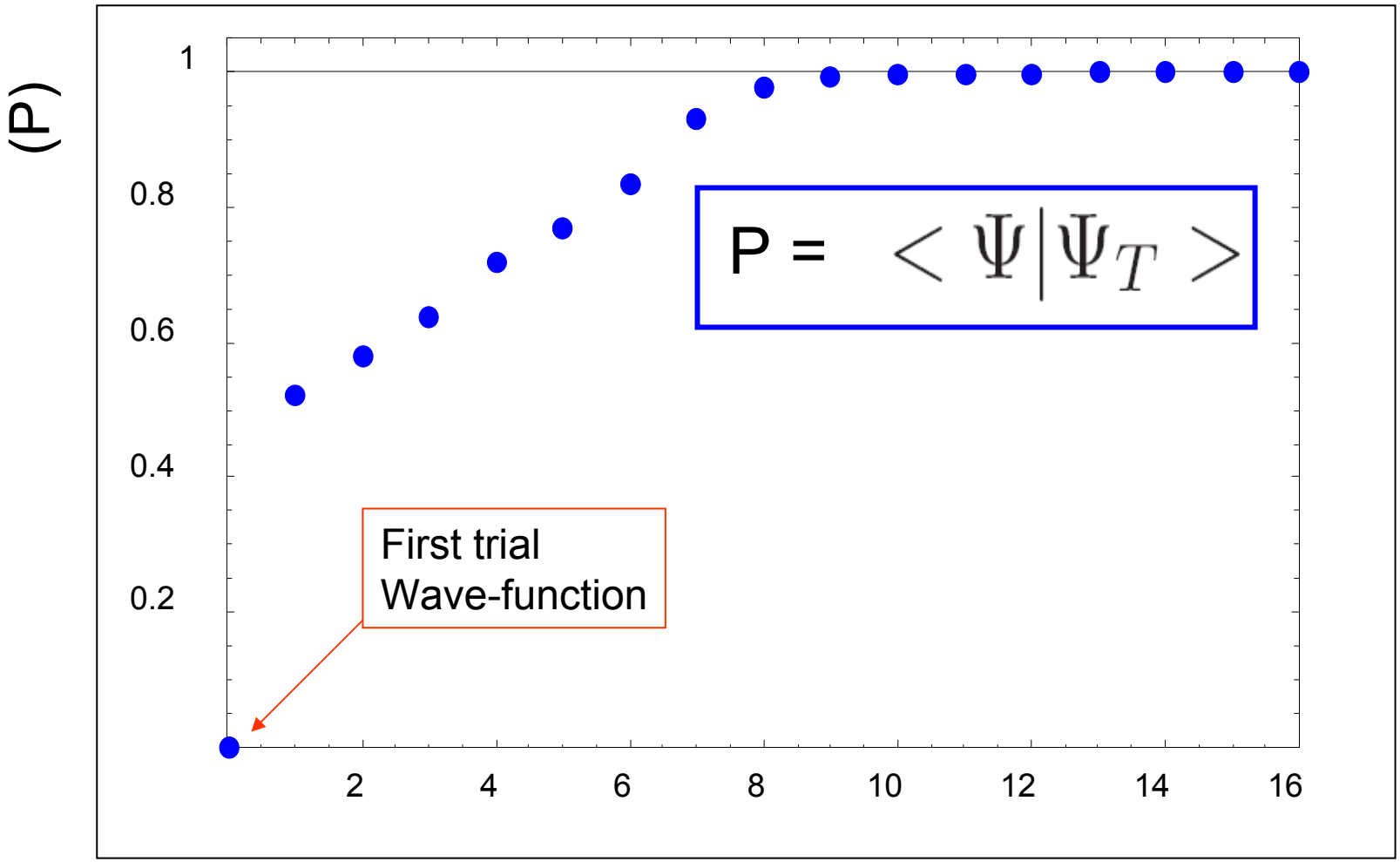
Expansion of the Ground-State Wave-Function (time evolution)



Systematic convergence of the wave-function towards the CI solution

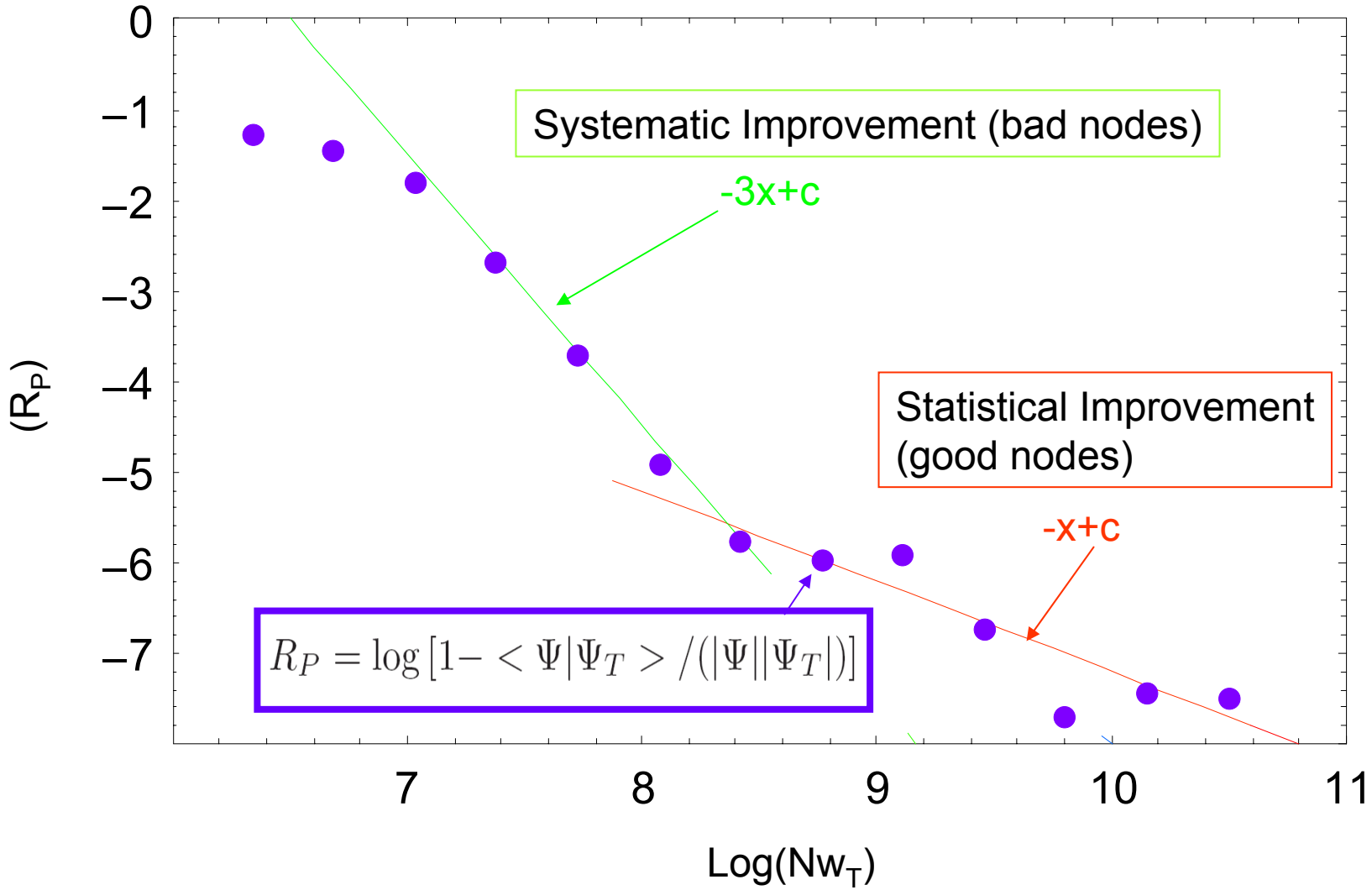
A Self-Healing DMC Simple Algorithm: **Results**

Projection of the SH-DMC WF on the CI Ground-State WF



A Self-Healing DMC Simple Algorithm: **Results**

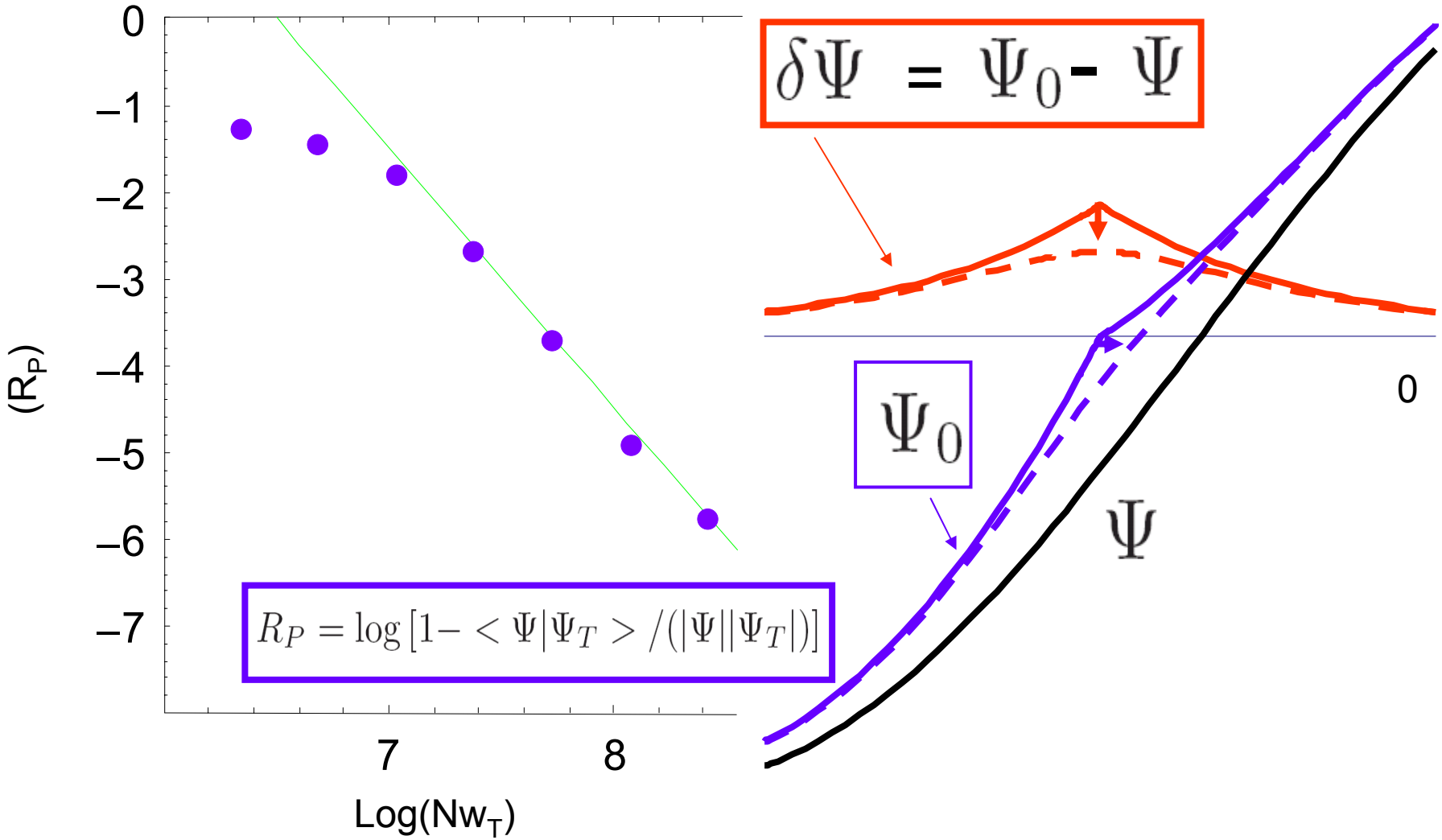
Projection of the SH-DMC WF on the CI Ground-State WF



We observe first a fast improvement followed by a slow improvement regime

A Self-Healing DMC Simple Algorithm: **Results**

Why does it work?



Truncation of high energy components moves the nodes in right direction

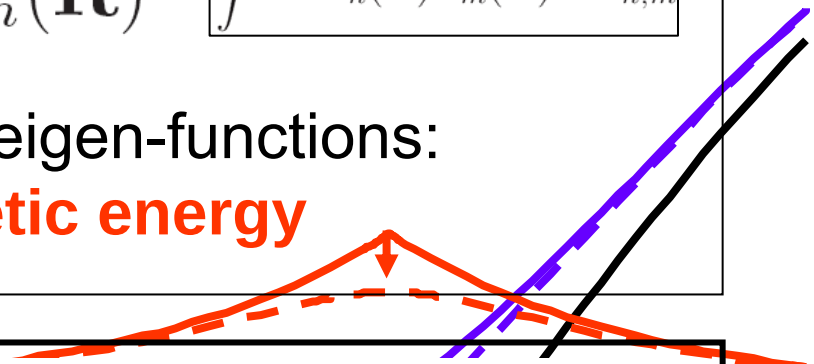
A Self-Healing DMC Simple Algorithm: **Results**

Why does it work?

1) $\Psi_0(\mathbf{R}) = e^{-J(\mathbf{R})} \sum_n \lambda_m \Phi_n(\mathbf{R})$ $\int d\mathbf{R}\Phi_n(\mathbf{R})\Phi_m(\mathbf{R}) = \delta_{n,m}$

$\Phi_n(\mathbf{R})$ Are non-interacting eigen-functions:

$\Longrightarrow$ **increasing kinetic energy**



2) $\lambda_n = 0$ if $\left| < \tilde{\lambda}_n > \right| < \dfrac{< \tilde{\sigma}_n >}{\sqrt{N_c - 1}}$ x 4

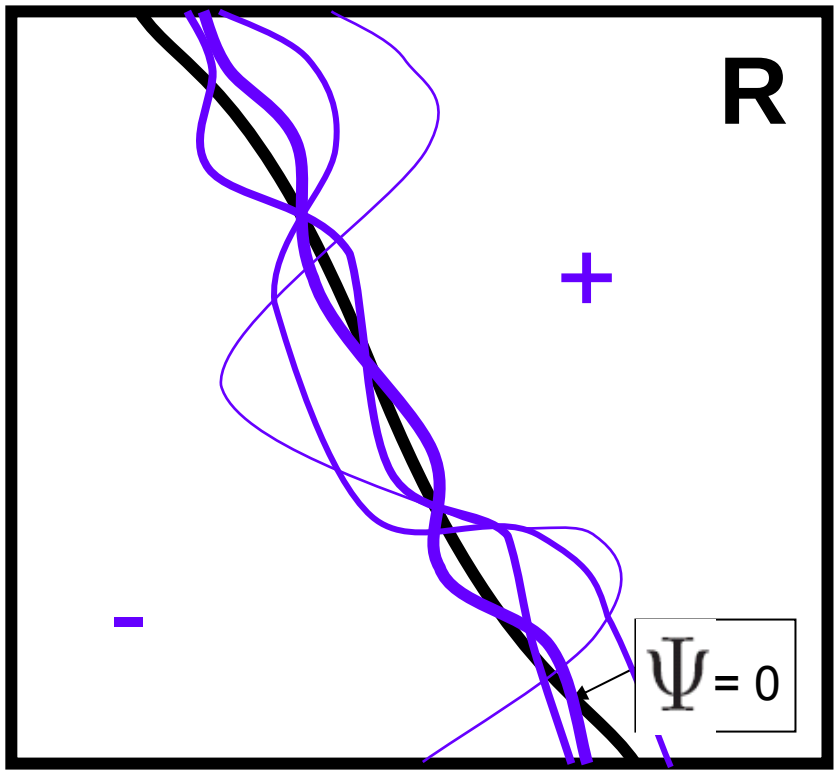
else $\lambda_n = < \hat{\lambda}_n >$

3) We set $\Psi_T(\mathbf{R}) = \Psi_0(\mathbf{R})$

Truncation of poorly resolved high energy components moves the nodes in right direction

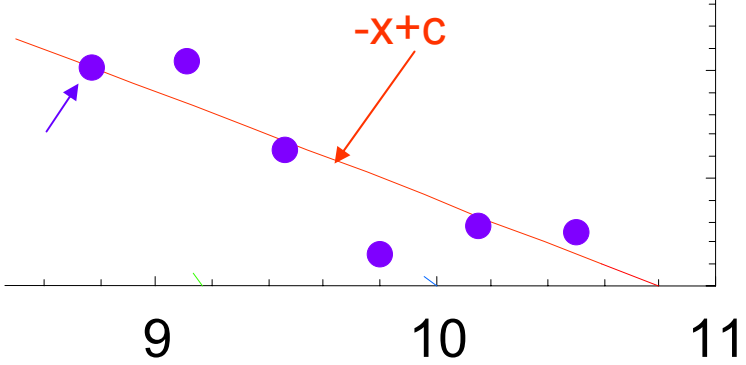
A Self-Healing DMC Simple Algorithm: **Results**

Why does it work?



$$R_P = \log\left[1 - < \Psi | \Psi_T > / (|\Psi||\Psi_T|)\right]$$

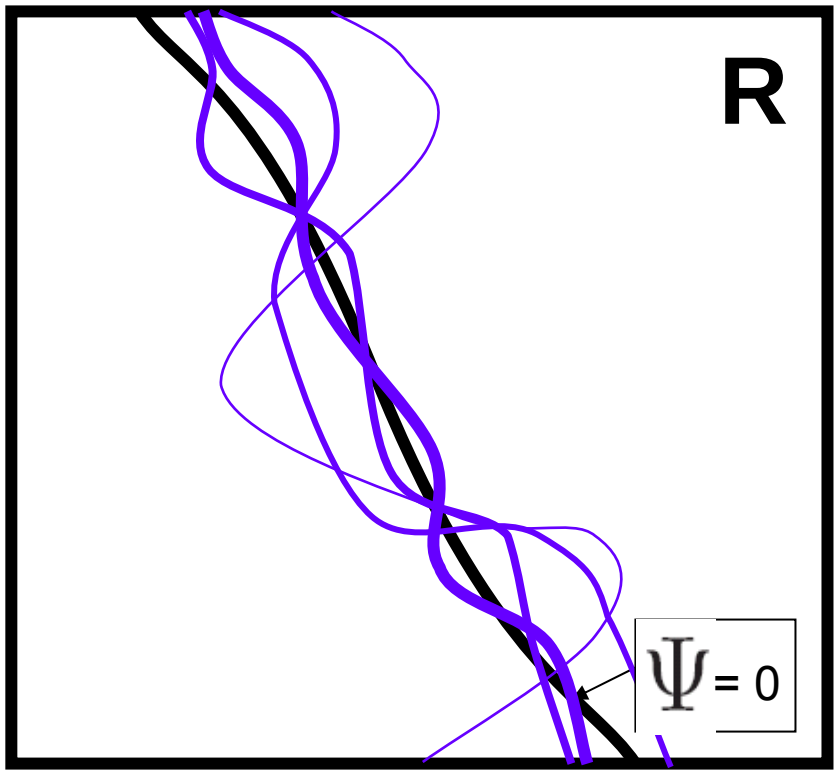
Statistical Improvement
(good nodes)

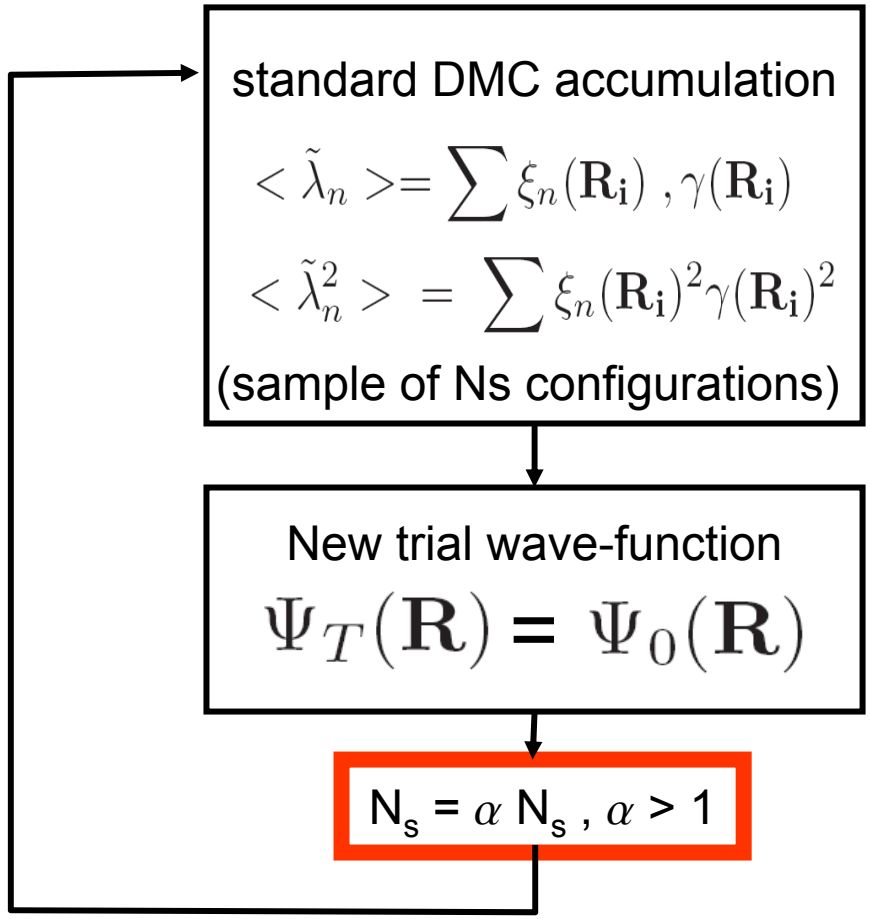


Noise in the coefficients plays the role of a temperature in a simulated annealing approach. Good fluctuations are reinforced bad ones are abandoned.

A Self-Healing DMC Simple Algorithm: **Results**

Why does it work?



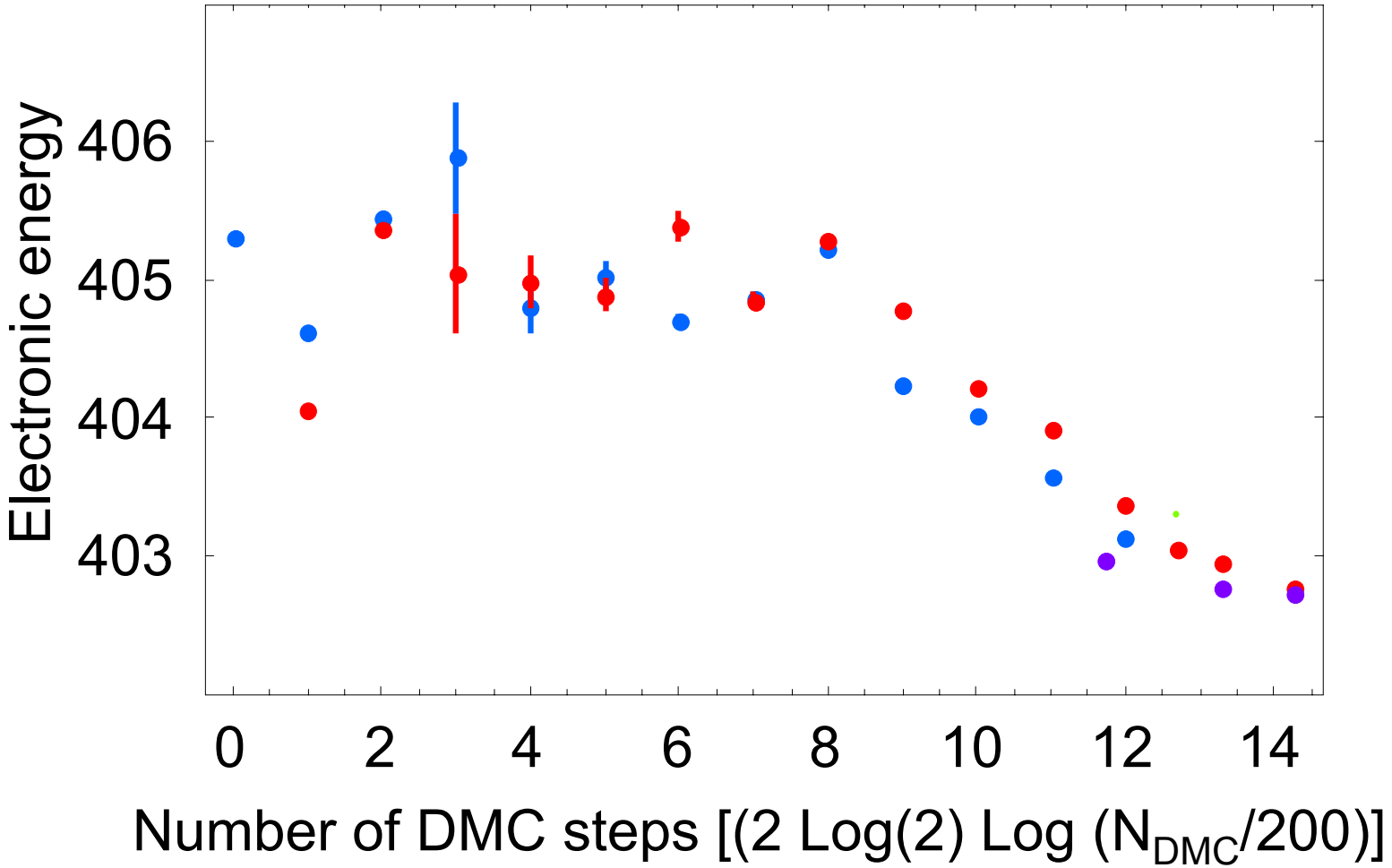


Noise in the coefficients plays the role of a temperature in a simulated annealing approach. Good fluctuations are reinforced bad ones are abandoned.

A Self-Healing DMC Simple Algorithm: **Results**

Case (2) Coulomb interaction $V = 20\ \pi^2\ 1/\mathrm{sqrt}[(x-x')^2+(y-y')^2]$

Expansion of the Ground-State Wave-Function

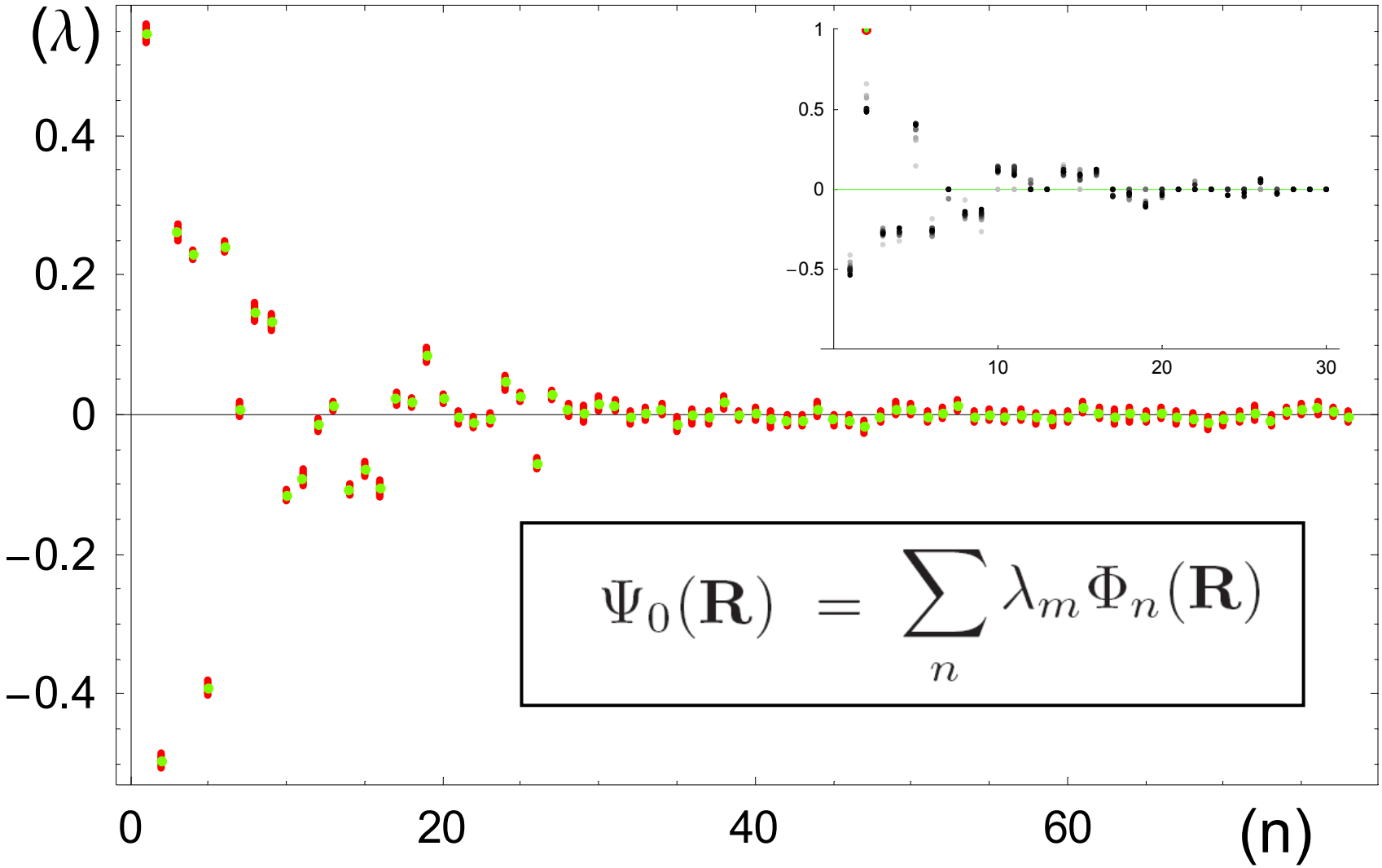


We obtain a systematic reduction of the energy (beyond error bar)

A Self-Healing DMC Simple Algorithm: **Results**

Case (2) Coulomb interaction $V = 20\ \pi^2\ 1/\mathrm{sqrt}[(x-x')^2+(y-y')^2]$

Expansion of the Ground-State Wave-Function



A Self-Healing DMC Simple Algorithm: **Results**

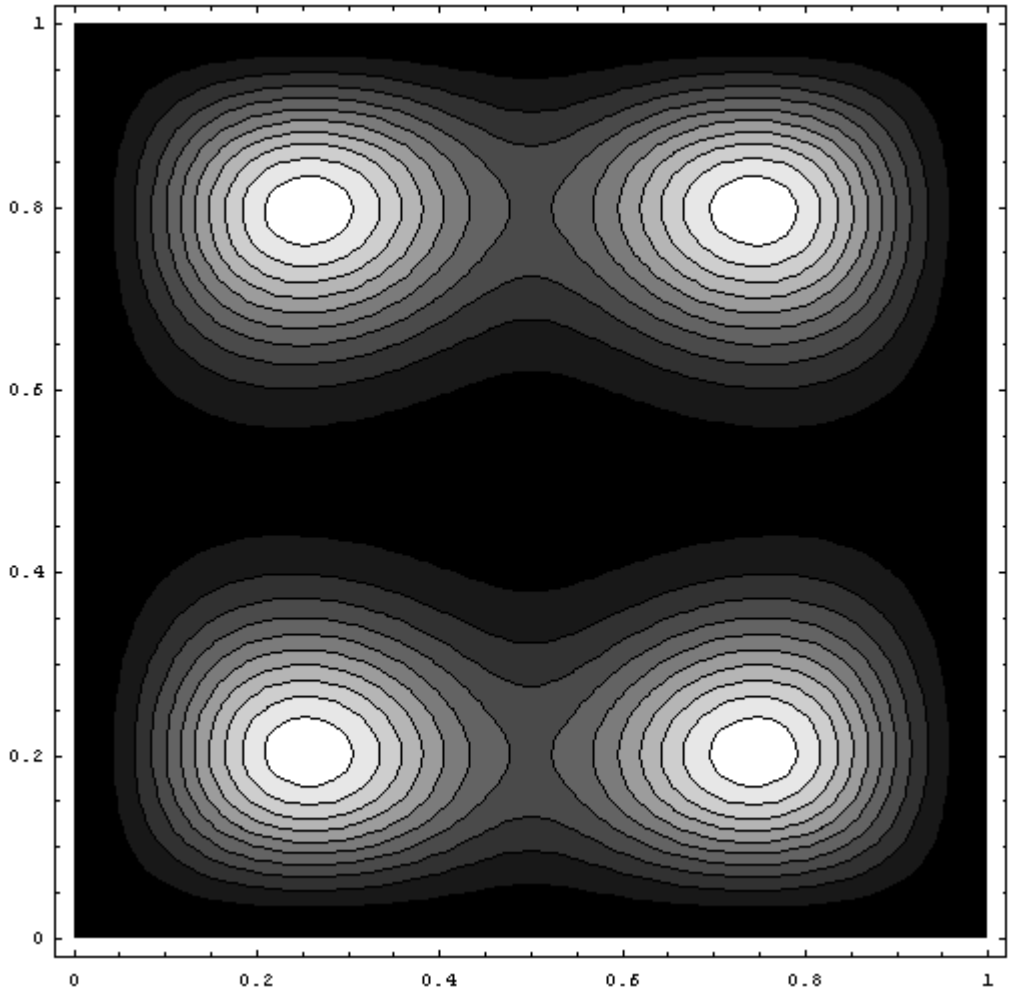
Case (2) Coulomb interaction $V = 20\ \pi^2\ 1/\mathrm{sqrt}[(x-x')^2+(y-y')^2]$

Interacting Ground-State: Electronic Density

$$e^{-J(\mathbf{R})} = 1$$

$$\rho(\mathbf{r}) = \sum_{n,\nu} \phi_n(\mathbf{r})\phi_\nu(\mathbf{r}) \sum_{k,l} \lambda_k \lambda_l < \Phi_k | c\dagger_n c_\nu | \Phi_l >$$

Initial trial wave function density →

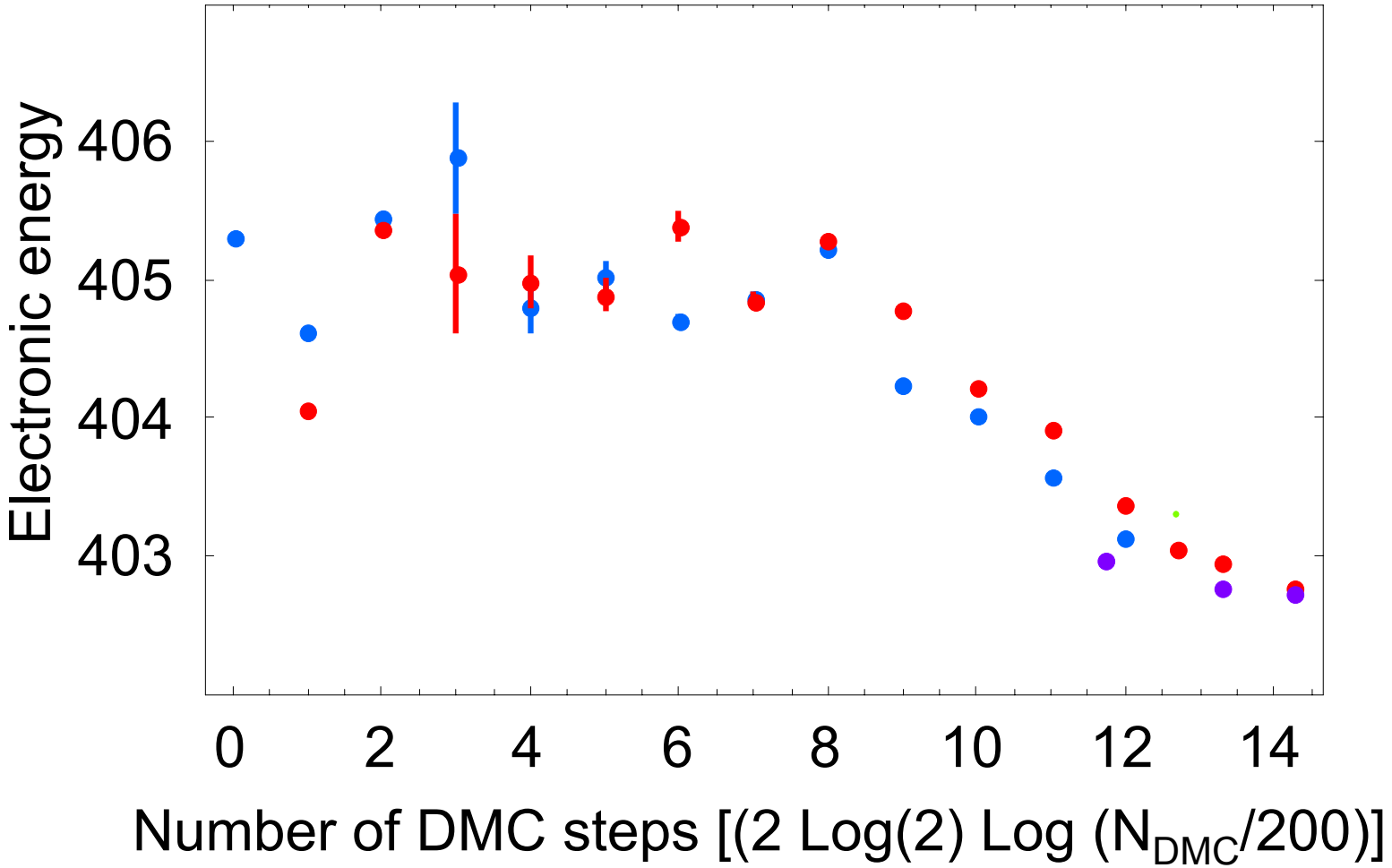


With the ground state wave function we can evaluate any observable

A Self-Healing DMC Simple Algorithm: **Results**

Case (2) Coulomb interaction $V = 20\ \pi^2\ 1/\mathrm{sqrt}[(x-x')^2+(y-y')^2]$

Expansion of the Ground-State Wave-Function



We obtain a systematic reduction of the energy (beyond error bar)

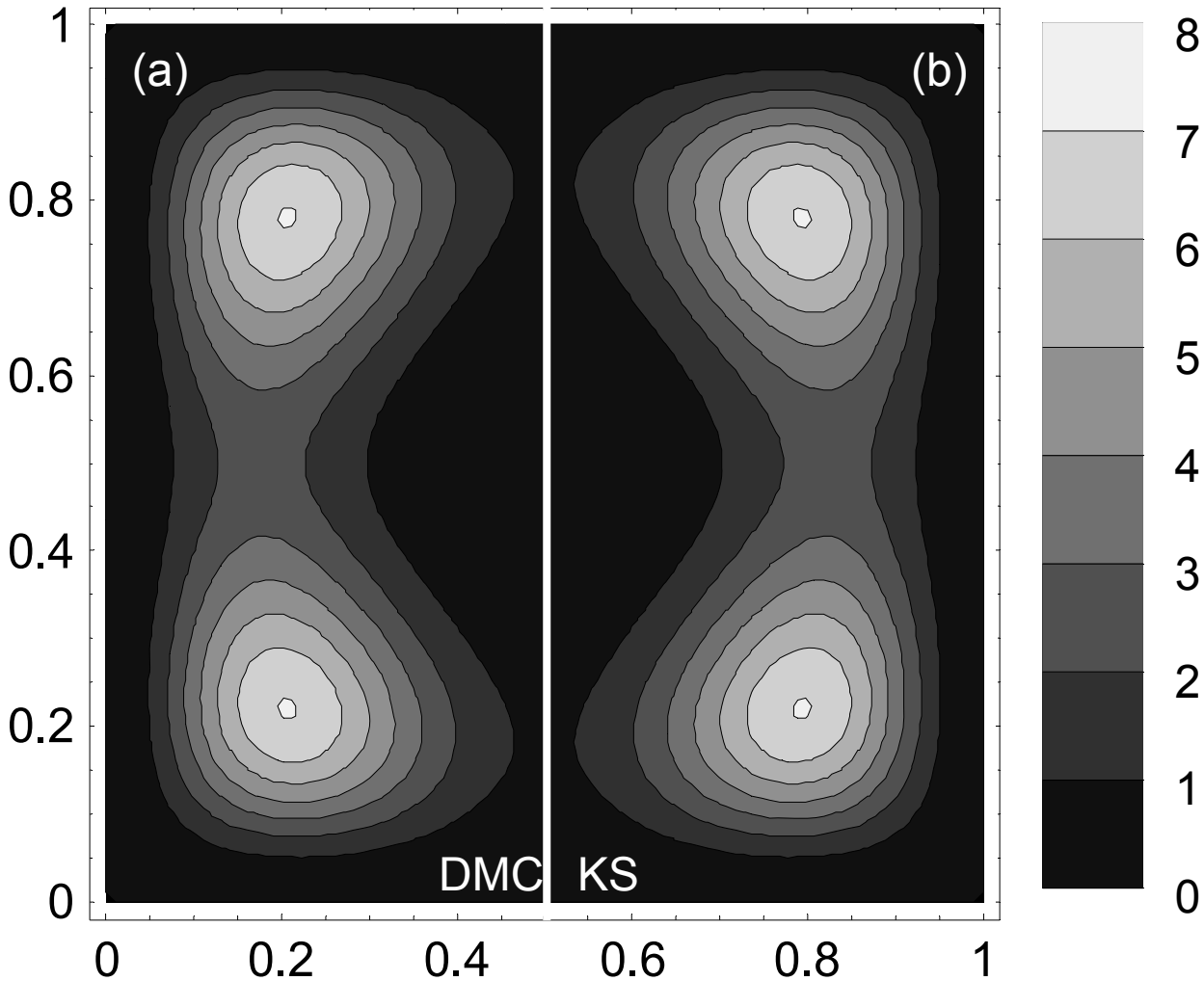
A Self-Healing DMC Simple Algorithm: **Results**

Case (2) Coulomb interaction $V = 20\ \pi^2\ 1/\mathrm{sqrt}[(x-x')^2+(y-y')^2]$

Non-Interacting Kohn-Sham Electronic Density

Reboredo & Kent
PRB 245110 (2008)

$$K_\rho = \frac{1}{2}\int \mathbf{dr}[\bar{\rho}(\mathbf{r}) - \rho(\mathbf{r})]^2$$



A Self-Healing DMC Simple Algorithm: **Results**

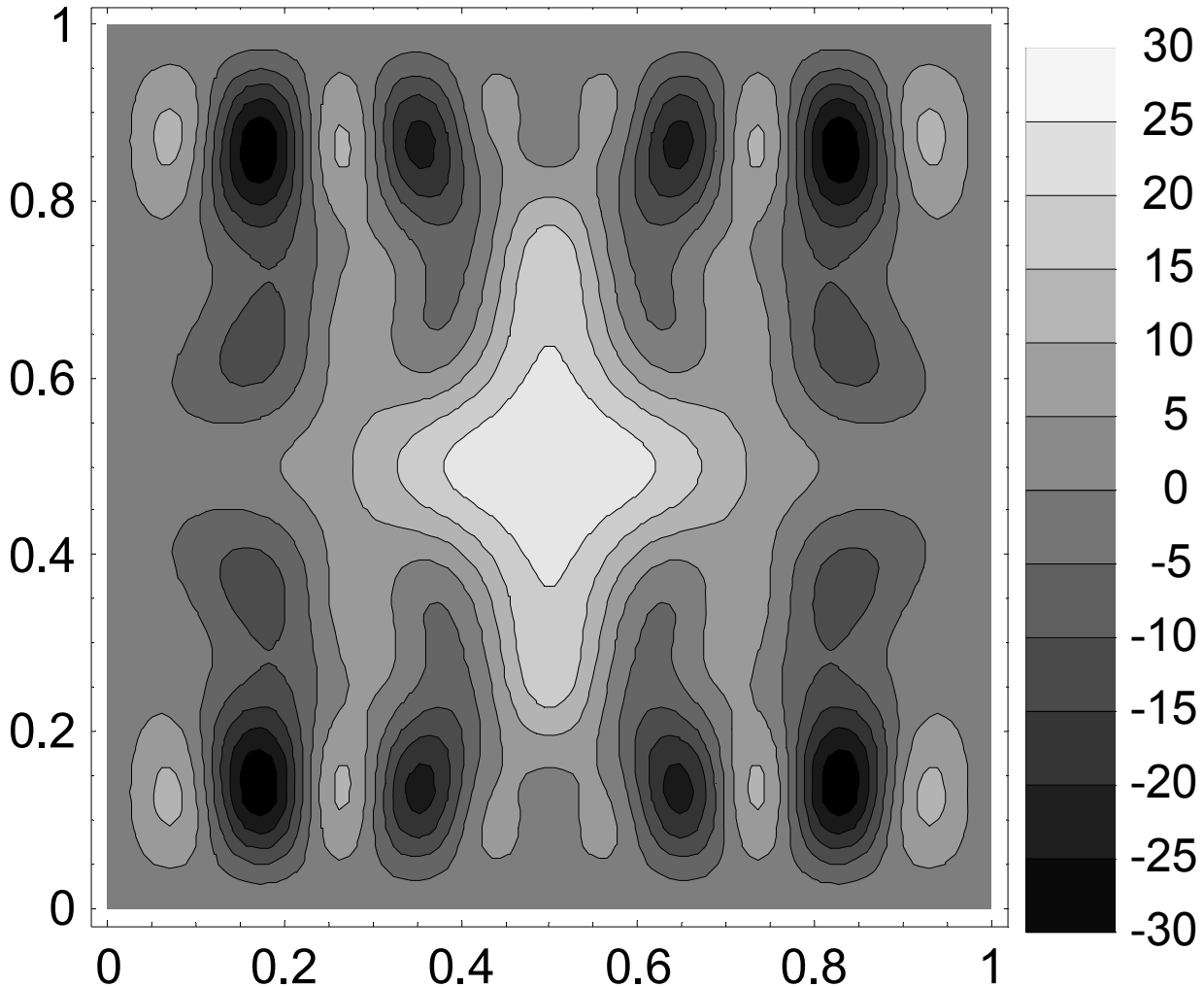
Case (2) Coulomb interaction $V = 20\ \pi^2\ 1/\mathrm{sqrt}[(x-x')^2+(y-y')^2]$

Kohn-Sham Potential

Reboredo & Kent
PRB 245110 (2008)

$$K_\rho = \frac{1}{2}\int \mathbf{dr}[\bar{\rho}(\mathbf{r}) - \rho(\mathbf{r})]^2$$

$$\Delta\bar{V}_{K_\rho}(\mathbf{r}) = \int \mathbf{dr}'[\rho(\mathbf{r}') - \bar{\rho}(\mathbf{r}')]\frac{\delta V(\mathbf{r}')}{\delta\rho(\mathbf{r})}$$



Summary

- The fixed node ground state wave function can be obtained directly from the walker distribution
- An iterative algorithm based on the update of the trial wave function leads to a systematic reduction of nodal errors
- The algorithm takes advantage of truncation and statistical errors to improve the trial wave function
- The Kohn-Sham potential can be obtained directly from a SH-DMC run
- Tests in larger systems are in progress