QMC and GW Calculations in Fullerenes

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•**Thanks A. J. Williamson, R. J. Needs, N. Drummond, M. Towler, J. Kim and M. Kalos**

DMC for fermions

$$\frac{\partial f}{\partial \tau} = \frac{\hbar^2}{2m}\left[\sum_{i=1}^{N}\nabla_i^2 f - \nabla_i\left(f\nabla_i \ln|\psi_T|^2\right)\right] - \left[\frac{H\psi_T}{\psi_T} - \varepsilon_0\right] f$$

Ceperley Alder PRL 1980

$$H = -\sum_i \frac{\hbar^2\nabla_i^2}{2m} + \sum_{i,j}\frac{e^2}{|\vec{r}_i - \vec{r}_j|} - \sum_{i,I}\frac{Z_I e^2}{|\vec{r}_i - \vec{R}_I|} + \sum_{J,I}\frac{Z_I Z_J e^2}{|\vec{R}_J - \vec{R}_I|}$$

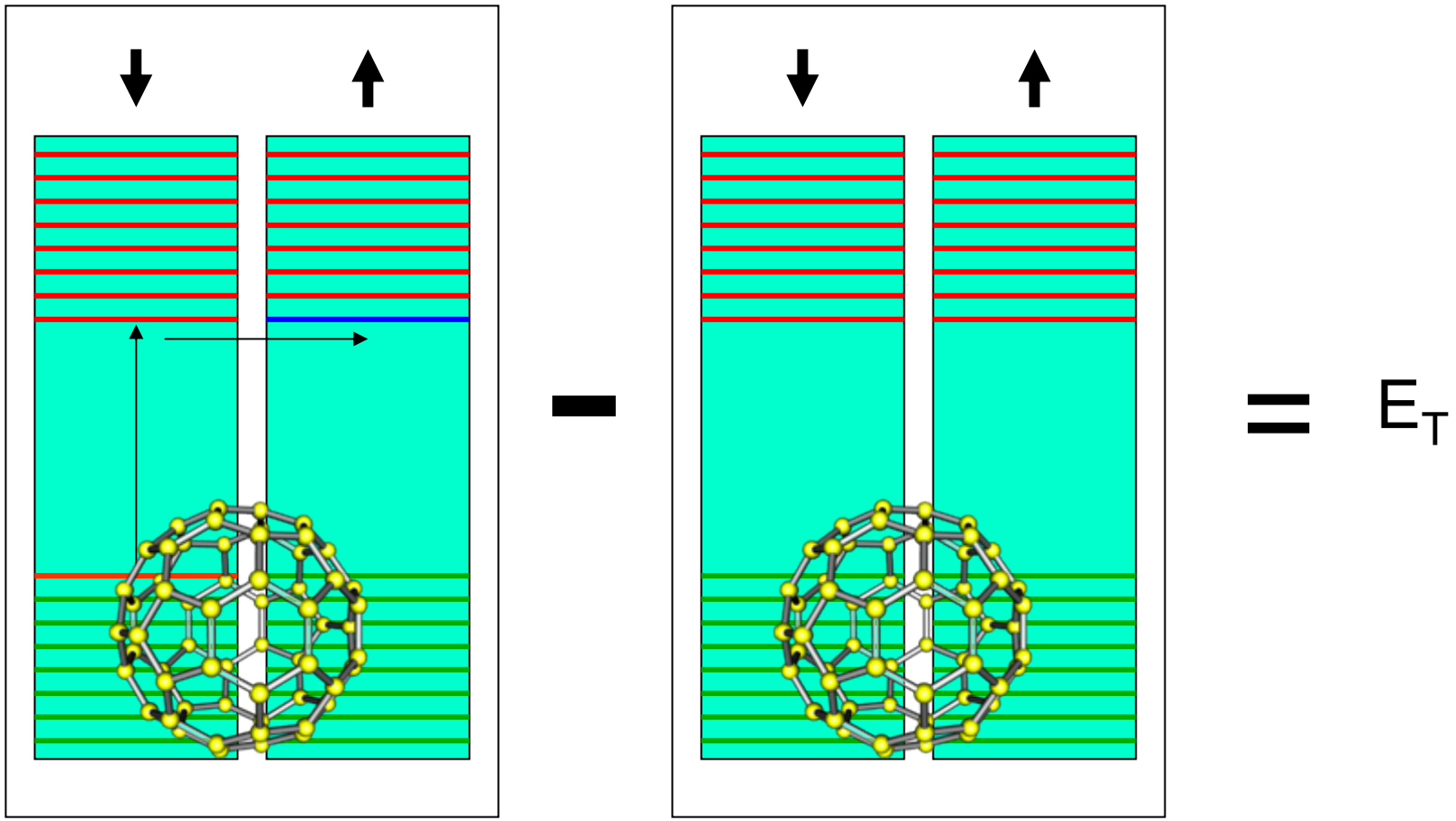
$$\Psi = \begin{vmatrix} \phi_1(\mathbf{r}_1) & \phi_1(\mathbf{r}_2) & \cdots \\ \phi_2(\mathbf{r}_1) & \phi_2(\mathbf{r}_2) & \\ \vdots & & \ddots \\ & & \phi_N(\mathbf{r}_N) \end{vmatrix} \cdot \exp\left[\sum_i^N \chi(\mathbf{r}_{iI}) - \sum_i^N u(\mathbf{r}_{ij})\right]$$

Slater Determinant
$O(N^3)$

Jastrow correlation function
$O(N^2)$

We use CASINO 2.1  **Cambridge Quantum Monte Carlo Code**

Approximations (1) pseudopotentials, (2) Fix Node (3) DFT structure



This is a very demanding test for DMC
Total energy differences require cancelation of errors on 0.01% or more

Levels of approximation of GW methods:

"DFT"

$$\Sigma = V_{xc}$$

Hybertsen & Louie (1985)

$$G_0(\mathbf{r},\mathbf{r}';E) = \sum_n \frac{\psi_n(\mathbf{r})\psi_n^\star(\mathbf{r}')}{E - E_n}$$

$$W \approx \epsilon^{-1}\frac{e^2}{|\mathbf{r}-\mathbf{r}'|}$$

G_0W_0 approximation

$$\Sigma = iG_0W_0$$

Del Sole et al. (1994)

Tiago et. al (2006)

G_0W_0 + vertex: G_0W_f approximation

$$\Sigma = iG_0W_0\Gamma_0$$

Self-consistent: GW approximation

$$\Sigma = iGW$$

Hedin's equations

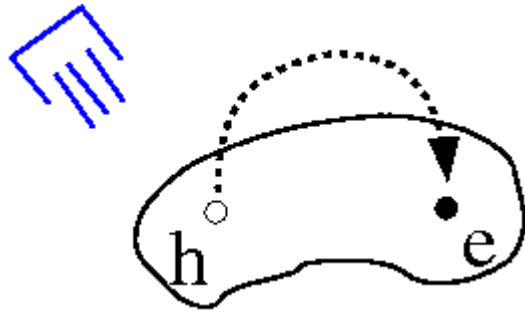
$$\begin{cases} W = V + VPW \\ P = -iGG\Gamma \\ \Sigma = iG\Gamma W \\ \Gamma = 1 + \frac{\delta\Sigma}{\delta G}GG\Gamma \end{cases}$$

G_0W_0 and G_0W_f approximations rely on DFT as a "good starting point".

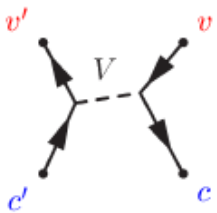
Optical Excitations: Bethe-Salpeter Equation

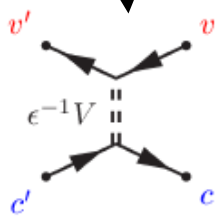
Eigenvalue problem:

$$\left(\varepsilon_c^{GW} - \varepsilon_v^{GW}\right) A_{cv}^S + \sum_{c'v'} \langle vc|K^{BSE}|c'v'\rangle A_{c'v'}^S = \Omega^S A_{cv}^S$$



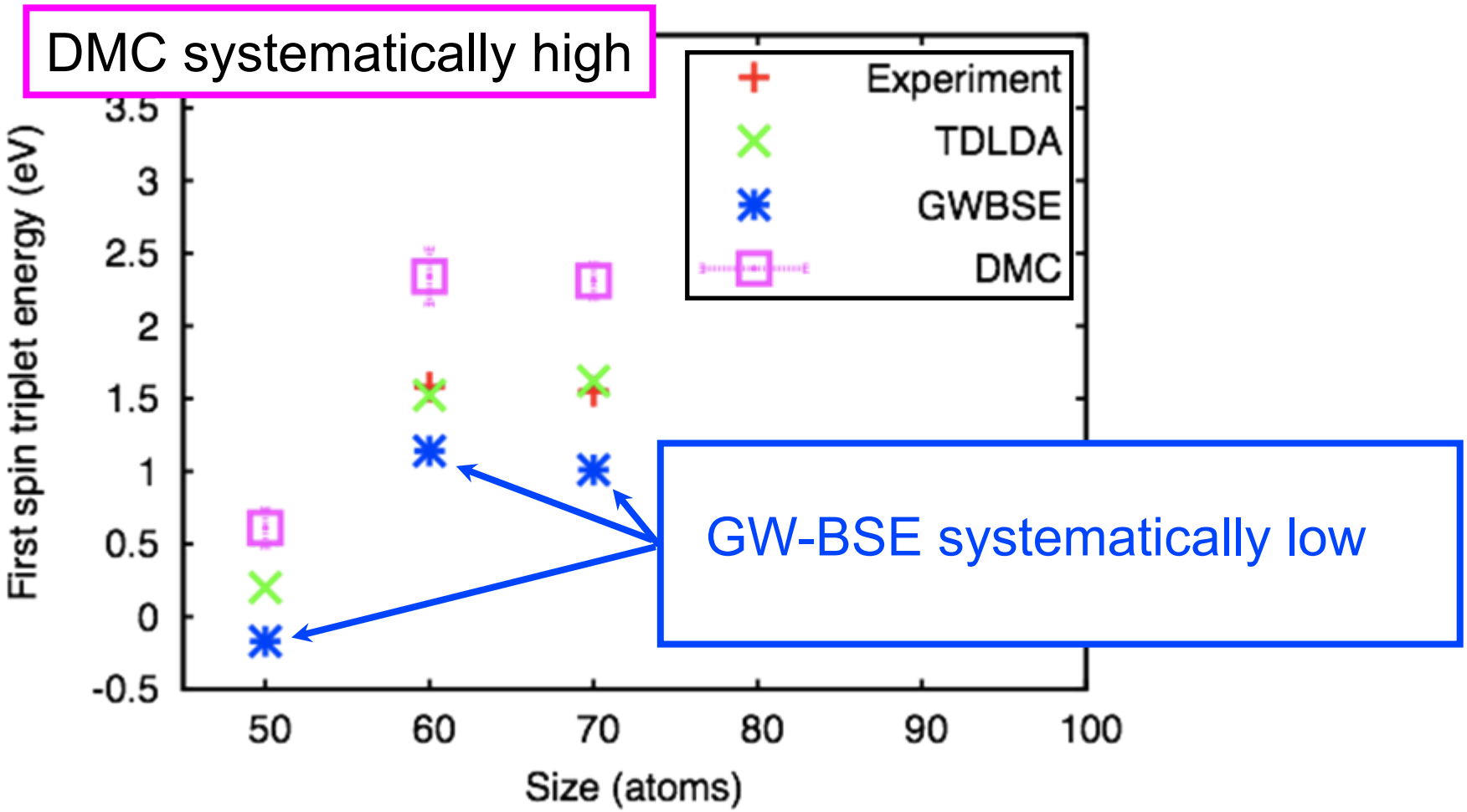
$$K^{BSE} = \frac{\delta}{\delta G}\left[1 \cdot V_{Coul} + \Sigma\right]$$





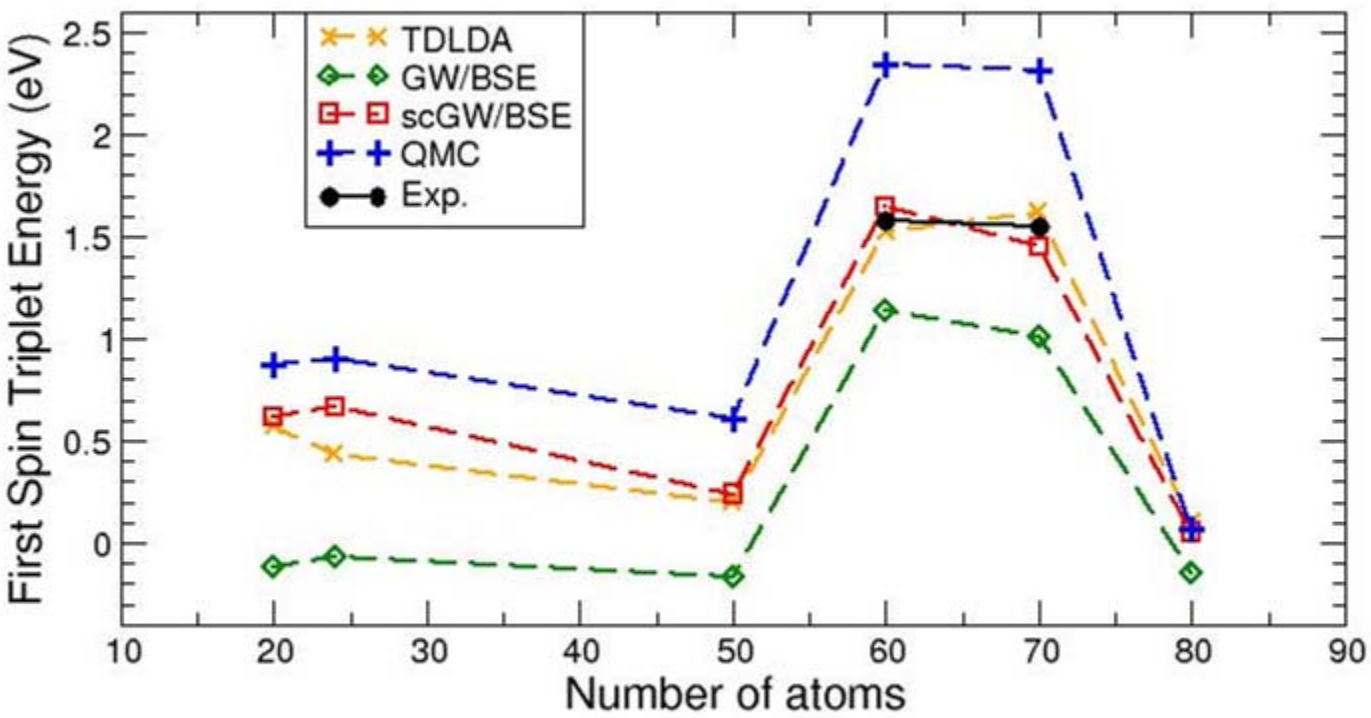
- Many-body expansion of the electron-hole propagator.
- Dynamics of electron-hole excitation obtained by solving the Bethe-Salpeter equation (BSE).
- Requires knowledge of quasiparticle orbitals (get from GW).

Results: First spin-triplet



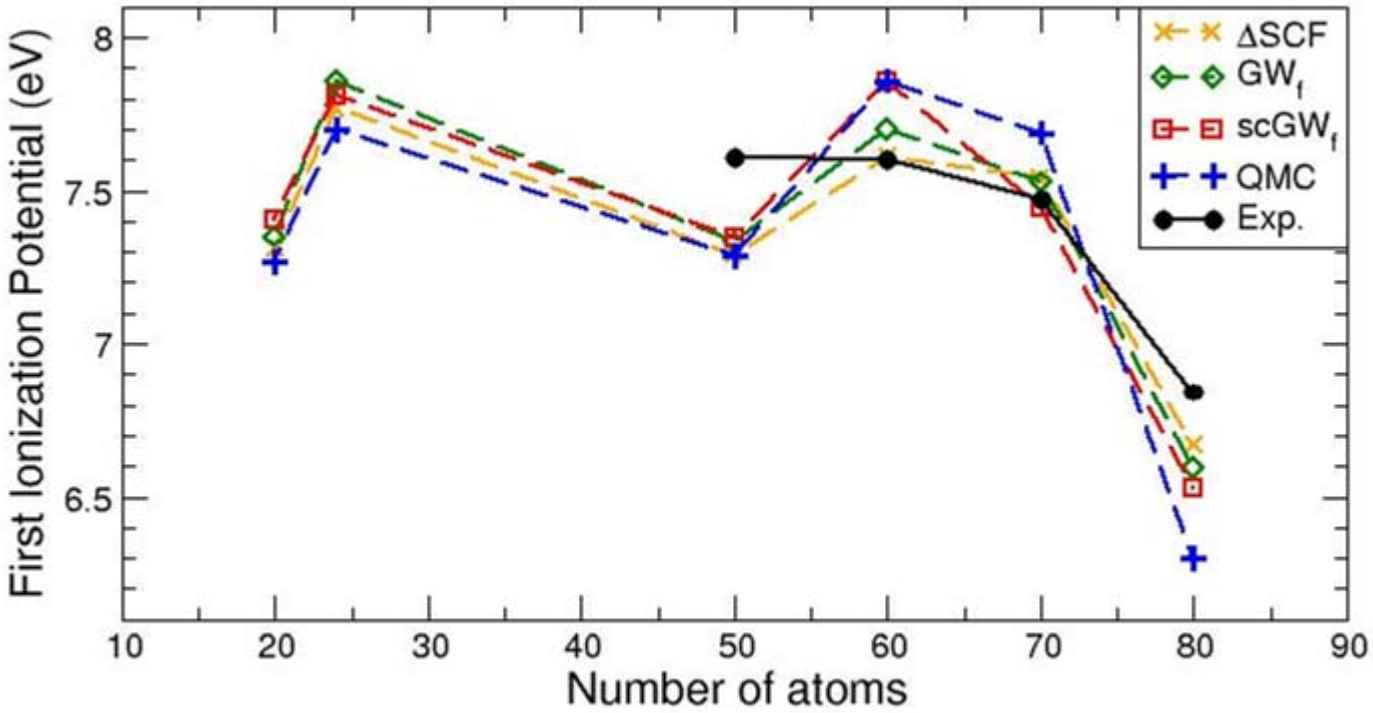
- Stoke's shifts estimated as max 0.2 eV from DFT not included in above data

Experimental data suggest incorporating self-consistency



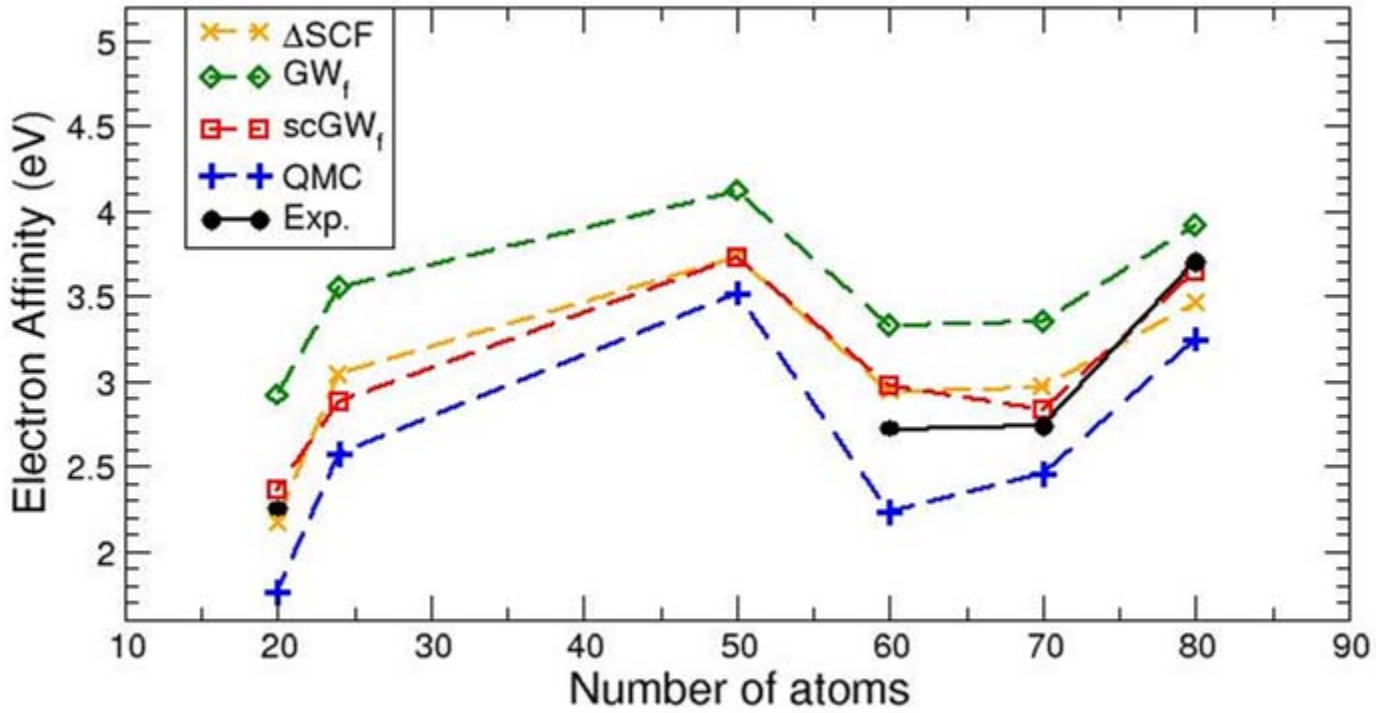
Scissors (eigen-values) self-consistency seems essential in GW/BSE.
DMC gives higher (~0.8 eV) triplet energies

First Ionization Potentials



We find good agreement for Ionization Potentials
ΔSCF (DFT) QMC and GW are similar.

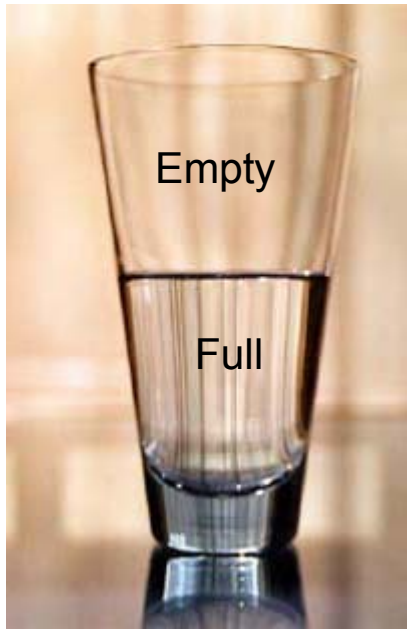
Electron Affinities



ΔSCF (DFT) is still not far from experimental data.
GW requires self-consistency
QMC systematically underestimates EA.

Is the glass full or empty?

- GW-BSE
  - Scissors self-consistent improves agreement with experiment
  - Has the approach predictive power in general?
- ΔSCF and TDLDA
  - Agree with experiment in fullerenes
  - They are known to disagree in carbon nanotubes
- QMC
  - Cancelations of the relative systematic errors < 10^{-5}
  - Need compact multiconfigurational expansions &/or orbital optimization for large systems
  - Pseudopotential evaluation related errors are small
- Experiment
  - Experiments in single molecules



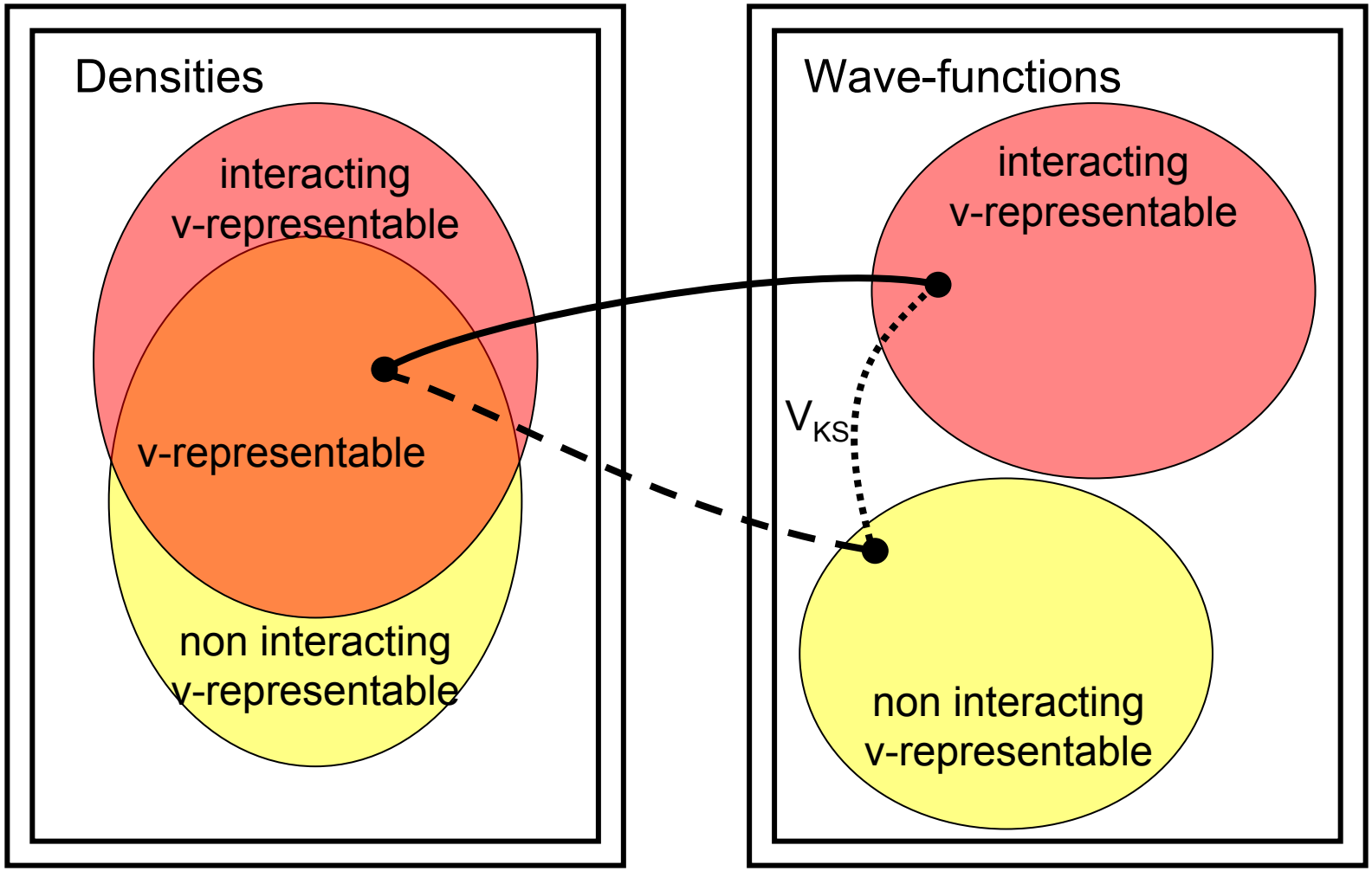
http://arxiv.org/abs/0803.0560

Motivation

- The Kohn-Sham formulation of DFT establishes an equivalence between interacting and non interacting densities.
- No other property of the interacting ground state wave-function is in principle retained.
- However, Kohn-Sham wave-functions are used as starting point for methods that go beyond DFT such as QMC or GW-BSE etc.

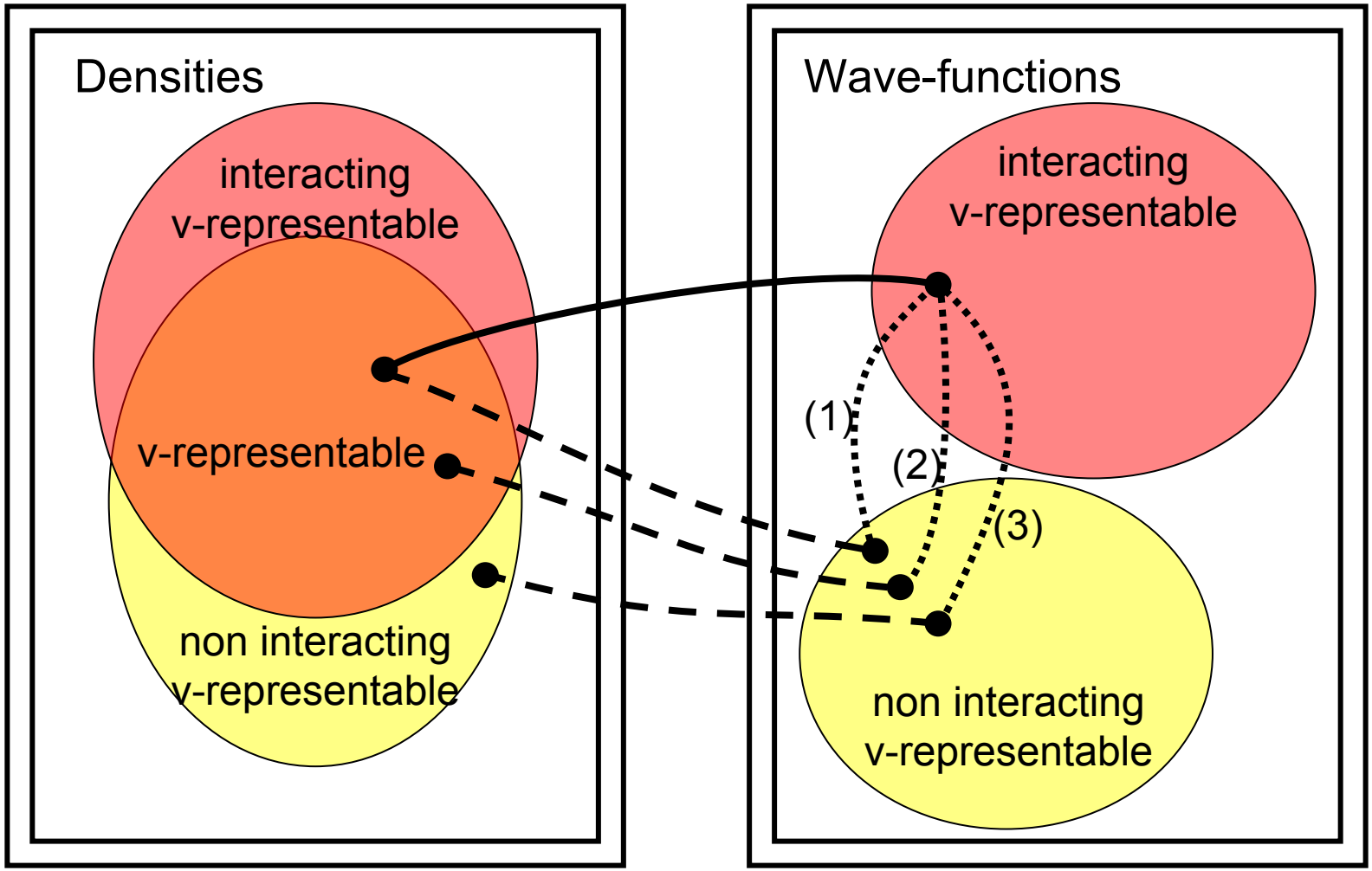
Are Kohn and Sham wave-functions any good? Do they retain any physical property beyond the density?

Kohn-Sham correspondence between interacting and non-interacting densities



For non-degenerate systems there is at most one Kohn-Sham wave-function with the interacting density

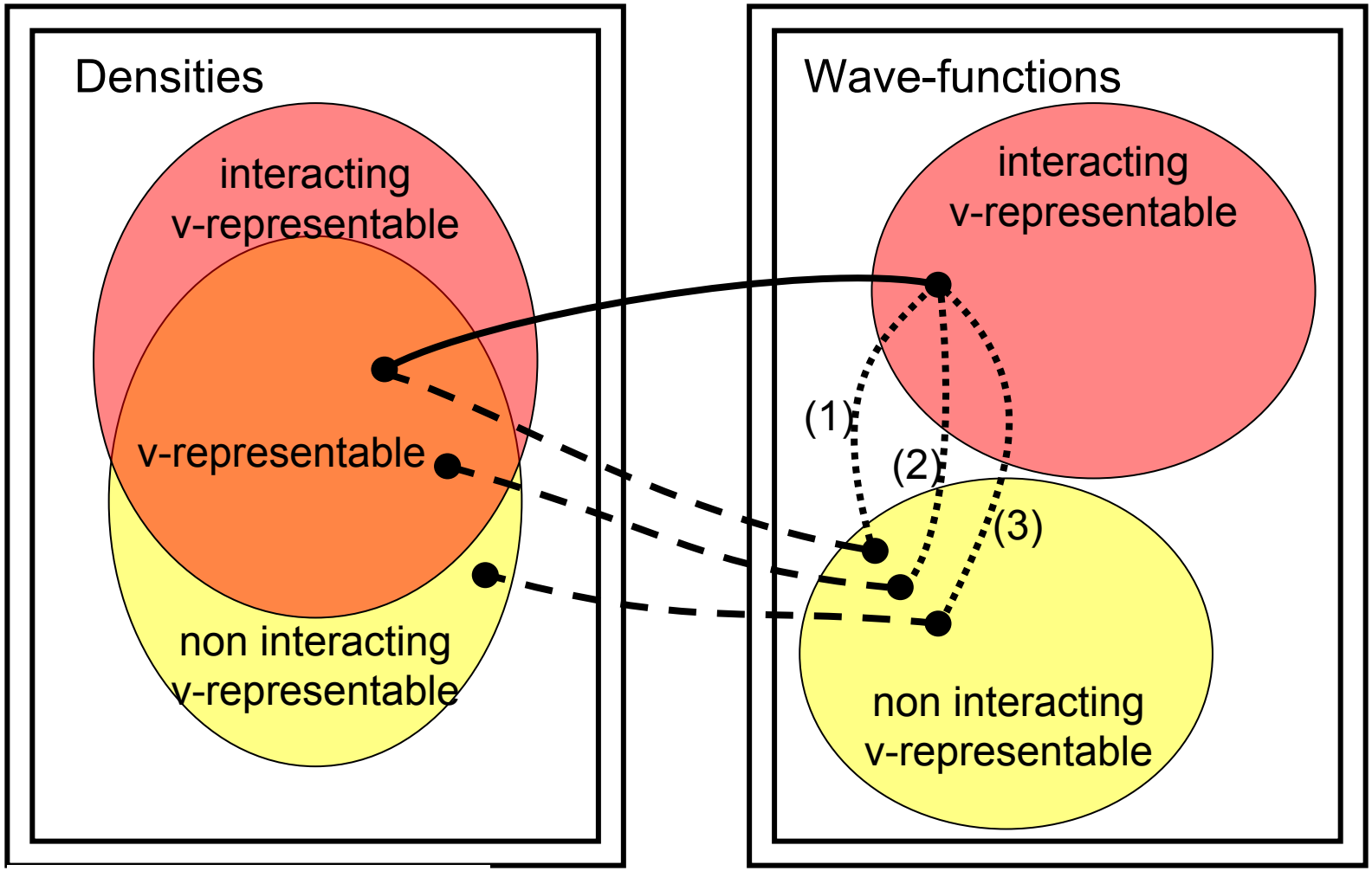
Retaining other properties of the interacting ground state in the non interacting wave-function



For non-degenerate systems there is at most one Kohn-Sham wave-function with the interacting density

Optimizing other properties thus requires to change the density

Retaining other properties of the interacting ground state
A density-density functional transformation must be found



$$\bar{\rho}_K(\mathbf{r}) = U_K\left[\rho(\mathbf{r})\right]$$

Reboredo & Kent PRB (2008)

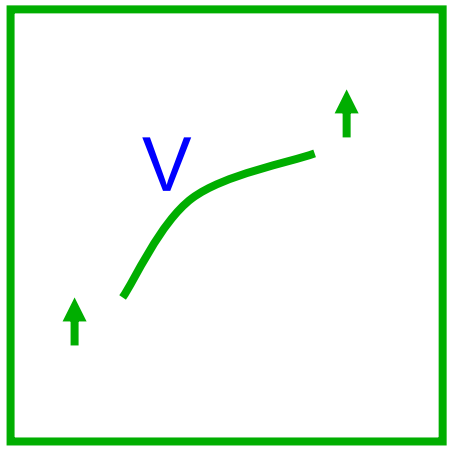
Optimizing other properties thus requires to change the density

Two interacting particles in a square box

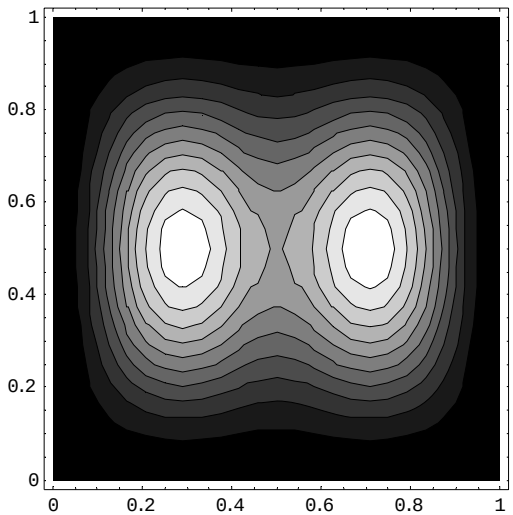
$V = 8\gamma \cos[\alpha\pi(x-x')] \cos[\alpha\pi(y-y')]$

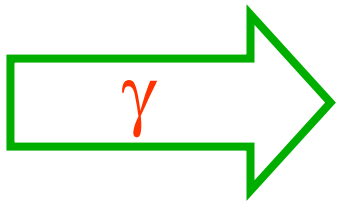
α and γ control the shape and strength of V

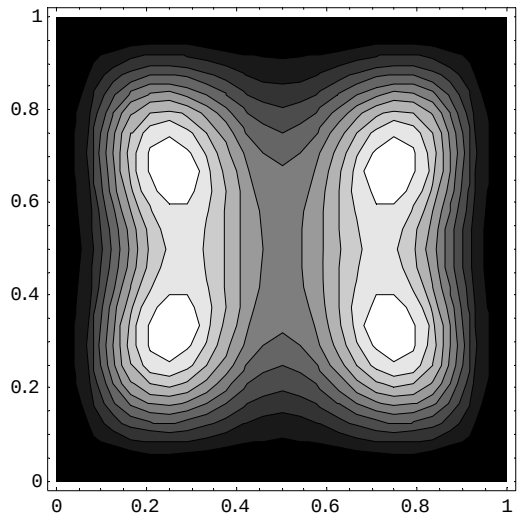
V is repulsive for $|\alpha| < 1/2$



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







Minimization of cost functions in the v-representable set

$$\left[-\frac{1}{2}\nabla^2 + \bar{V}(\mathbf{r})\right]\phi_\nu(\mathbf{r}) = \varepsilon_\nu \phi_\nu(\mathbf{r})$$

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

Kohn-Sham DFT

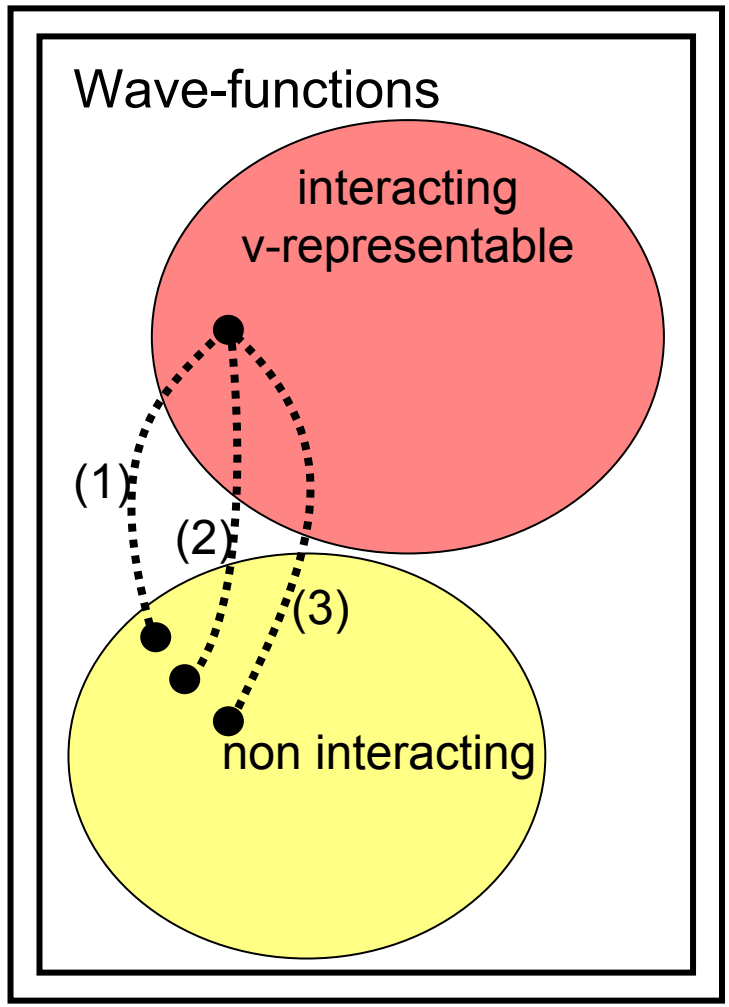
$$\Delta\bar{V}_{K_\rho}(\mathbf{r}) = \int d\mathbf{r}'\,[\rho(\mathbf{r}') - \bar{\rho}(\mathbf{r}')]\,\frac{\delta V(\mathbf{r}')}{\delta\rho(\mathbf{r})}$$

$$K_{Det} = -\left|\langle\Psi\,|\Phi_T\rangle\right|^2$$

$$\delta V_{K_{Det}}(\mathbf{r}) = \epsilon\,\langle\Psi\,|\Phi_T\rangle\sum_\nu^o\sum_n^u\langle\Psi|\,c_n^\dagger c_\nu\,|\Phi_T\rangle\,\frac{\phi_n(\mathbf{r})\phi_{nu}(\mathbf{r})}{\varepsilon_\nu - \varepsilon_n}$$

$$K_{S_0} = \int_{S_0} d\mathbf{S}\,|\Phi_T(\mathbf{R})|^2$$

$$\delta V_{K_{Det}}(\mathbf{r}) = \epsilon\sum_\nu^o\sum_n^u\int_{S_0} d\mathbf{S}\Phi_T^{n,\nu}(\mathbf{R})\Phi_T(\mathbf{R})\,\frac{\phi_n(\mathbf{r})\phi_{nu}(\mathbf{r})}{\varepsilon_\nu - \varepsilon_n}$$



Different properties imply different cost functions and different potentials

The density is depends strongly on the cost function

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

Exact Kohn-Sham

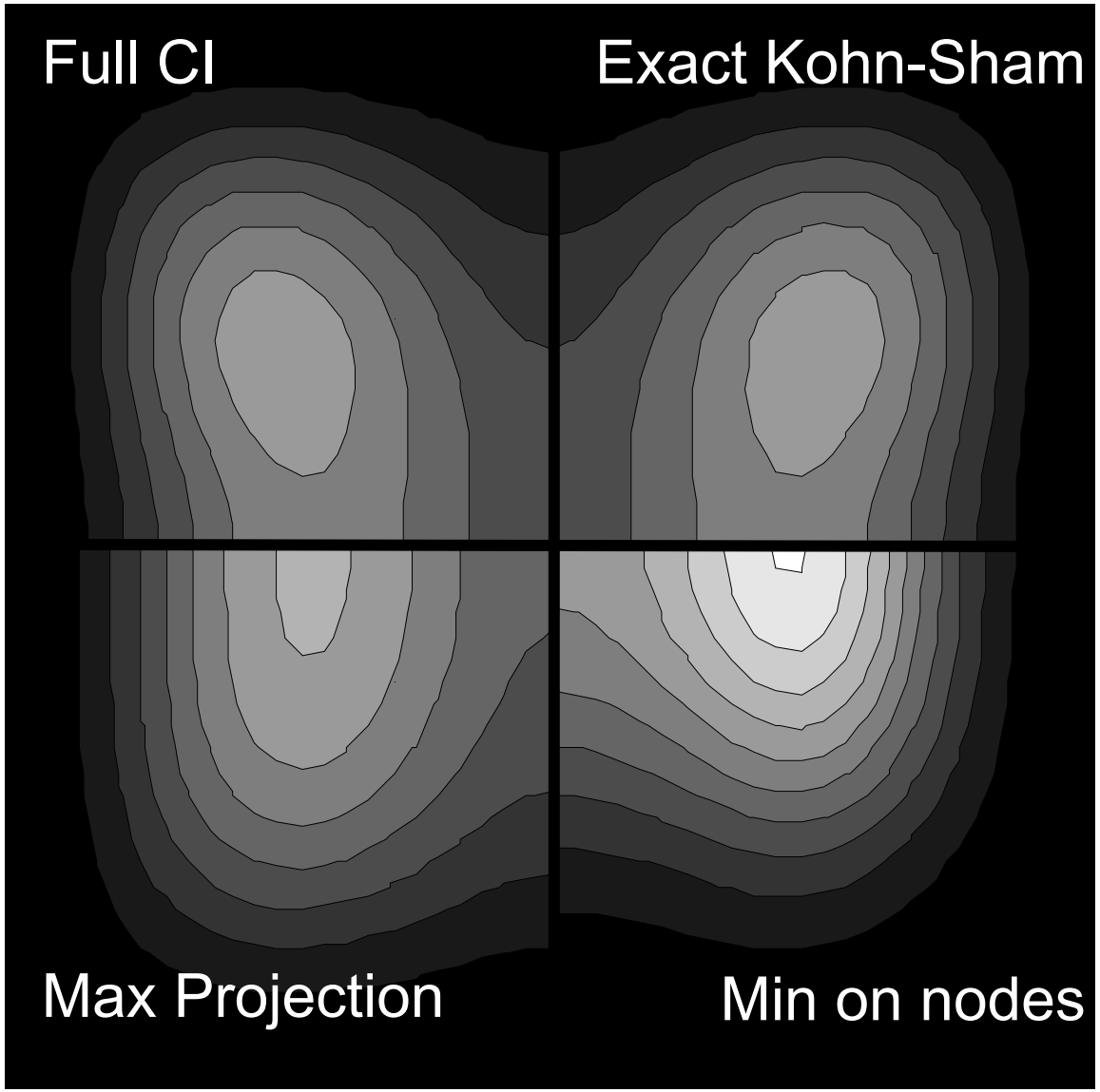
$$K_{Det} = -\left|\langle \Psi \,|\Phi_T\rangle\right|^2$$

Max Projection

$$K_{S_0} = \int_{S_0} \mathrm{dS}\,|\Phi_T(\mathrm{R})|^2$$

Min on nodes

$$\bar{\rho}_K(\mathrm{r}) = U_K\,[\rho(\mathrm{r})$$



A density-density functional must be found to optimize other properties

Optimized effective potentials

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

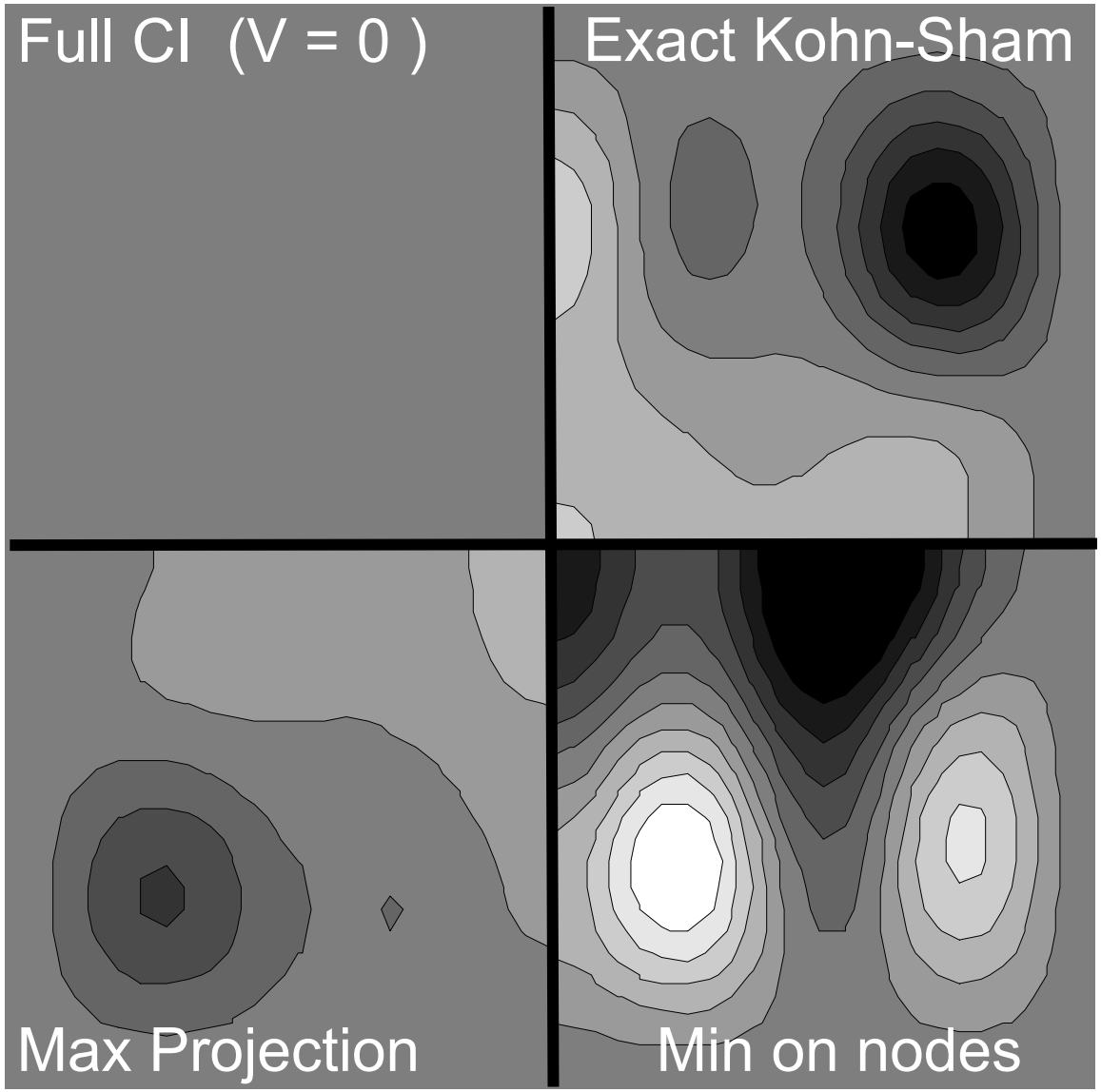
Exact Kohn-Sham

$$K_{Det} = -\left|\langle \Psi\,|\Phi_T\rangle\right|^2$$

Max Projection

$$K_{S_0} = \int_{S_0} \mathrm{dS}\,|\Phi_T(\mathrm{R})|^2$$

Min on nodes



Effective potentials depend strongly on the many-body property retained

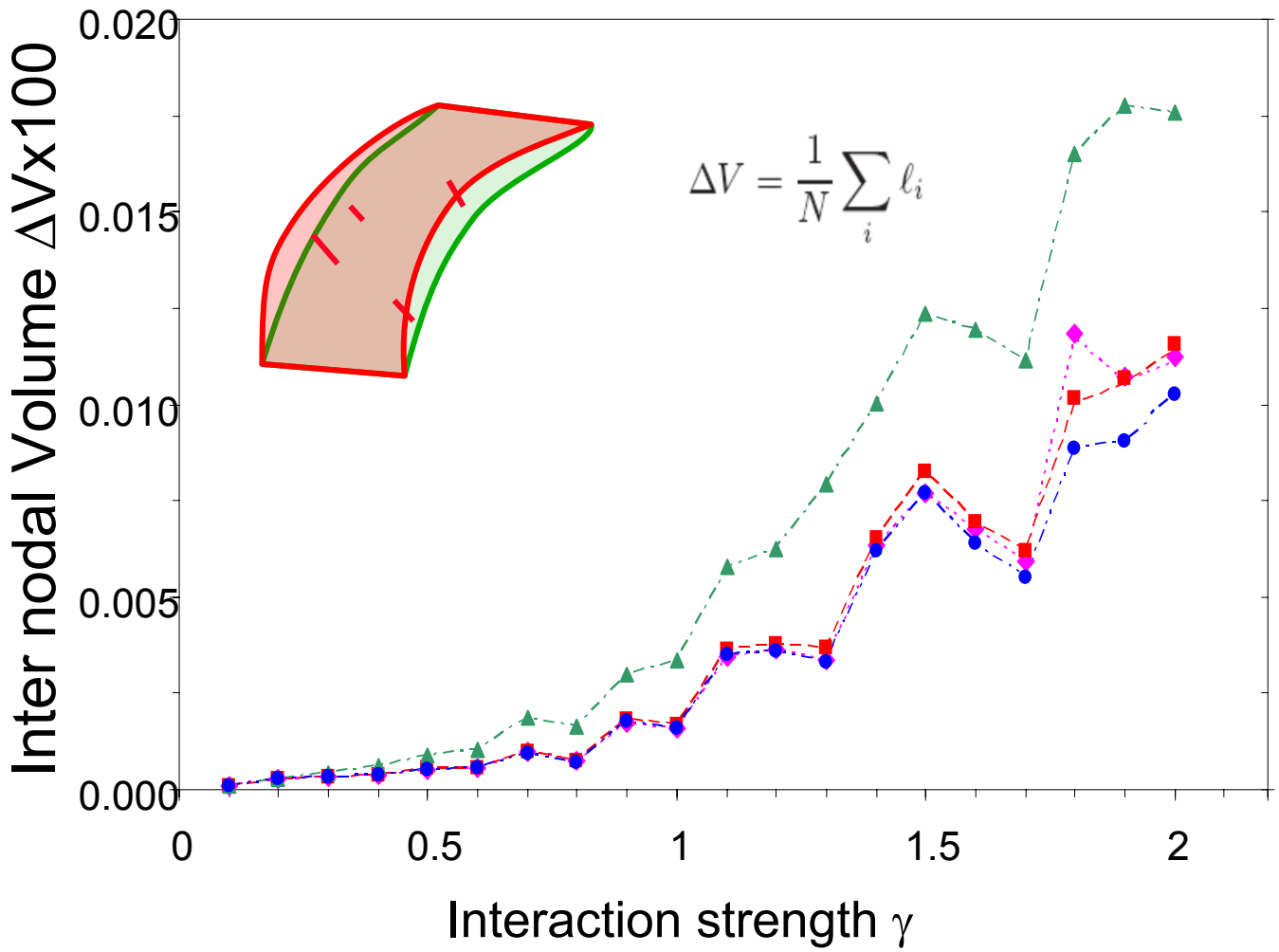
Volume between interacting and non-interacting nodes

Exact Kohn-Sham

Max Projection

Min on nodes

Non interacting



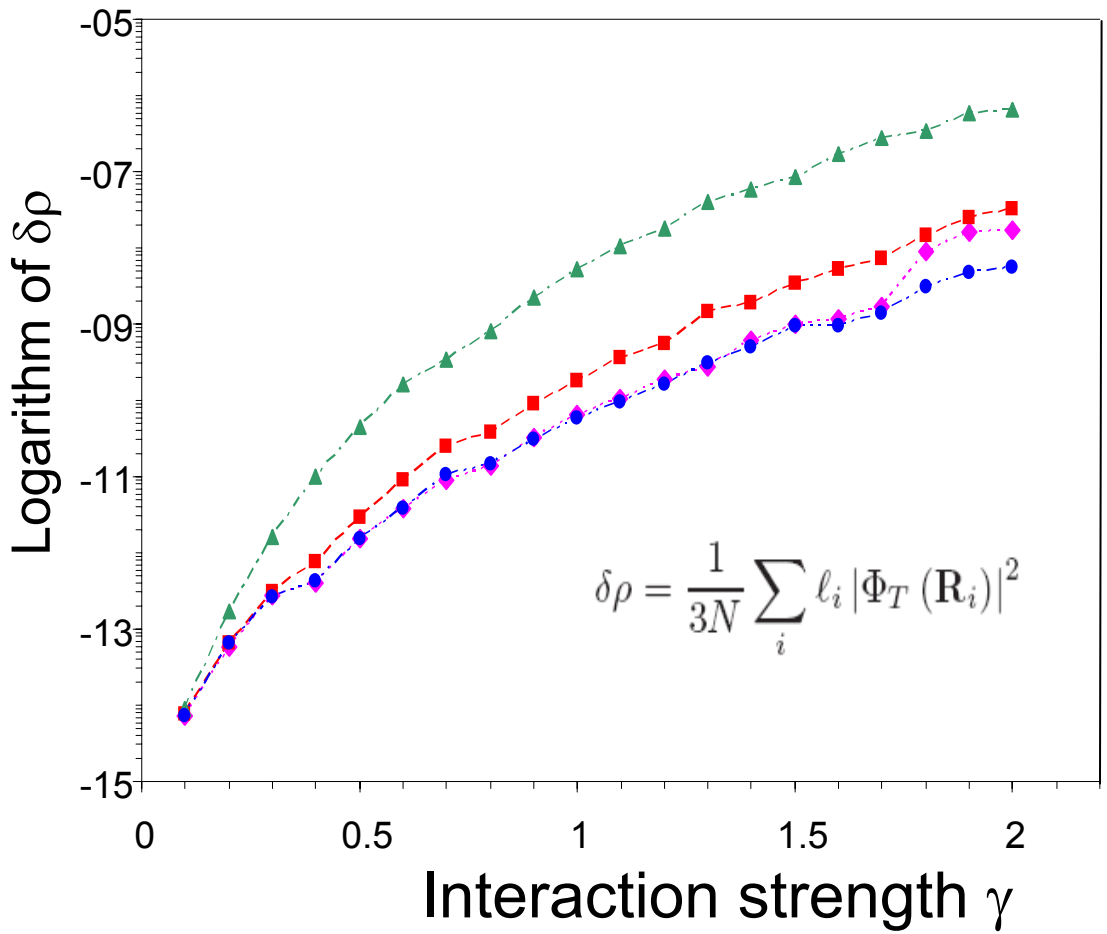
Volume between interacting and non-interacting nodes

Exact Kohn-Sham

Max Projection

Min on nodes

Non interacting

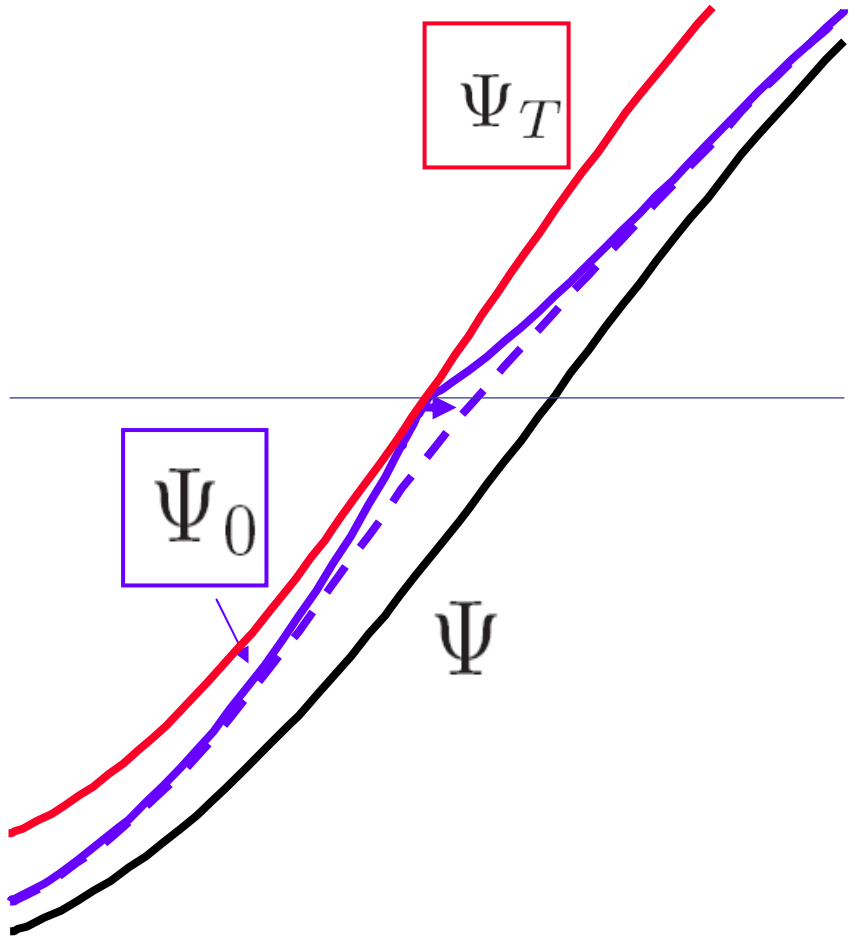


For this model exact DFT is
the worst description of the nodes !

How do we get good nodes for large systems?

How do we transform a complex wave-function With good properties into a simpler-function with the same properties ?

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

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

Number of configurations

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

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

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

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

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

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

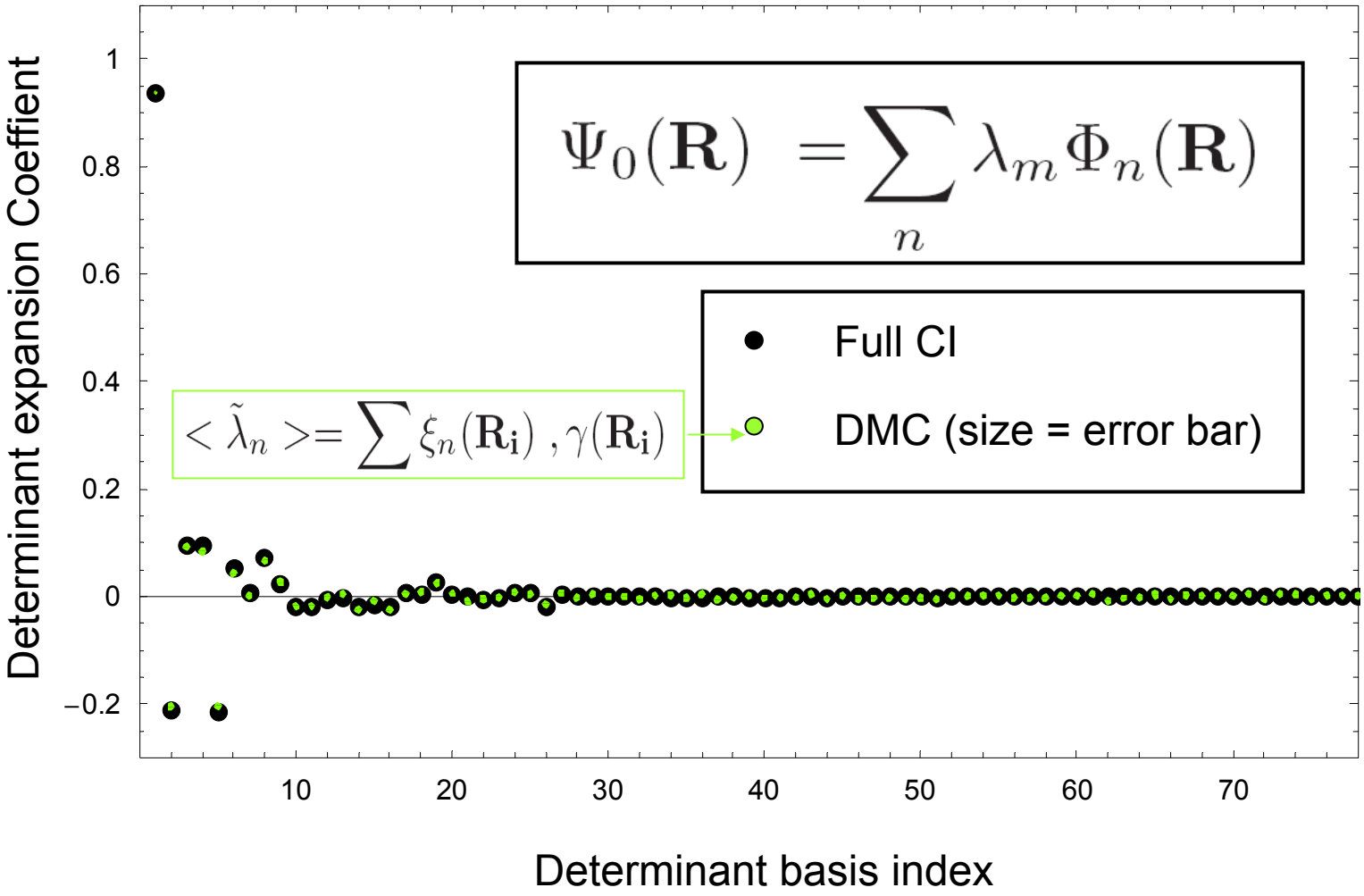
DMC sampling

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

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

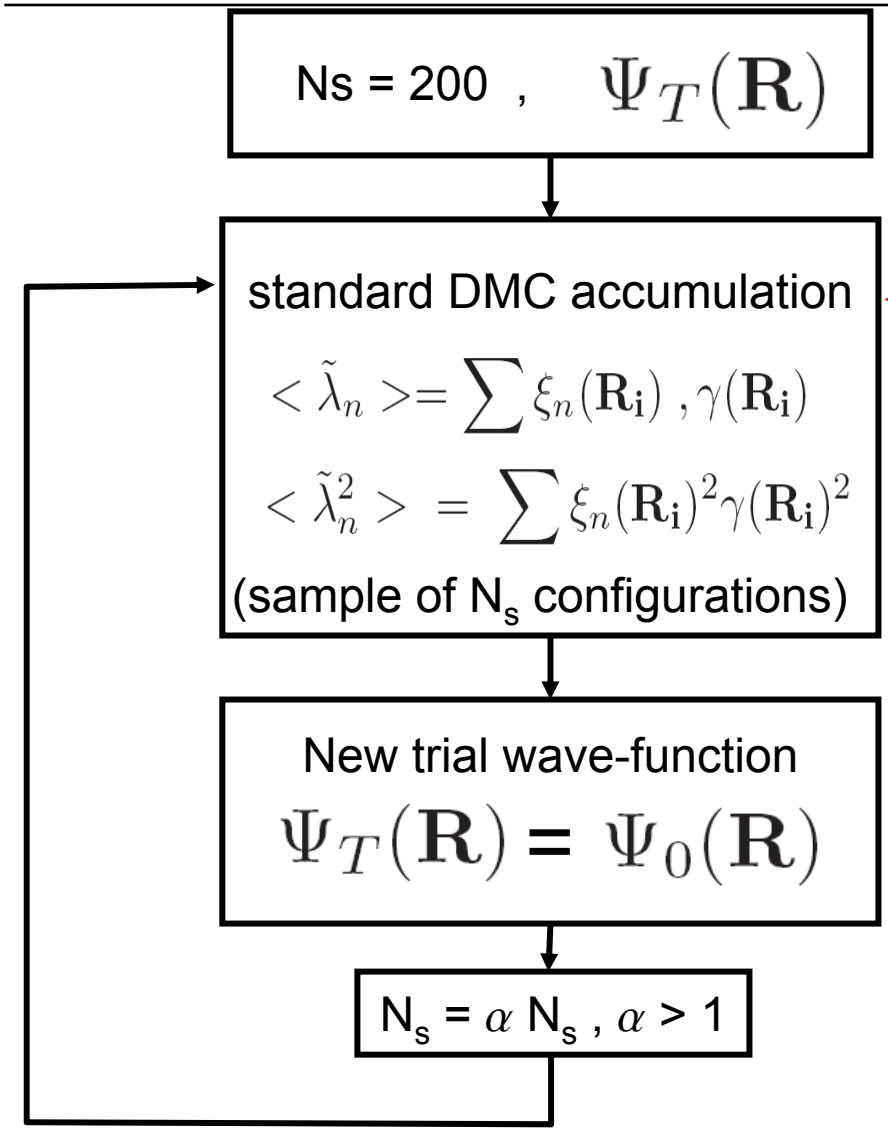
A Simple Self-Healing DMC Algorithm: **Results**

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

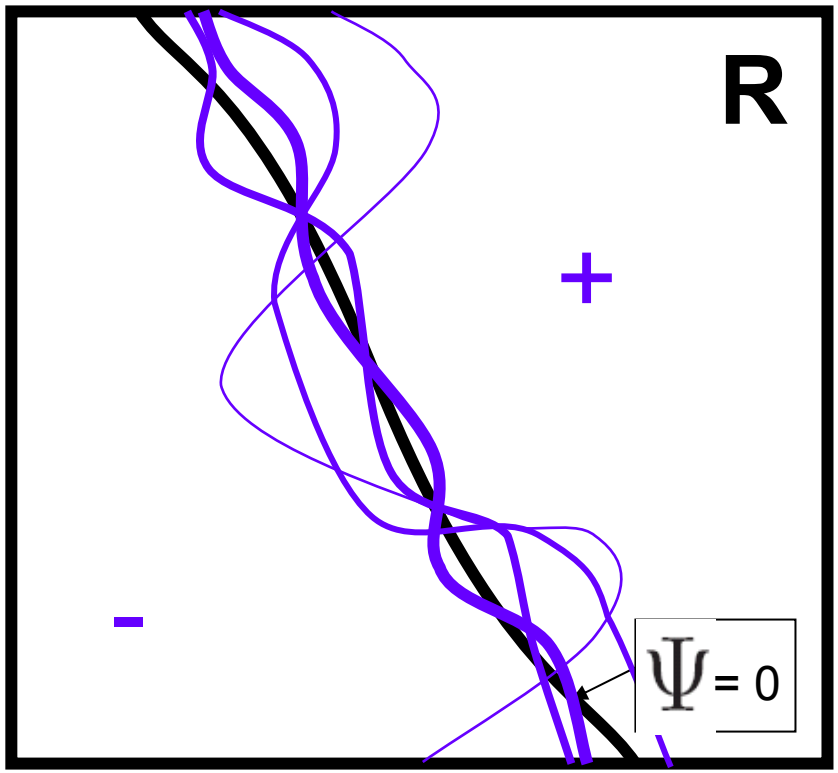


starting trial wave function: **anything**

How do we simplify the wave-function ?

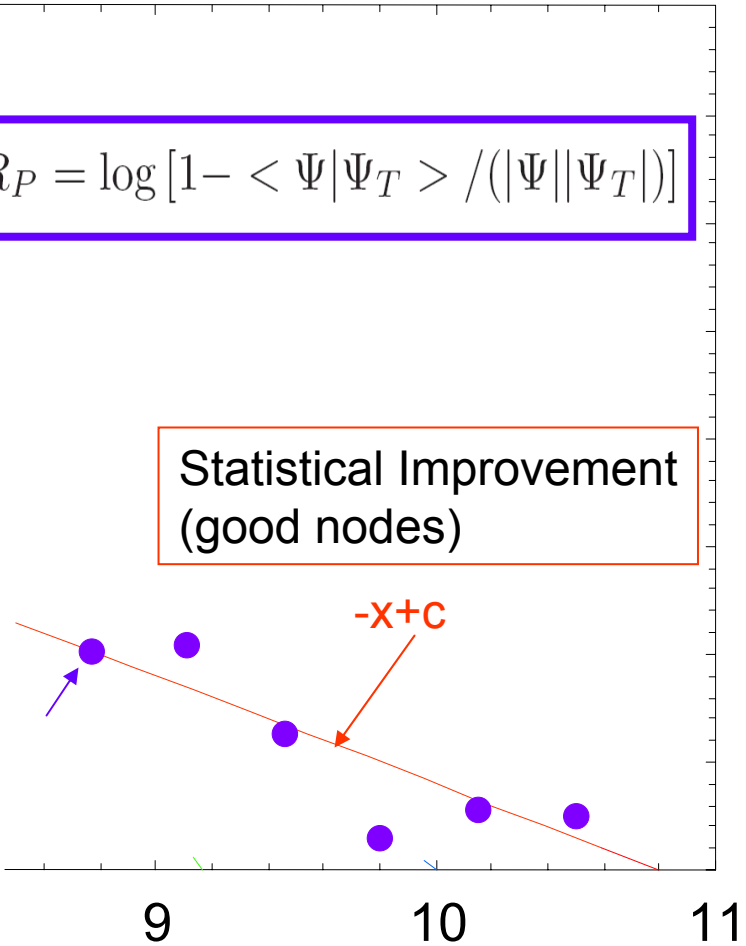
How do we construct a faster one?

Conjecture (2) Noise in the coefficients plays the role of a temperature in a simulated annealing approach. Good fluctuations are reinforced bad ones are abandoned.



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

Statistical Improvement
(good nodes)



Conjecture (3) Removing the high energy contribution removes the kink at the node and improves it

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

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

A cost function for optimization of trial wave functions for Importance Sampling

Chi-Squared distribution

$$\chi^2 = \sum_i^M \frac{\left[n_i - N_c \Omega_i \bar{p}(\mathbf{R}_i)\right]^2}{N_c \Omega_i \bar{p}(\mathbf{R}_i)}$$

Relative errors have the same Impact for every bin

How close are two probability densities?

$$K_{pq} = \int \mathbf{dr} \frac{\left[q(\mathbf{R}) - p(\mathbf{R})\right]^2}{p(\mathbf{R})}$$

$$K_{DMC} = \int \mathbf{dR} \frac{\left[\frac{N_c}{\tilde{\nu}} \tilde{\Psi}_T(\mathbf{R}) \Psi_T(\mathbf{R}) - f(\mathbf{R})\right]^2}{\left|\frac{N_c}{\tilde{\nu}} \tilde{\Psi}_T(\mathbf{R}) \Psi_T(\mathbf{R})\right|^{\alpha}} \times \theta\left[f(\mathbf{R}) - \eta\right]$$

This cost function extended to the full Hilbert space by the | | and the θ[ ]

A cost function for optimization of trial wave functions for Importance Sampling

$$K_{DMC} = \int \mathbf{dR} \frac{\left[\frac{N_c}{\tilde{\nu}}\tilde{\Psi}_T(\mathbf{R})\Psi_T(\mathbf{R}) - f(\mathbf{R})\right]^2}{\left|\frac{N_c}{\tilde{\nu}}\tilde{\Psi}_T(\mathbf{R})\Psi_T(\mathbf{R})\right|} \times \theta\left[f(\mathbf{R}) - \eta\right]$$

$$f(\mathbf{R}) = \frac{N_c}{\nu_T}\Psi_0(\mathbf{R})\Psi_T(\mathbf{R}) \qquad \tilde{\nu} = \int \mathbf{dR}\tilde{\Psi}_T(\mathbf{R})\Psi_T(\mathbf{R})$$

Any expression of the Ground State Wave-Function
- Single determinant
- Multi determinant
- Back flow
- Pfaffian
- etc

$$\delta V_K(\mathbf{r}) = -\epsilon \sum_{\nu}^{occ} \int \mathbf{dr}' \frac{\delta K}{\delta \phi_\nu(\mathbf{r}')} \frac{\delta \phi_\nu(\mathbf{r}')}{\delta \bar{V}(\mathbf{r})}$$

$$\left[-\frac{1}{2}\nabla^2 + \bar{V}(\mathbf{r})\right]\phi_\nu(\mathbf{r}) = \varepsilon_\nu \phi_\nu(\mathbf{r})$$

wave functions can be optimized
via an effective field potential (v-representable set)

A cost function for optimization of trial wave functions via an effective field DFT-like potential

$$K_{DMC} = \int \mathbf{dR} \frac{\left[\frac{N_c}{\tilde{\nu}}\tilde{\Psi}_T(\mathbf{R})\Psi_T(\mathbf{R}) - f(\mathbf{R})\right]^2}{\left|\frac{N_c}{\tilde{\nu}}\tilde{\Psi}_T(\mathbf{R})\Psi_T(\mathbf{R})\right|} \times \theta\left[f(\mathbf{R}) - \eta\right]$$

$$f(\mathbf{R}) = \frac{N_c}{\nu_T}\Psi_0(\mathbf{R})\Psi_T(\mathbf{R}) \qquad \tilde{\nu} = \int \mathbf{dR}\tilde{\Psi}_T(\mathbf{R})\Psi_T(\mathbf{R})$$

$$\delta V_K(\mathbf{r}) = -\epsilon \sum_{\nu}^{occ} \int \mathbf{dr}' \frac{\delta K}{\delta \phi_\nu(\mathbf{r}')} \frac{\delta \phi_\nu(\mathbf{r}')}{\delta \bar{V}(\mathbf{r})}$$

$$\frac{\delta K_{DMC}}{\delta \phi_\nu(\mathbf{r}')} = \int \mathbf{dR} W(\mathbf{R}) e^{-\tilde{J}(\mathbf{R})} \frac{\delta \tilde{\Phi}(\mathbf{R})}{\delta \phi_\nu(\mathbf{r}')}$$

$$W(\mathbf{R}) = \frac{\delta K_{DMC}}{\delta \tilde{\Psi}(\mathbf{R})}$$

A cost function for optimization of trial wave functions via an effective field DFT-like potential

$$K_{DMC} = \int \mathbf{dR} \frac{\left[\frac{N_c}{\tilde{\nu}}\tilde{\Psi}_T(\mathbf{R})\Psi_T(\mathbf{R}) - f(\mathbf{R})\right]^2}{\left|\frac{N_c}{\tilde{\nu}}\tilde{\Psi}_T(\mathbf{R})\Psi_T(\mathbf{R})\right|} \times \theta\left[f(\mathbf{R}) - \eta\right]$$

$$f(\mathbf{R}) = \frac{N_c}{\nu_T}\Psi_0(\mathbf{R})\Psi_T(\mathbf{R}) \qquad \tilde{\nu} = \int \mathbf{dR}\tilde{\Psi}_T(\mathbf{R})\Psi_T(\mathbf{R})$$

$$\delta V_{K_{DMC}}(\mathbf{r}) = \epsilon \sum_{\nu}^{o}\sum_{n}^{u} \frac{\phi_n(\mathbf{r})\phi_{nu}(\mathbf{r})}{\varepsilon_\nu - \varepsilon_n}\beta_\nu^n + c.c.$$

$$\beta_\nu^n = \int \mathbf{dR} W(\mathbf{R}) e^{-\tilde{J}(\mathbf{R})}\tilde{\Phi}_\nu^n(\mathbf{R}) \,,$$

$$W(\mathbf{R}) = \frac{2\Delta(\mathbf{R})\alpha(\mathbf{R}) - \Delta(\mathbf{R})^2}{|\alpha(\mathbf{R})|^2} sign(\alpha(\mathbf{R})) \times \left[1 - \alpha(\mathbf{R})\right]\psi_T(\mathbf{R})\frac{N_c}{\tilde{\nu}}\theta\left[f(\mathbf{R}) - \eta\right]$$

$$\Delta(\mathbf{R}) = f(\mathbf{R}) - \alpha(\mathbf{R})$$

$$\alpha(\mathbf{R}) = \frac{N_c}{\tilde{\nu}}\tilde{\Psi}_T(\mathbf{R})\Psi_T(\mathbf{R})$$

Optimization of the Jastrow Parameters directly from the DMC run

$$K_{DMC} = \int \mathbf{dR} \frac{\left[\frac{N_c}{\tilde{\nu}}\tilde{\Psi}_T(\mathbf{R})\Psi_T(\mathbf{R}) - f(\mathbf{R})\right]^2}{\left|\frac{N_c}{\tilde{\nu}}\tilde{\Psi}_T(\mathbf{R})\Psi_T(\mathbf{R})\right|} \times \theta\left[f(\mathbf{R}) - \eta\right]$$

$$f(\mathbf{R}) = \frac{N_c}{\nu_T}\Psi_0(\mathbf{R})\Psi_T(\mathbf{R}) \qquad \tilde{\nu} = \int \mathbf{dR}\tilde{\Psi}_T(\mathbf{R})\Psi_T(\mathbf{R})$$

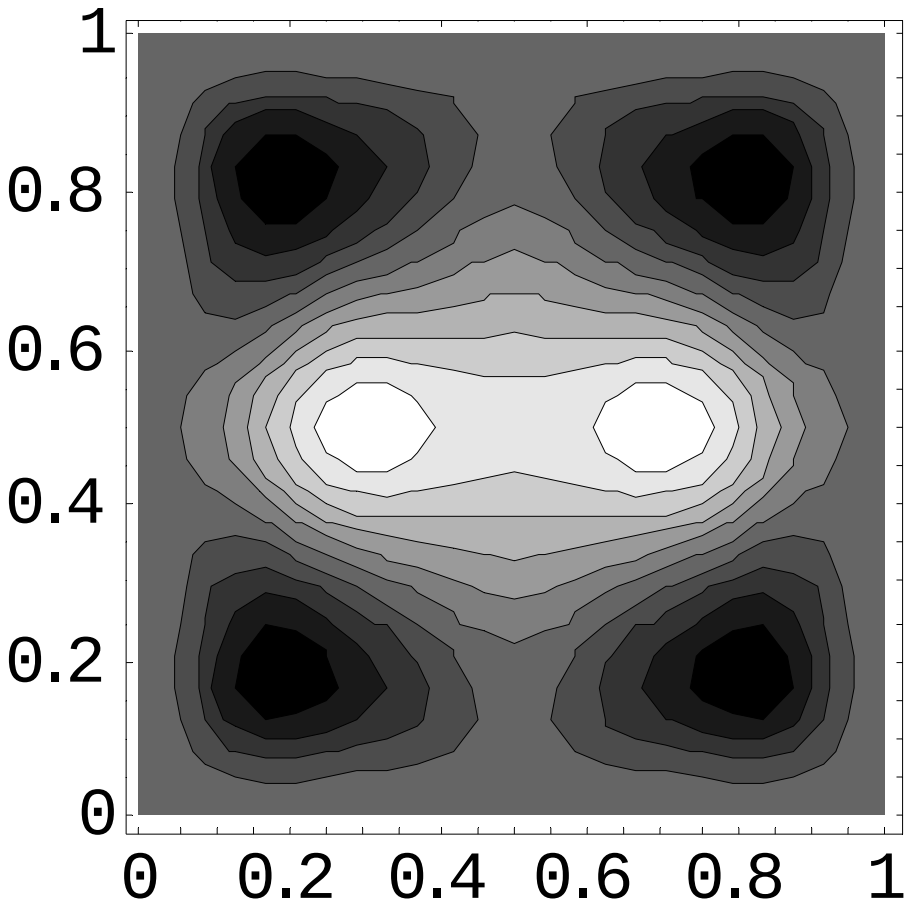
$$\frac{dK_{DMC}}{d\gamma_n} = -\int \mathbf{dR} W(\mathbf{R}) e^{-\tilde{J}(\mathbf{R})}\tilde{\Phi}_T(\mathbf{R})\frac{dJ(\mathbf{R})}{d\gamma_n}$$

$$W(\mathbf{R}) = \frac{2\Delta(\mathbf{R})\alpha(\mathbf{R}) - \Delta(\mathbf{R})^2}{|\alpha(\mathbf{R})|^2} sign(\alpha(\mathbf{R})) \times \left[1 - \alpha(\mathbf{R})\right]\psi_T(\mathbf{R})\frac{N_c}{\tilde{\nu}}\theta\left[f(\mathbf{R}) - \eta\right]$$

$$\Delta(\mathbf{R}) = f(\mathbf{R}) - \alpha(\mathbf{R})$$

$$\alpha(\mathbf{R}) = \frac{N_c}{\tilde{\nu}}\tilde{\Psi}_T(\mathbf{R})\Psi_T(\mathbf{R})$$

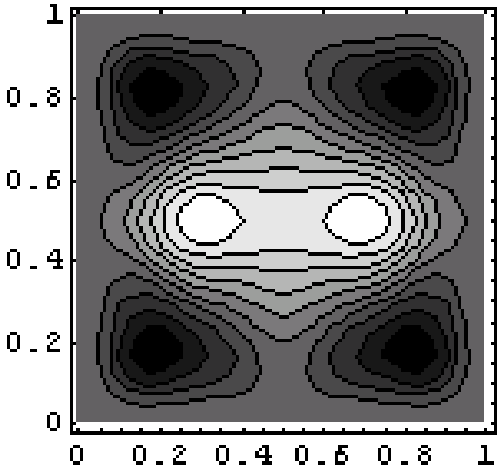
Nodal Effective potential

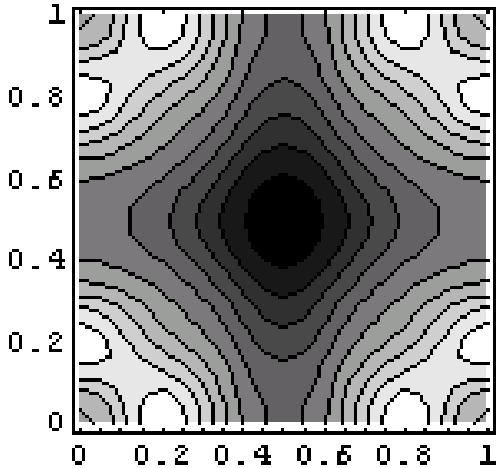


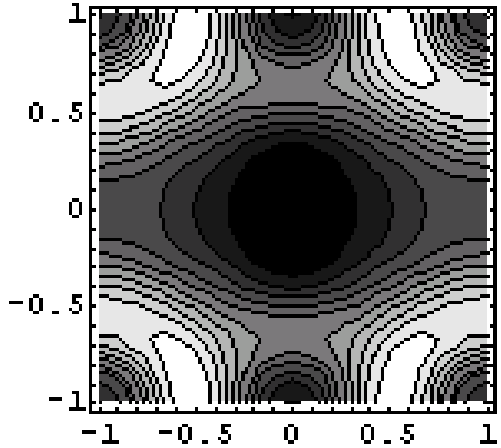
V-representable nodal surfaces

The wave function can be optimized directly from the DMC run

V(r) χ(r) J^2(r)







Optimization of Back Flaw Parameters directly from the DMC run

$$K_{DMC} = \int \mathbf{dR} \frac{\left[\frac{N_c}{\tilde{\nu}}\tilde{\Psi}_T(\mathbf{R})\Psi_T(\mathbf{R}) - f(\mathbf{R})\right]^2}{\left|\frac{N_c}{\tilde{\nu}}\tilde{\Psi}_T(\mathbf{R})\Psi_T(\mathbf{R})\right|} \times \theta\left[f(\mathbf{R}) - \eta\right]$$

$$\tilde{\nu} = \int \mathbf{dR}\tilde{\Psi}_T(\mathbf{R})\Psi_T(\mathbf{R}) \qquad f(\mathbf{R}) = \frac{N_c}{\nu_T}\Psi_0(\mathbf{R})\Psi_T(\mathbf{R})$$

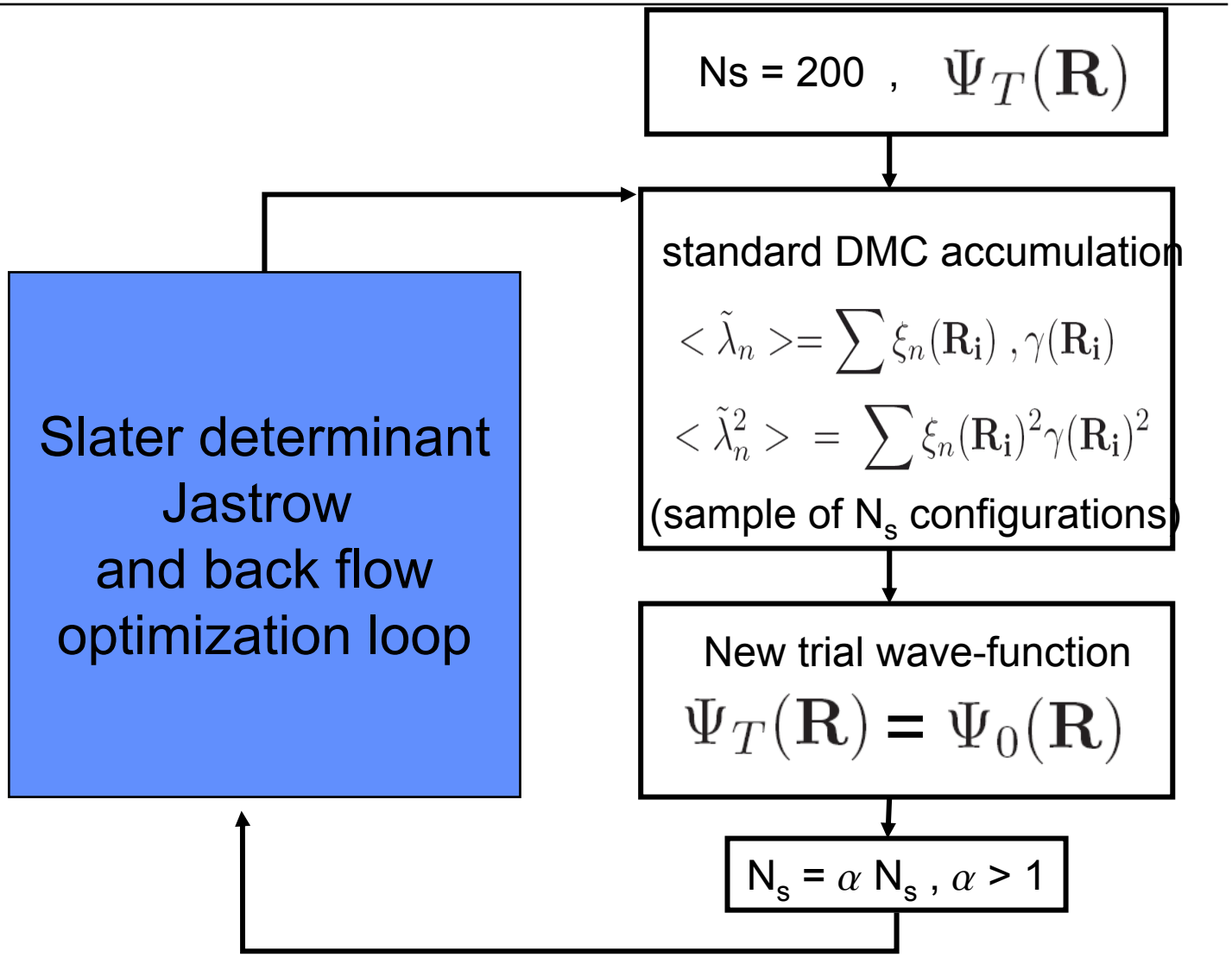
$$\frac{dK_{DMC}}{da_n} = -\int \mathbf{dR} W(\mathbf{R}) e^{-\tilde{J}(\mathbf{R})} \sum_{\nu}^{occ} \frac{\delta\tilde{\Phi}(\mathbf{R})}{\delta\phi_\nu} \quad \nabla\phi_\nu(\mathbf{r}).(\delta\mathbf{r}/da_n|_{\mathbf{r}})$$

$$W(\mathbf{R}) = \frac{2\Delta(\mathbf{R})\alpha(\mathbf{R}) - \Delta(\mathbf{R})^2}{|\alpha(\mathbf{R})|^2} sign(\alpha(\mathbf{R})) \times \left[1 - \alpha(\mathbf{R})\right]\psi_T(\mathbf{R})\frac{N_c}{\tilde{\nu}}\theta\left[f(\mathbf{R}) - \eta\right]$$

$$\Delta(\mathbf{R}) = f(\mathbf{R}) - \alpha(\mathbf{R})$$

$$\alpha(\mathbf{R}) = \frac{N_c}{\tilde{\nu}}\tilde{\Psi}_T(\mathbf{R})\Psi_T(\mathbf{R})$$

The **Complete** Self-Healing DMC Algorithm



Conclusions

- The fixed node ground state wave-function can be obtained directly by sampling over the walker distribution of a DMC run
- Single determinant Wave functions with backflow can be optimized directly from the DMC run reducing the impact of non-polynomial costs
- Conjecture (1) Removing the kink in the Fixed node wave-function always improves the nodes globally
- Conjecture (2) Random errors in the wave-function expansion improve the nodes in a simulating annealing-like process
- Conjecture (3) Removing the high energy contribution removes the kink at the node and improves it
- Provided that conjectures (1) to (3) are true, the sign problem can be circumvented accepting a finite error
- The cost of reducing this error grows exponentially with the number of particles

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