Dynamical imaginary time correlations from Auxiliary Fields Quantum Monte Carlo

E. Vitali, M. Motta, D. E. Galli

S. Moroni

Università degli Studi di Milano

CNR-INFM DEMOCRITOS and SISSA, Trieste, Italy

Projection onto the Ground State

$$U(\tau)\left|\psi_T\right\rangle \xrightarrow[\tau\to+\infty]{} \left|\Psi_0\right\rangle$$

Static properties: E_0, g(r), S(q), …

$$U(\tau) = \exp(-\tau(\hat{H} - E_0))$$

T=0 QUANTUM MONTE CARLO

Imaginary time correlation functions

$$\left\langle\Psi_0\right|\hat{A}\,U(\tau)\,\hat{B}\left|\Psi_0\right\rangle$$

Dynamical properties: $\omega(q)$, $S(q,\omega)$, $\chi(q)$, …

In Auxiliary Fields Quantum Monte Carlo methods

$$U(\tau) = \exp(-\tau(\hat{H} - E_0))$$

is dealt with in the abstract Hilbert Space of the physical system, relying on the single-particle formalism

The starting point is an interacting hamiltonian:

$$H = \sum_{i} T_i a_i^+ a_i + \sum_{i,j,k,l} V_{ijlk} a_i^+ a_j^+ a_k a_l$$

written in second quantization formalism, relying on a finite one particle basis:

$$\left\{ \left| i \right\rangle \right\}_{i=1,\dots,M}$$

Equivalent expression:

$$H = H_0 + \sum_{\alpha} A_{\alpha}^2 \qquad H_0, A_{\alpha}$$

One particle operators

Trotter decomposition:

$$U(\tau) = \left(U(\delta\tau)\right)^n, \qquad \tau = n\,\delta\tau$$

AUXILIARY FIELDS
QUANTUM
MONTE CARLO

Primitive approximation:

$$U(\delta\tau) \cong \exp(-\frac{1}{2}\delta\tau H_0)\prod_{\alpha}\boxed{\exp(-\delta\tau A_{\alpha}^2)}\exp(-\frac{1}{2}\delta\tau H_0)$$

TWO-BODY PROPAGATOR

$$U(\delta\tau) = \int d\eta\, g(\eta)\, G(\eta)$$

HUBBARD-STRATONOVICH TRANSFORMATION

$$g(\eta) = \frac{\exp\left(-\frac{1}{2}|\eta|^2\right)}{(2\pi)^{M^2}}$$

$2M^2$ dimensional standard normal probability density

AUXILIARY FIELDS QUANTUM MONTE CARLO

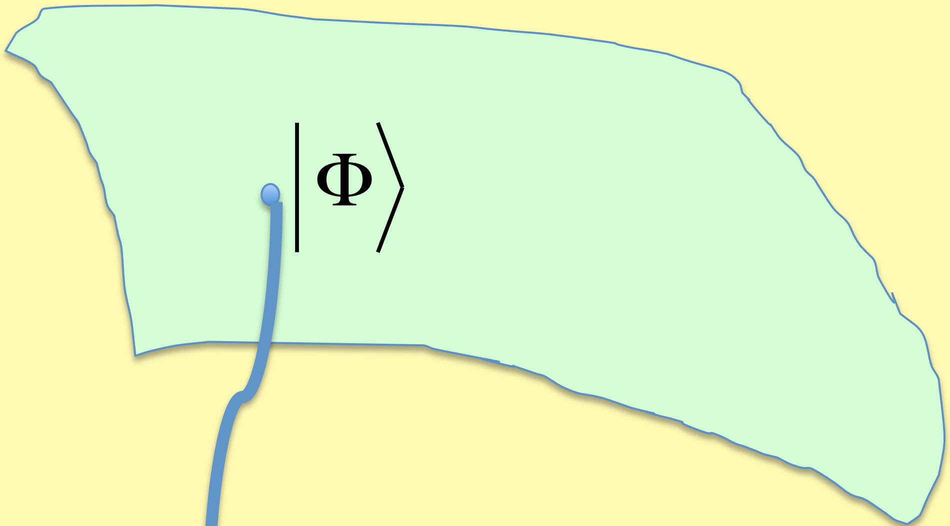
$$G(\eta) = \exp(-\frac{1}{2}\delta\tau H_0)\prod_{\alpha}\exp(i\sqrt{\delta\tau}\,\eta_\alpha A_\alpha)\exp(-\frac{1}{2}\delta\tau H_0)$$

ONE BODY PROPAGATOR

N fermions, Slater determinants

One particle wave functions

$$|\Phi\rangle = \frac{1}{N!} \sum_{\sigma \in S(N)} (-1)^{\sigma} |\varphi_{\sigma(1)}\rangle \otimes \ldots \otimes |\varphi_{\sigma(N)}\rangle$$



AUXILIARY FIELDS QUANTUM MONTE CARLO

Manifold of Slater determinants

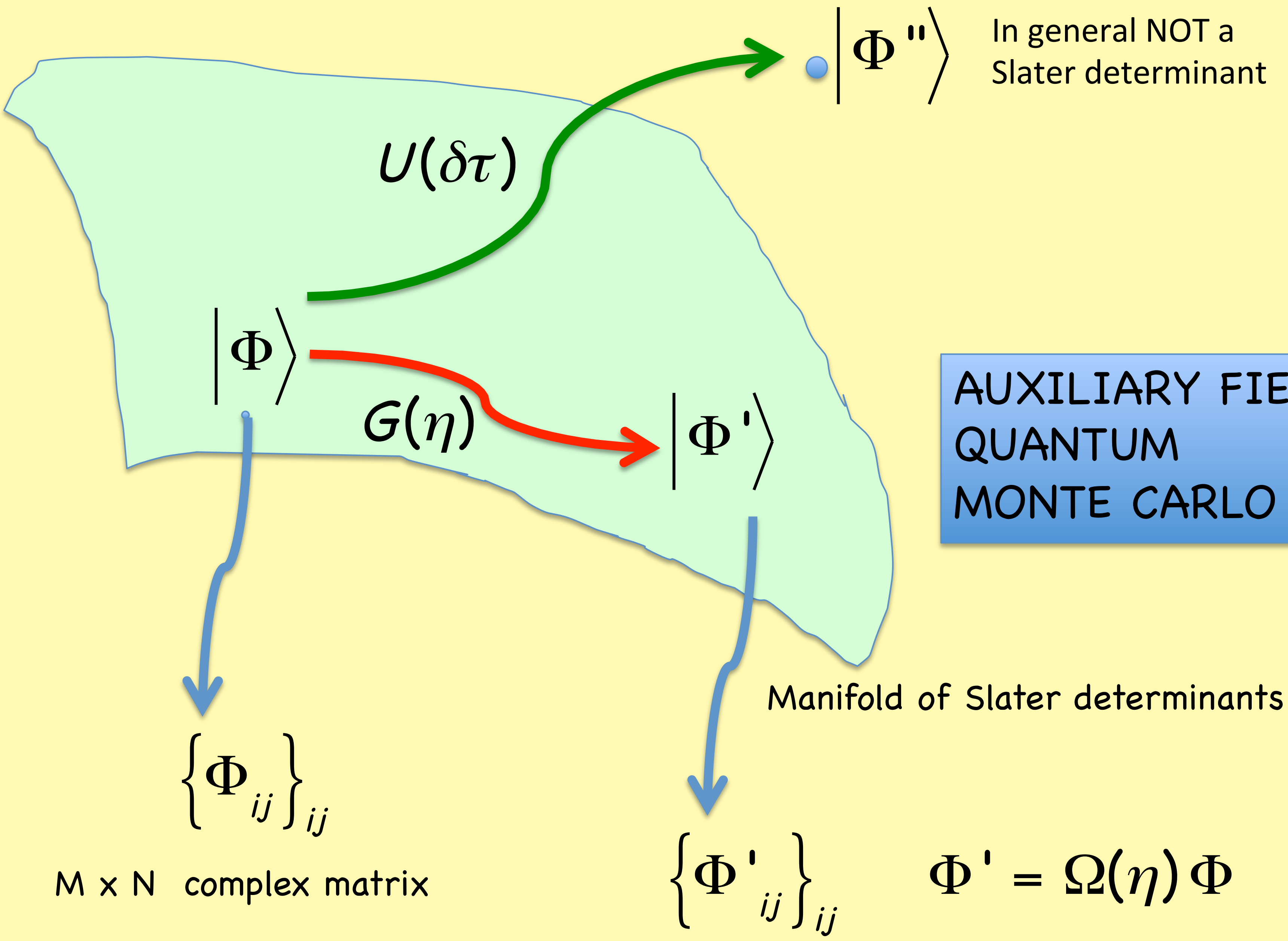
$$\left\{ \Phi_{ij} = \langle i | \varphi_j \rangle \right\}_{ij}$$

M x N complex matrix

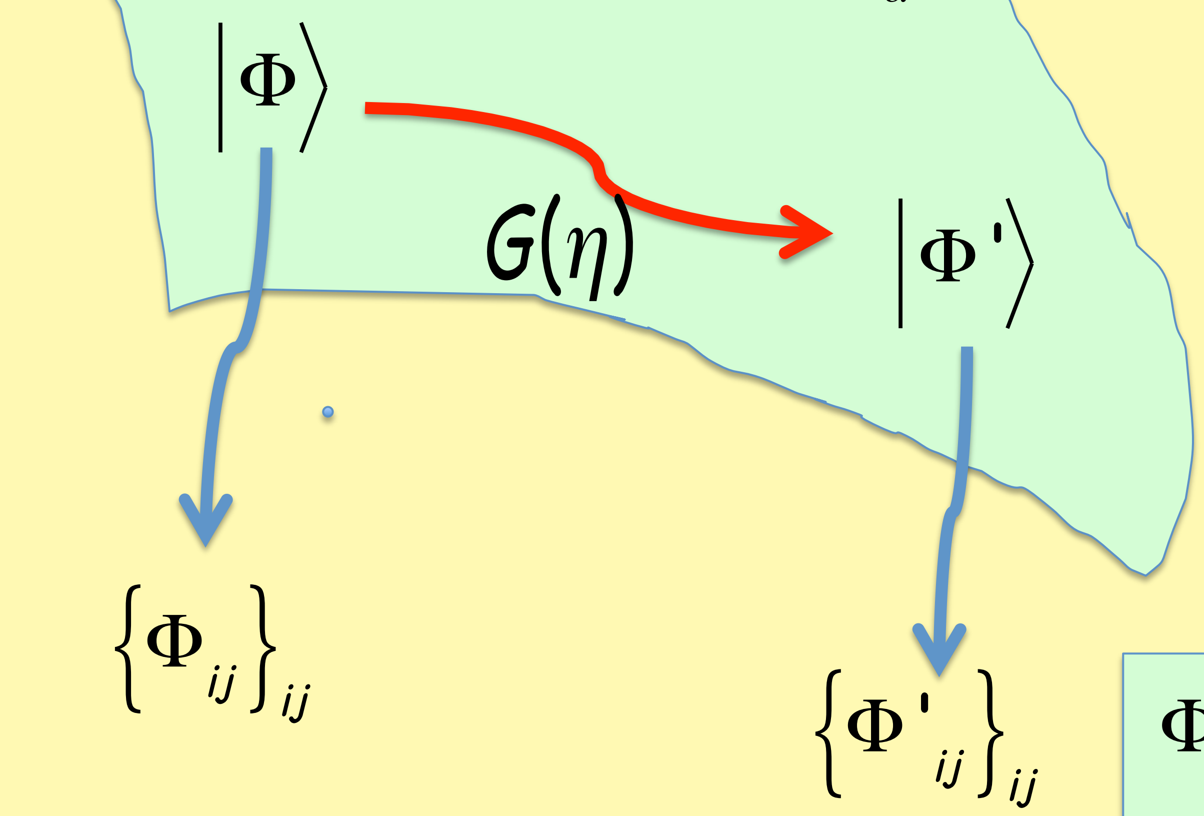
BASIS LABEL

PARTICLE LABEL

AUXILIARY FIELDS QUANTUM MONTE CARLO



$$G(\eta) = \exp(-\frac{1}{2}\delta\tau H_0)\prod_{\alpha}\exp(i\sqrt{\delta\tau}\,\eta_\alpha A_\alpha)\exp(-\frac{1}{2}\delta\tau H_0)$$



$$H_0 = \sum_i (H_0)_i a_i^+ a_i$$

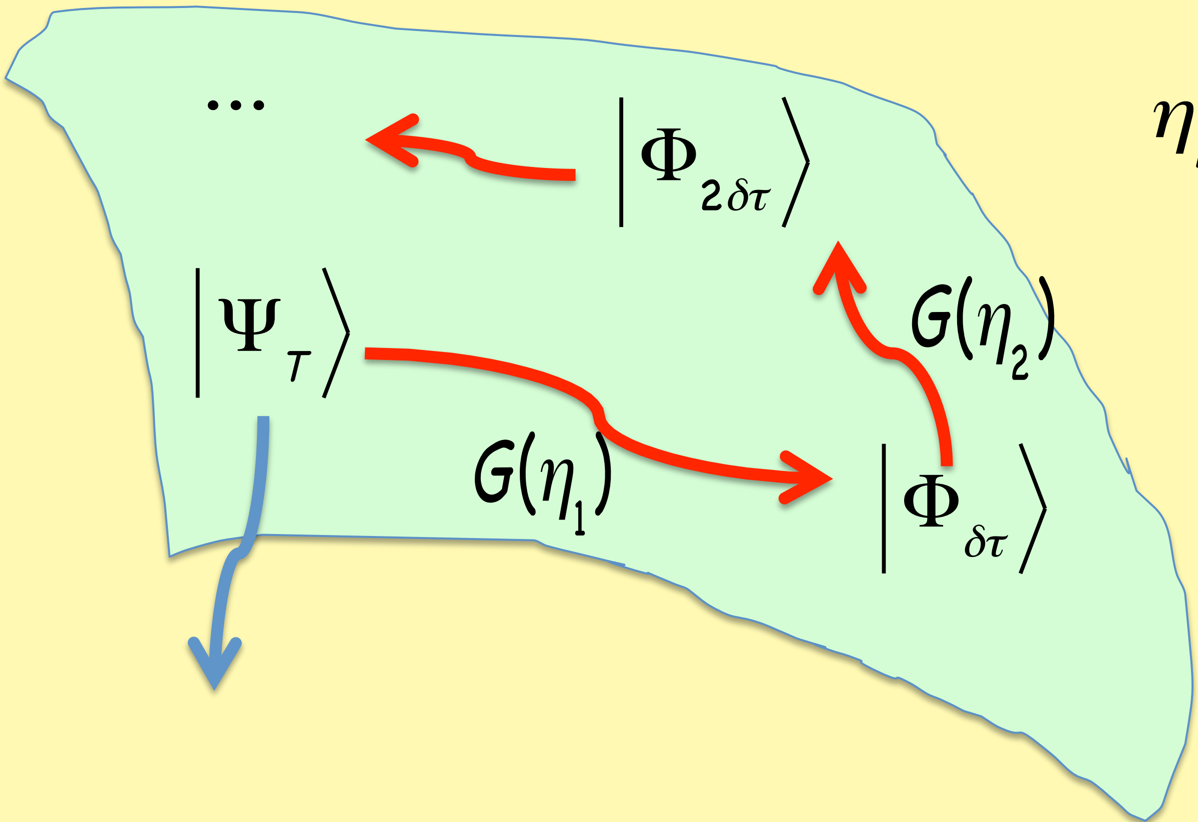
$$A_\alpha = \sum_{ij} (A_\alpha)_{ij} a_i^+ a_j$$

AUXILIARY FIELDS QUANTUM MONTE CARLO

$$\Phi' = \Omega(\eta)\,\Phi$$

$$(\Omega(\eta))_{ij} = \exp(-\frac{1}{2}\delta\tau (H_0)_i)\left(\exp(\sum_\alpha i\sqrt{\delta\tau}\,\eta_\alpha A_\alpha)\right)_{ij}\exp(-\frac{1}{2}\delta\tau (H_0)_j)$$

EXPONENTIALS OF COMPLEX MATRICES



η_i realizations of standard independent Normal random variable

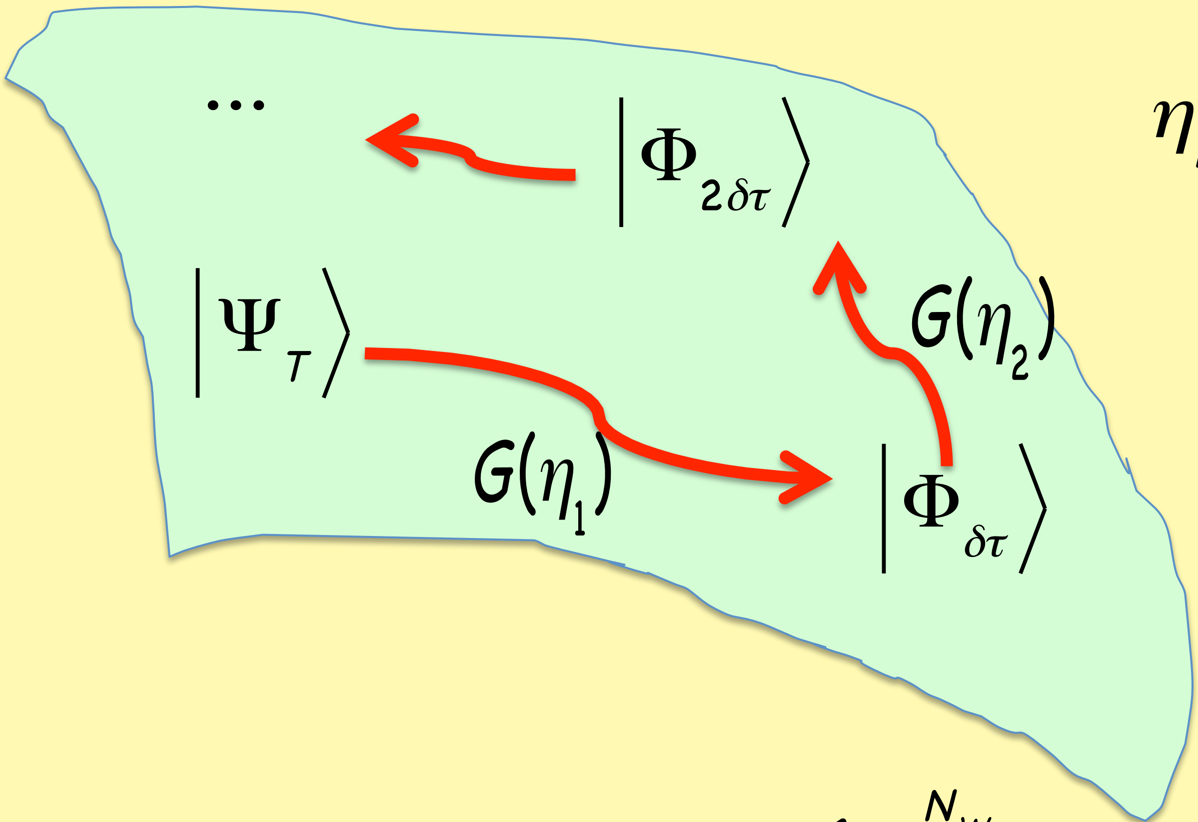
AUXILIARY FIELDS QUANTUM MONTE CARLO

Starting point: for example, Hartree-Fock solution

$$|\Psi_0\rangle \cong \int d\eta_1 \ldots d\eta_L \, g(\eta_1 \ldots \eta_L) \prod_{i=1}^{L} G(\eta_i) |\Psi_T\rangle = \text{L big enough}$$

$$= \left\langle \Phi_{L\delta\tau} \right\rangle_{\substack{\text{auxiliary fields} \\ \eta_1 \ldots \eta_L}}$$

AUXILIARY FIELDS QUANTUM MONTE CARLO



η_i realizations of standard independent Normal random variable

$$\left|\Psi_0\right\rangle \cong \left\langle \Phi_{L\delta\tau} \right\rangle_{\substack{\text{auxiliary fields} \\ \eta_1 \dots \eta_L}} \approx \frac{1}{N_W} \sum_{w=1}^{N_W} \left| \Phi_{L\delta\tau}^{w} \right\rangle$$

N_W independent samplings of the auxiliary fields configurations

RANDOM WALK ON THE SLATER DETERMINANTS MANIFOLD

Quantum Monte Carlo method using phase-free random walks with Slater determinants

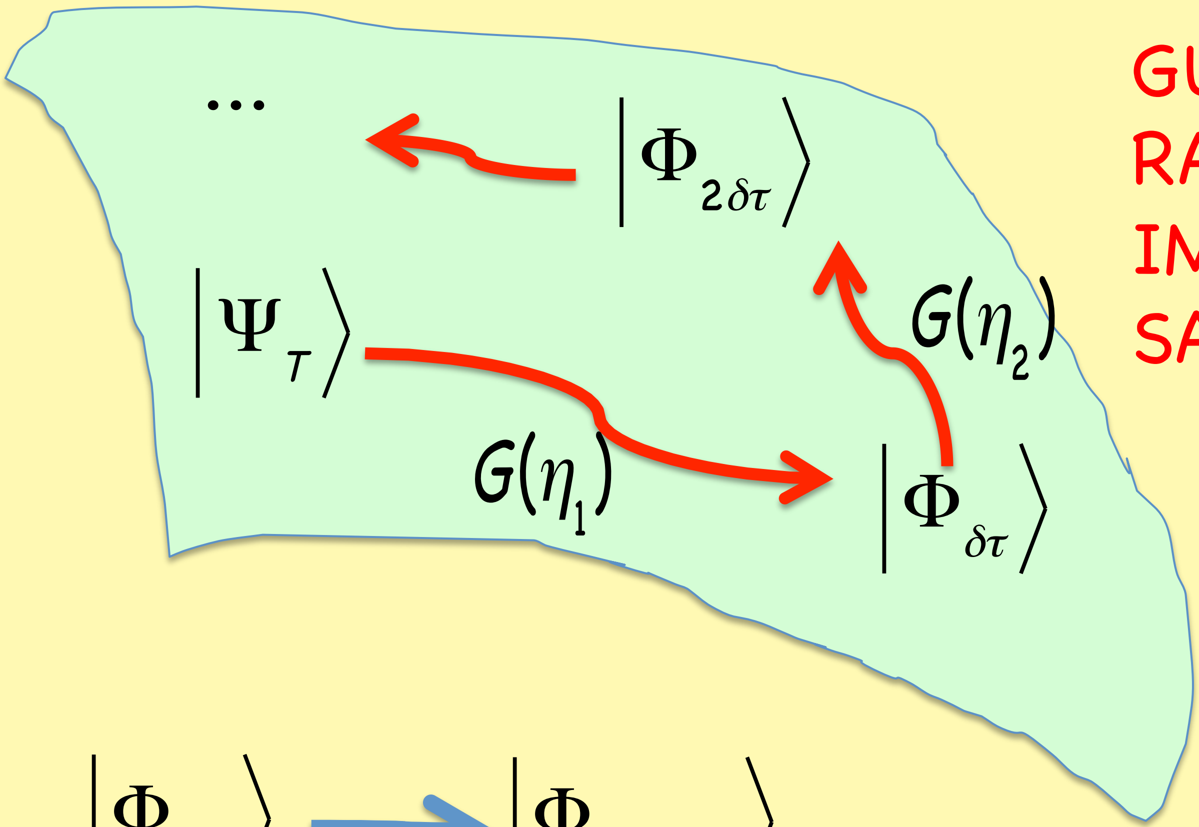
Shiwei Zhang and Henry Krakauer
Department of Physics, College of William and Mary, Williamsburg, VA 23187-8795
(Dated: February 1, 2008)

We develop a quantum Monte Carlo method for many fermions that allows the use of *any* one-particle basis. It projects out the ground state by random walks in the space of Slater determinants. An approximate approach is formulated to control the phase problem with a trial wave function $|\Psi_T\rangle$. Using plane-wave basis and non-local pseudopotentials, we apply the method to Si atom, dimer, and 2, 16, 54 atom (216 electrons) bulk supercells. Single Slater determinant wave f from density functional theory calculations were used as $|\Psi_T\rangle$ with no additional optimizati calculated binding energy of Si_2 and cohesive energy of bulk Si are in excellent agreem experiments and are comparable to the best existing theoretical results.

PACS numbers: 02.70.Ss, 71.15.-m, 31.25.-v

AUXILIARY FIELDS
QUANTUM
MONTE CARLO

We follow the algorithm invented by Shiwei Zhang .....



GUIDING THE RANDOM WALK …
IMPORTANCE SAMPLING

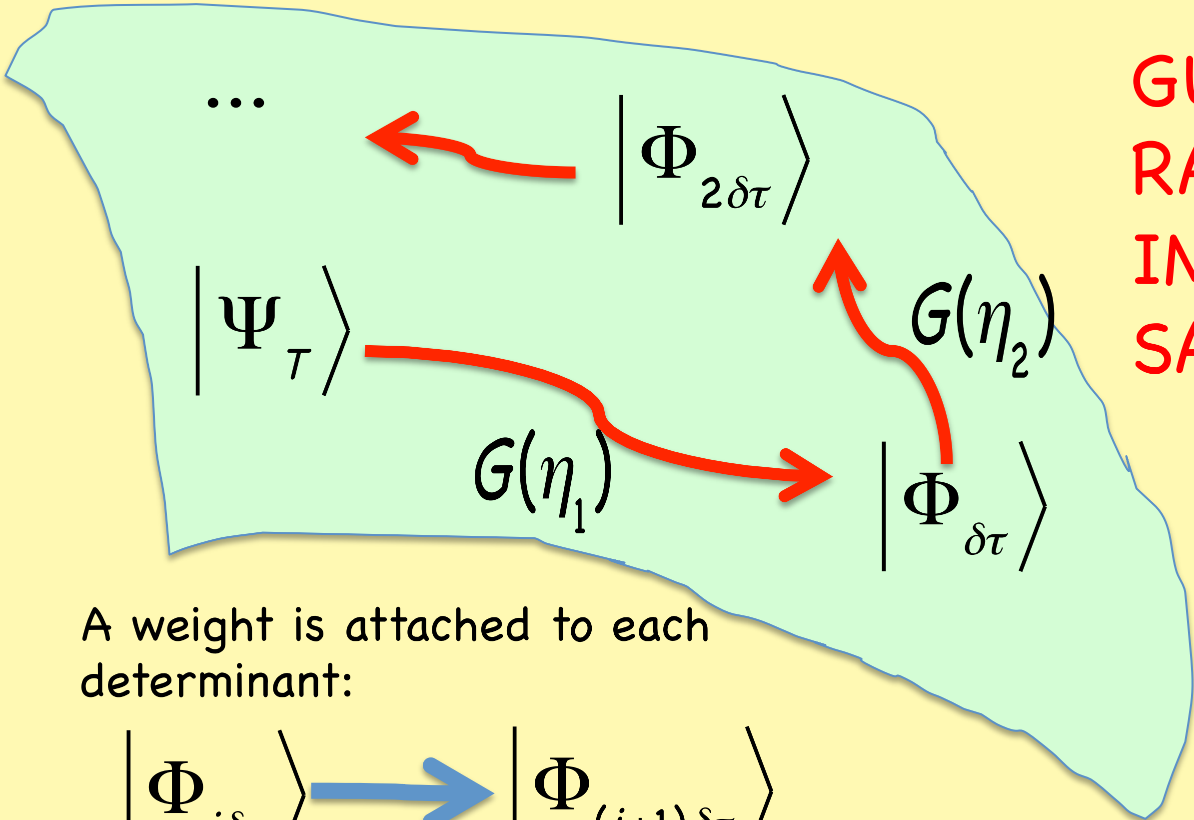
AUXILIARY FIELDS QUANTUM MONTE CARLO

$$\left|\Phi_{i\delta\tau}\right\rangle \rightarrow \left|\Phi_{(i+1)\delta\tau}\right\rangle$$

$$G(\eta - \xi(\Phi_{i\delta\tau}))$$ SHIFT PARAMETER

The precise expression (chosen to minimize some fluctuations) is ….

$$\xi_\alpha = -i\sqrt{\delta\tau}\,\frac{\left\langle \Psi_T \middle| A_\alpha \middle| \Phi_{i\delta\tau} \right\rangle}{\left\langle \Psi_T \middle| \Phi_{i\delta\tau} \right\rangle}$$



GUIDING THE RANDOM WALK …

IMPORTANCE SAMPLING

A weight is attached to each determinant:

$$\left|\Phi_{i\delta\tau}\right\rangle \rightarrow \left|\Phi_{(i+1)\delta\tau}\right\rangle$$

$$w_{(i+1)\delta\tau} = f \exp(-\delta\tau E_{local}(\Phi_{i\delta\tau}))w_{i\delta\tau}$$

AUXILIARY FIELDS QUANTUM MONTE CARLO

REAL LOCAL ENERGY APPROXIMATION

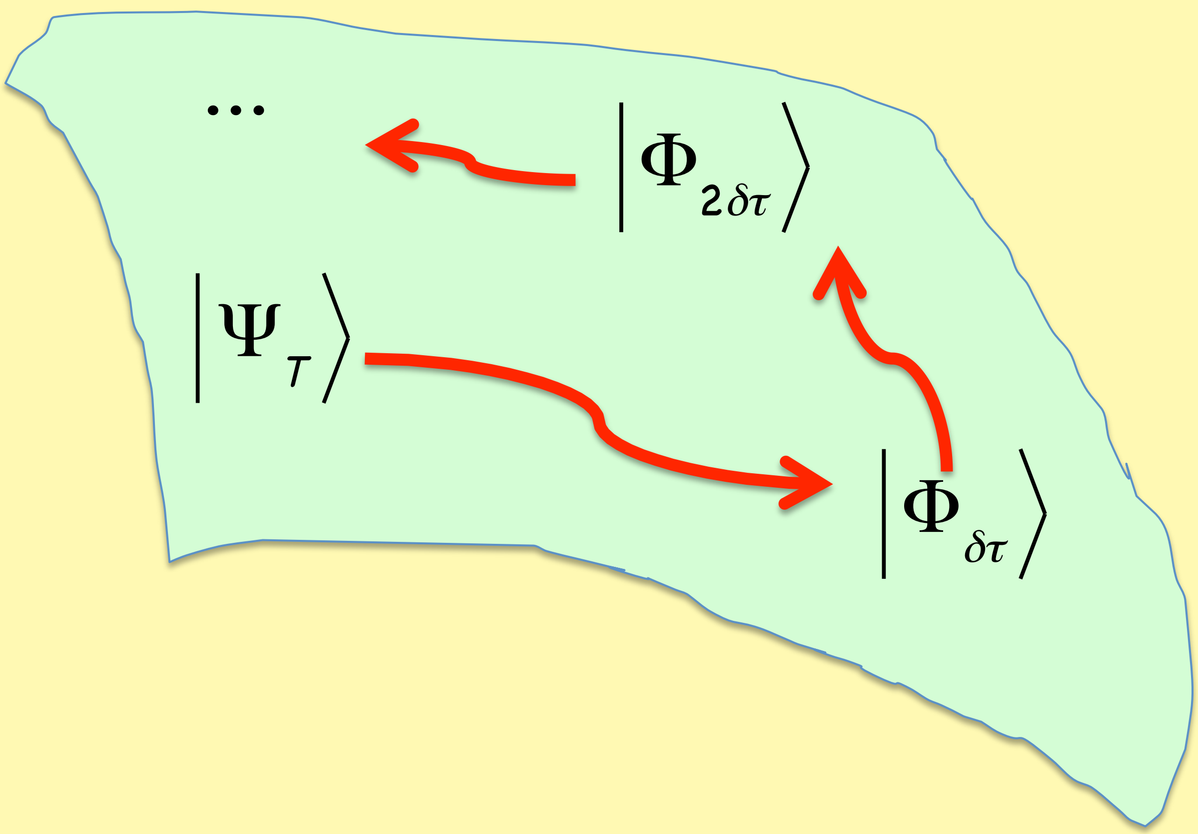
PHASE CONTROL

$$f = \max(0, \cos(\Delta\theta))$$

↓

Flip of the phase of the determinant

$$E_{local} = \Re \frac{\left\langle \Psi_T \middle| H \middle| \Phi_{i\delta\tau} \right\rangle}{\left\langle \Psi_T \mid \Phi_{i\delta\tau} \right\rangle}$$



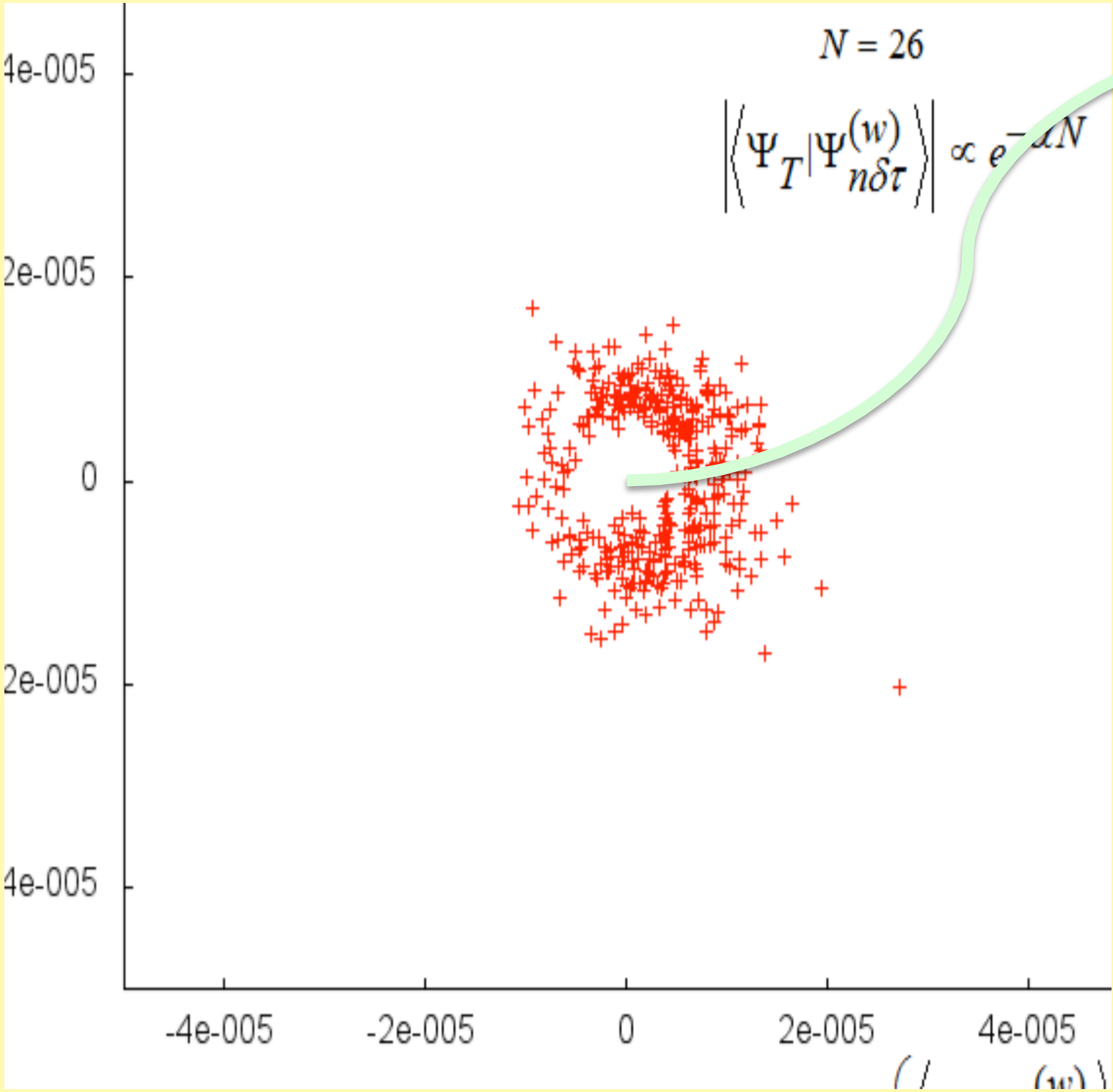
PHASELESS
AUXILIARY FIELDS
QMC

$$|\Psi_0\rangle \approx \frac{1}{N_W}\sum_{w=1}^{N_W} w_{L\delta\tau}^{w}\,\frac{|\Phi_{L\delta\tau}^{w}\rangle}{\langle\Psi_T|\Phi_{L\delta\tau}^{w}\rangle}$$

$$\left|\Psi_0\right\rangle \approx \frac{1}{N_w}\sum_{w=1}^{N_w} w^{w}_{L\delta\tau}\,\frac{\left|\Phi^{w}_{L\delta\tau}\right\rangle}{\left\langle\Psi_T\middle|\Phi^{w}_{L\delta\tau}\right\rangle}$$

ZEROS IN THE COMPLEX PLANE ARE AVOIDED

$$\left\langle\Psi_T\middle|\Phi^{w}\right\rangle$$



SIGN PROBLEM AND IMPORTANCE SAMPLING

$$\frac{\langle \Psi_T | A | \Psi_0 \rangle}{\langle \Psi_T | \Psi_0 \rangle} \approx \frac{\sum_{w=1}^{N_W} W_{L\delta\tau}^{w} \dfrac{\langle \Psi_T | A | \Phi_{L\delta\tau}^{w} \rangle}{\langle \Psi_T | \Phi_{L\delta\tau}^{w} \rangle}}{\sum_{w=1}^{N_W} W_{L\delta\tau}^{w}}$$

Such estimations provide Ground State expectations if

$$[A, H] = 0$$

MIXED ESTIMATES

To compute these matrix elements we perform linear algebra operations on the matrices of Ψ_T, Φ and A

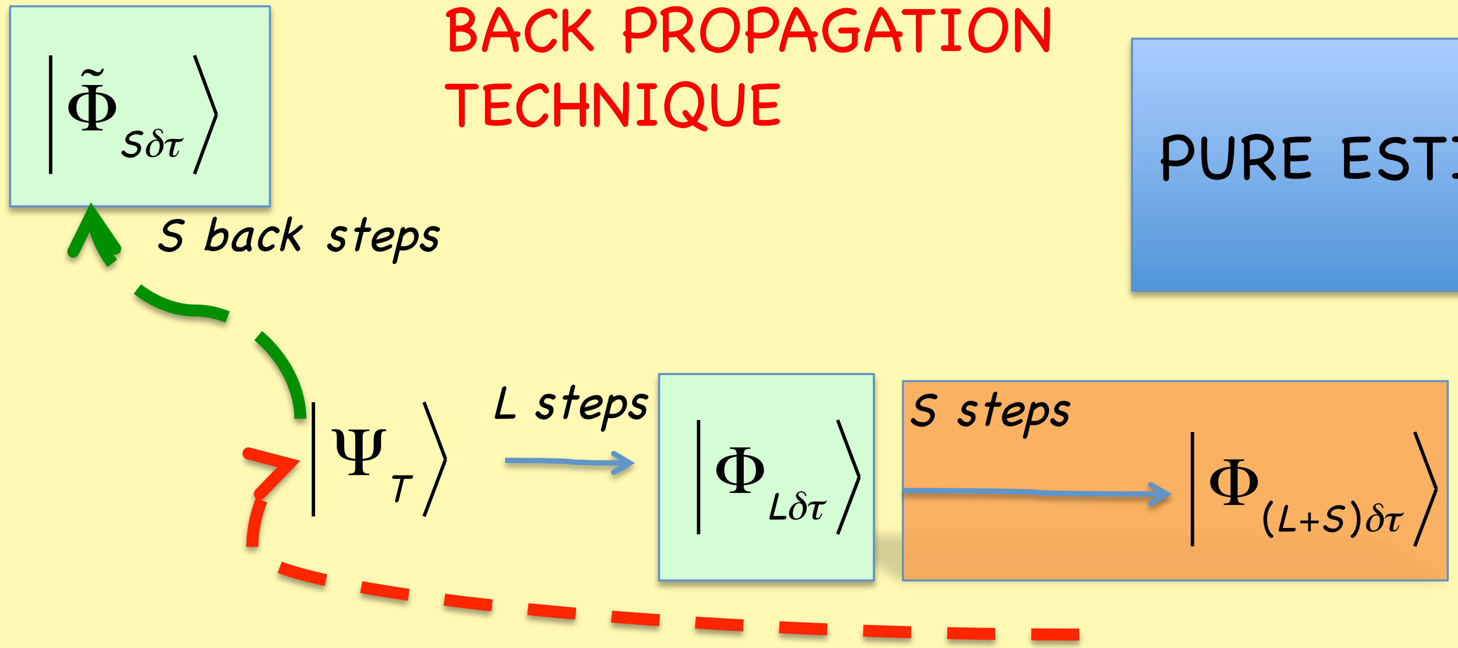
$$\frac{\left\langle \Psi_T \middle| U(S\delta\tau) A \middle| \Psi_0 \right\rangle}{\left\langle \Psi_T \middle| U(S\delta\tau) \middle| \Psi_0 \right\rangle} \approx \frac{\sum_{w=1}^{N_W} W^{w}_{(L+s)\delta\tau} \dfrac{\left\langle \tilde{\Phi}^{w}_{S\delta\tau} \middle| A \middle| \Phi^{w}_{L\delta\tau} \right\rangle}{\left\langle \tilde{\Phi}^{w}_{S\delta\tau} \middle| \Phi^{w}_{L\delta\tau} \right\rangle}}{\sum_{w=1}^{N_W} W^{w}_{(L+S)\delta\tau}}$$

$$\left| \tilde{\Phi}_{S\delta\tau} \right\rangle \cong \left(G(\eta_{L+S}) \ldots G(\eta_{L+1}) \right)^{+} \left| \Psi_T \right\rangle$$

$$\left[A, H \right] \neq 0$$

BACK PROPAGATION TECHNIQUE

PURE ESTIMATES



For the evaluation of imaginary time correlation functions, we start from the following work ...

PHYSICAL REVIEW B, VOLUME 63, 073105

Efficient calculation of imaginary-time-displaced correlation functions in the projector auxiliary-field quantum Monte Carlo algorithm

M. Feldbacher and F. F. Assaad
Institut für Theoretische Physik III, Universität Stuttgart, Pfaffenwaldring 57, D-70550 Stuttgart, Germany
(Received 28 September 2000; published 29 January 2001)

The calculation of imaginary-time-displaced correlation functions with the auxiliary-field projector quantum Monte Carlo algorithm provides valuable insight (such as spin and charge gaps) into the model under consideration. One of the authors and M. Imada proposed a numerically stable method to compute those quantities [J. Phys. Soc. Jpn. **65**, 189 (1996)]. Although precise, this method is expensive in CPU time. Here we present an alternative approach which is an order of magnitude quicker, just as precise, and very simple to implement. The method is based on the observation that for a given auxiliary field the equal-time Green-function matrix G is a projector: $G^2 = G$.

DOI: 10.1103/PhysRevB.63.073105 PACS number(s): 71.27.+a, 71.10.−w, 71.10.Fd

$$f_A(\tau) = \frac{\langle \Psi_0 | A\, U(\tau)\, A^+ | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle}$$

$A = a_i$ Dynamical Green function ...

$A = \sum_{i,j} A_{ij} a_i^+ a_j$ Density-Density Response function ...

in general $\left[A, G(\eta) \right] \neq 0$

some $G(\eta)$ remain "trapped"

$$G(\eta) = \exp(-\frac{1}{2}\delta\tau H_0) \prod_\alpha \exp(i\sqrt{\delta\tau}\ \eta_\alpha A_\alpha) \exp(-\frac{1}{2}\delta\tau H_0)$$

$$(\Omega(\eta))_{ij} = \exp(-\frac{1}{2}\delta\tau (H_0)_i) \left(\exp(i\sqrt{\delta\tau}\ \eta_\alpha A_\alpha) \right)_{ij} \exp(-\frac{1}{2}\delta\tau (H_0)_j)$$

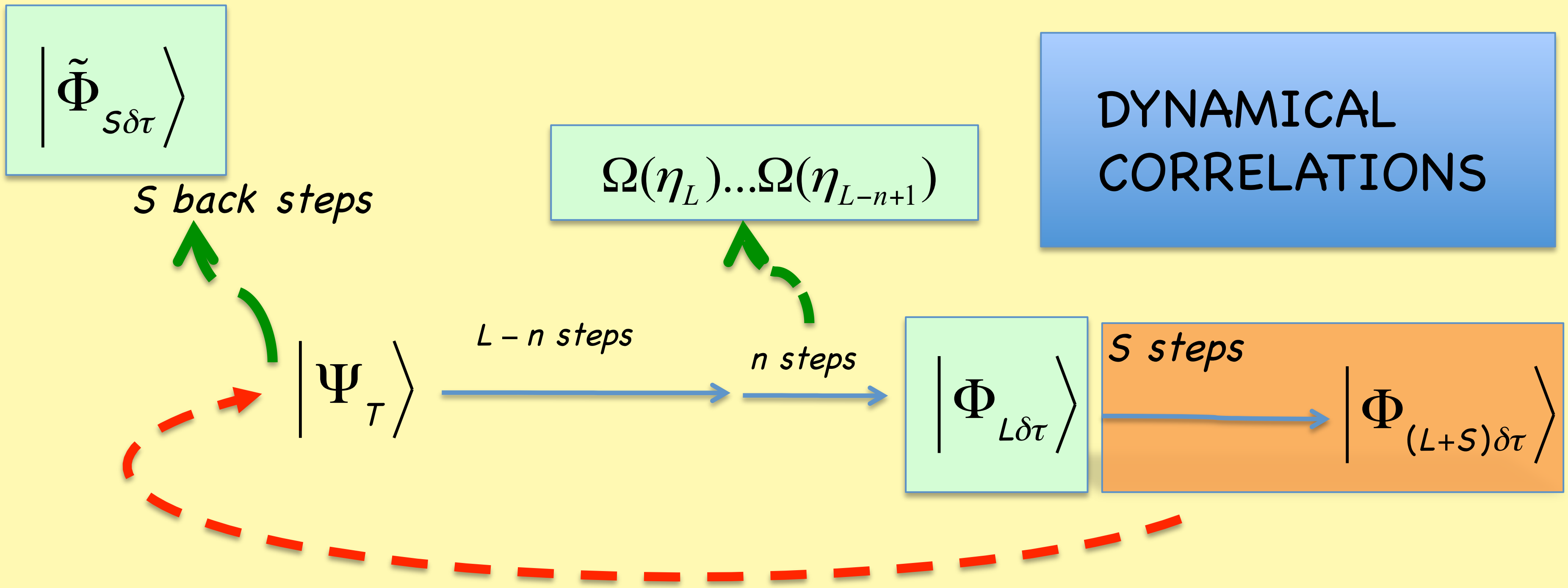
DYNAMICAL CORRELATIONS

$$G(\eta_n)...G(\eta_1) a_i^+ a_j =$$

$$\sum_{kl} \left[\Omega(\eta_n)...\Omega(\eta_1) \right]^{-1}_{ki} a_k^+ a_l \left[\Omega(\eta_n)...\Omega(\eta_1) \right]_{jl} G(\eta_n)...G(\eta_1)$$

$$f_A(n\delta\tau) \approx \frac{\left\langle \Psi_T \middle| U(S\delta\tau) A U(n\delta\tau)\, A^{+} U((L-n)\delta\tau) \middle| \Psi_0 \right\rangle}{\left\langle \Psi_T \,|\, U((S+L-n)\delta\tau) \,|\, \Psi_T \right\rangle} \approx$$

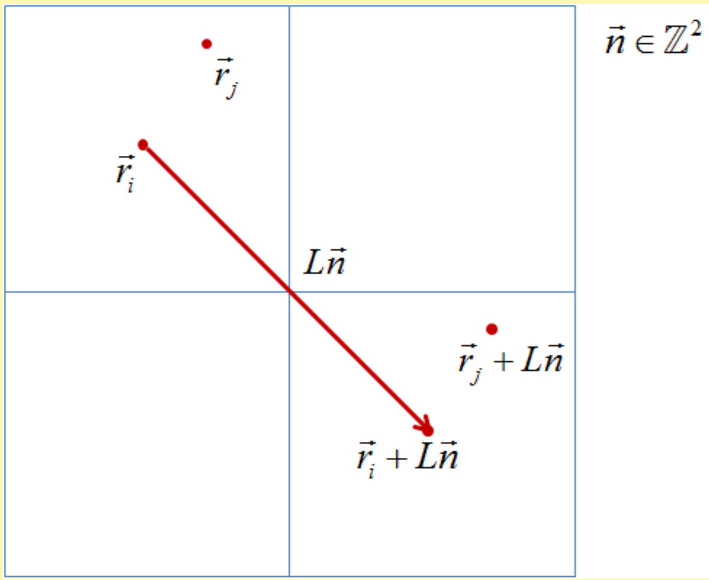
$$\frac{\displaystyle\sum_{w=1}^{N_W} W^{w}_{(L+S)\delta\tau} \sum_{kl=1}^{M} \frac{\left\langle \tilde{\Phi}^{w}_{S\delta\tau} \middle| A a_k^{+} a_l \middle| \Phi^{w}_{L\delta\tau} \right\rangle}{\left\langle \tilde{\Phi}^{w}_{S\delta\tau} \middle| \Phi^{w}_{L\delta\tau} \right\rangle} \Big[\big[\Omega(\eta_L)\ldots\Omega(\eta_{L-n+1}) \big]^{-1} A^{+}\, \Omega(\eta_L)\ldots\Omega(\eta_{L-n+1}) \Big]_{kl}}{\displaystyle\sum_{w=1}^{N_W} W^{w}_{(L+S-n)\delta\tau}}$$



The algorithm at work …

A test case …. The <u>2D Jellium model</u>

N ½-spin fermions interacting via an 1/r pair potential: Electrons in a uniform background of positive charges, moving inside a 2D box of surface V, in periodic boundary conditions



$$H = \sum_{k\sigma} \frac{|k|^2}{2} a^+_{k\sigma} a_{k\sigma} + \frac{N}{2}\xi + \frac{1}{2V} \sum_{kk'pp'\sigma\sigma'} \delta_{p-k,k'-p'} \, \phi_{k-p} \, a^+_{k\sigma} a^+_{k'\sigma'} a_{p'\sigma'} a_{p\sigma}$$

$$\phi_q = \begin{cases} 0 & q = 0 \\ \dfrac{2\pi}{|q|} & q \neq 0 \end{cases}$$

Coulomb potential

$$\xi = \frac{1}{L}\left[\sum_{n \neq 0} \frac{erfc(\pi |n| / \alpha)}{|n|} + \frac{erfc(\alpha |n|)}{|n|} - \frac{2\alpha}{\sqrt{\pi}} - \frac{2\sqrt{\pi}}{\alpha} \right]$$

Ewald constant

2D JELLIUM

Energy in Hartree, lenght in Bohr radius units.

$$H = \sum_{\vec{k} \in B_K} \sum_{\sigma = \uparrow,\downarrow} \left(\frac{|\vec{k}|^2}{2} + \mu_{\vec{k}} \right) a^+_{\vec{k},\sigma} a_{\vec{k},\sigma} + \frac{N}{2}\xi + \frac{1}{2} \sum_{\vec{q} \in B_Q} \left(A^2_{1,\vec{q}} + A^2_{2,\vec{q}} \right)$$

Cutoff in Kinetic energy

$$\mu_k = \frac{1}{2V} \sum_p \phi_{k-p}$$

Transferred wave vectors

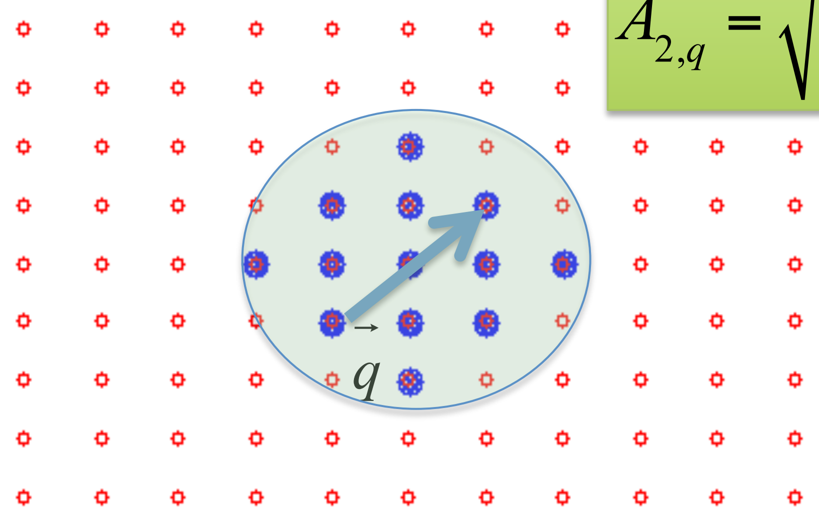
$$\rho_q = \sum_{k\sigma} a^+_{p-q\sigma} a_{p\sigma}$$

density fluctuation

$$A_{1,q} = \sqrt{\frac{\phi_q}{4V}} \left(\rho_q + \rho_{-q} \right)$$

$$A_{2,q} = \sqrt{\frac{\phi_q}{4V}} \left(i\rho_q - i\rho_{-q} \right)$$

2D JELLIUM



$$\rho_q = \sum_{k\sigma} a^+_{p-q\sigma} a_{p\sigma}$$

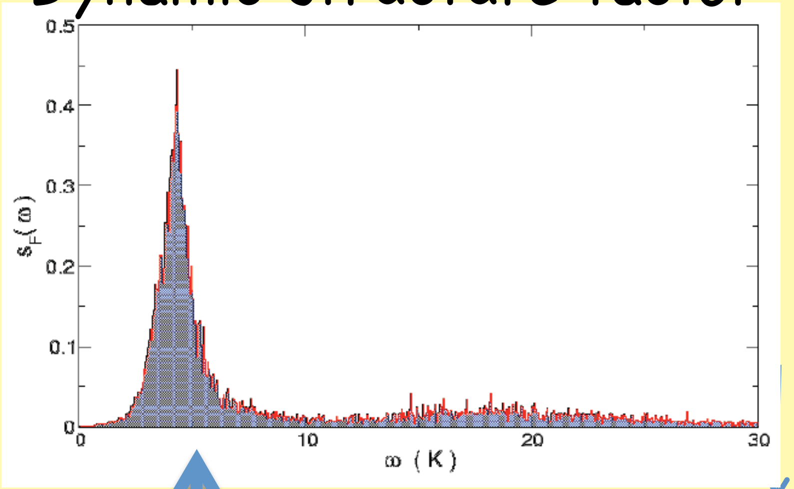
$$F(q,\tau) = \langle \Psi_0 | \rho_q U(\tau) \rho_{-q} | \Psi_0 \rangle$$

$$F(q,\tau) = \int_0^\infty e^{-\tau\omega} S(q,\omega)$$

$$\int_0^\infty d\tau\, F(q,\tau) \propto \chi(q)$$

Density response function

Dynamic structure factor



2D JELLIUM: DENSITY-DENSITY CORRELATION FUNCTION

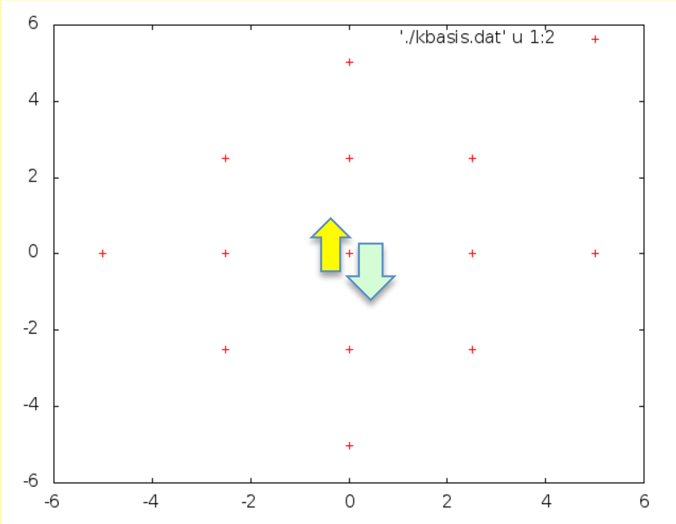
$\omega(q)$ Excitation spectrum of the system

The algorithm at work …

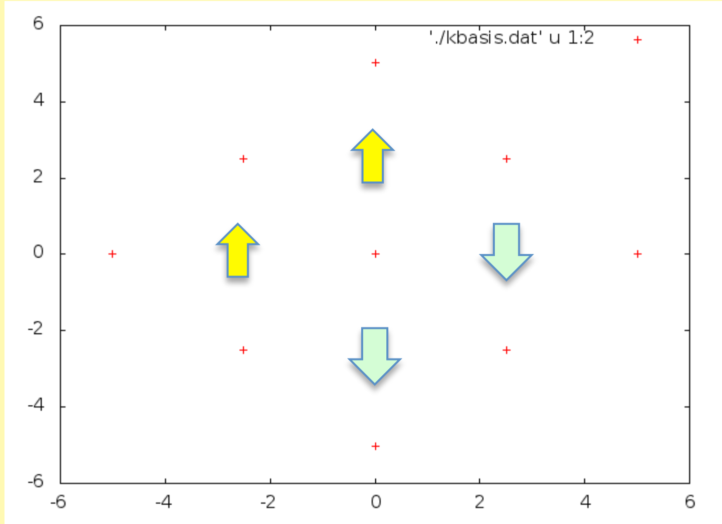
Simple situations: comparison between AFQMC and exact solutions

N = 2 electrons, “small” numbers of plane waves

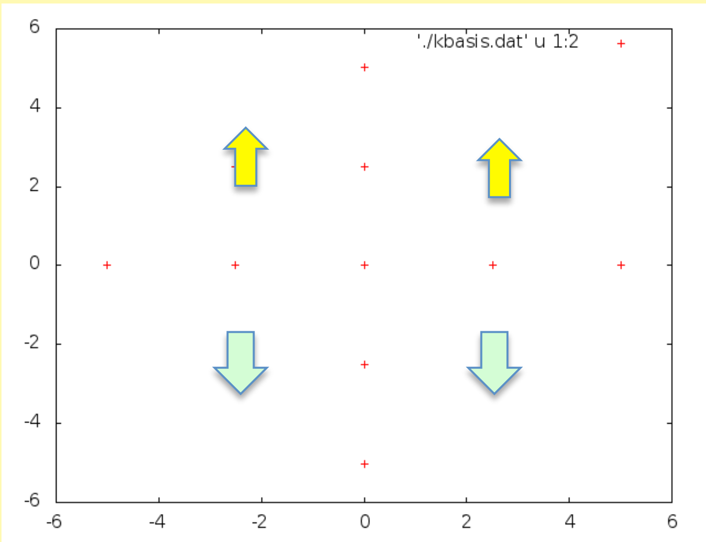
$$\left|\Psi_0\right\rangle = \alpha$$



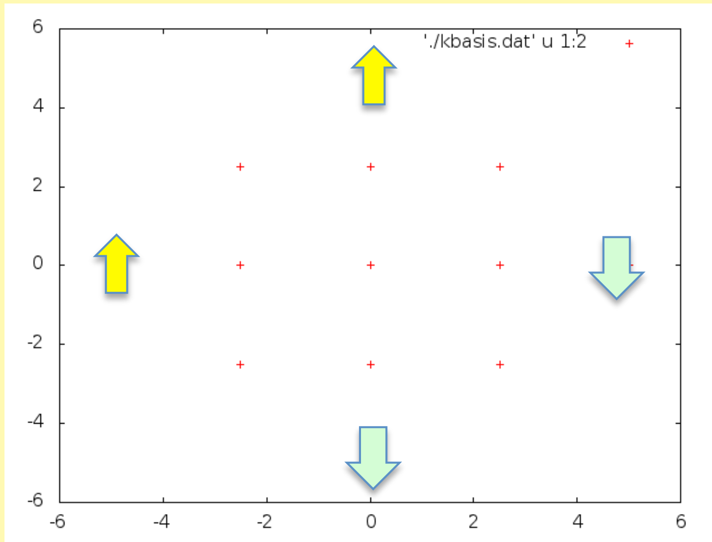
$$+\beta$$



$$+\gamma$$



$$+\delta$$

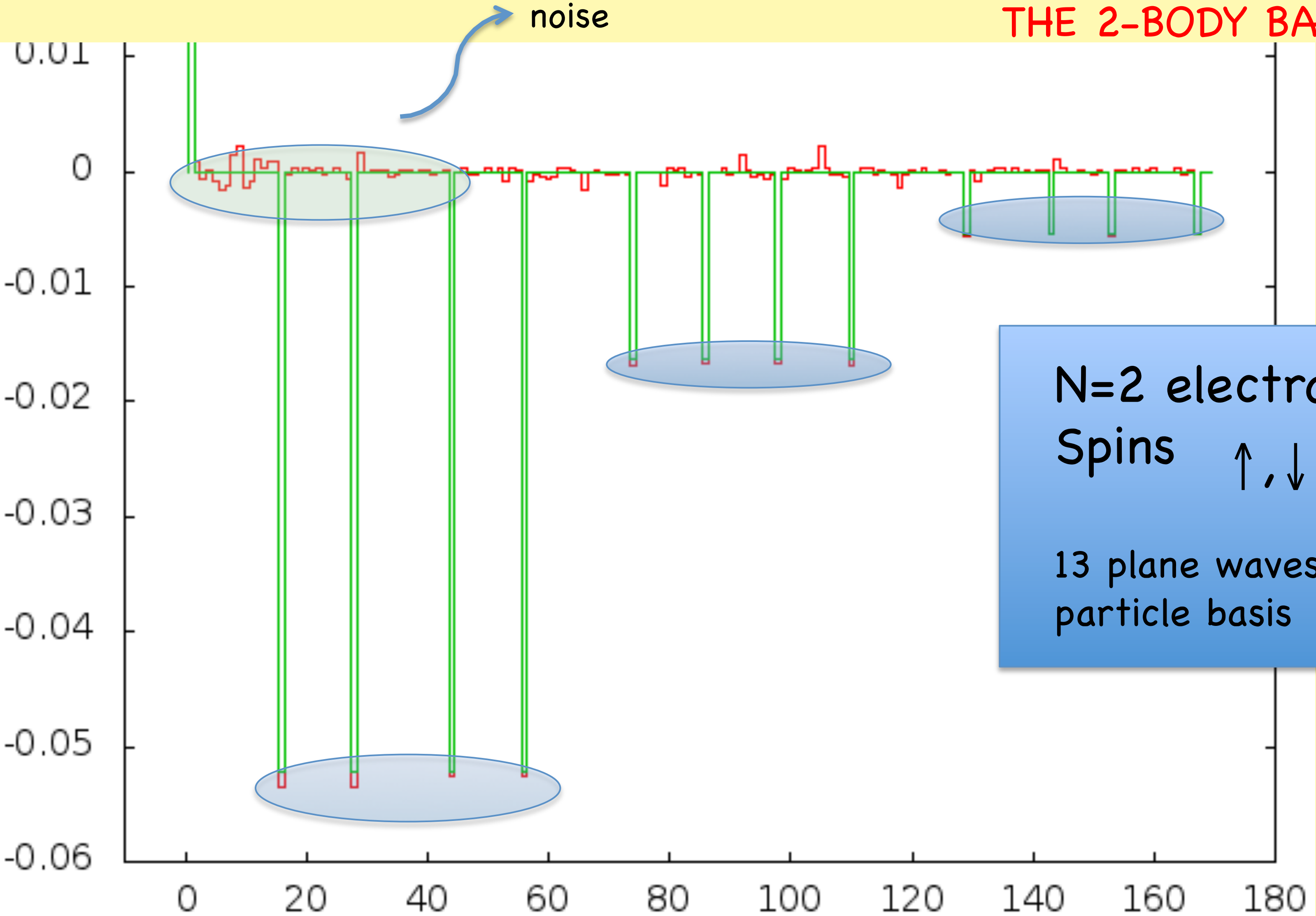


$\alpha \approx 0.994$ $\beta \approx -0.052$ $\gamma \approx -0.016$ $\delta \approx -0.005$

$$\left|\Psi_0\right\rangle \approx \frac{1}{N_W}\sum_{w=1}^{N_W} w^w_{L\delta\tau}\frac{\left|\Phi^w_{L\delta\tau}\right\rangle}{\left\langle\Psi_T\middle|\Phi^w_{L\delta\tau}\right\rangle}$$

$$\left\langle i_1\uparrow, i_2\downarrow\middle|\Psi_0\right\rangle$$

COMPONENTS OF THE GROUND STATE ON THE 2-BODY BASIS

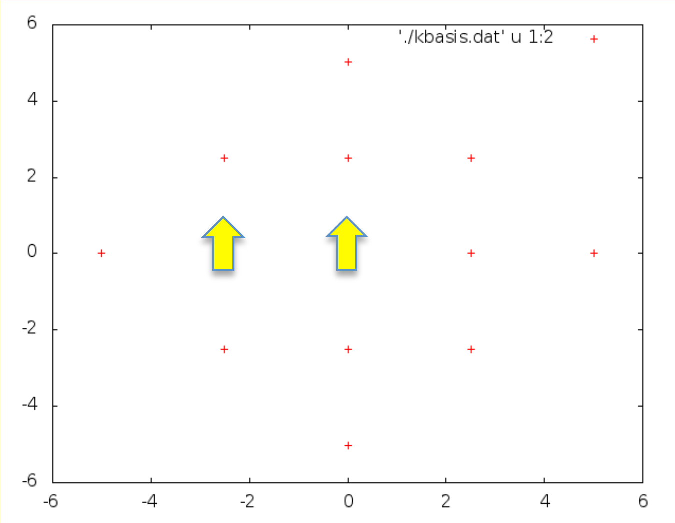


N=2 electrons, rs=1

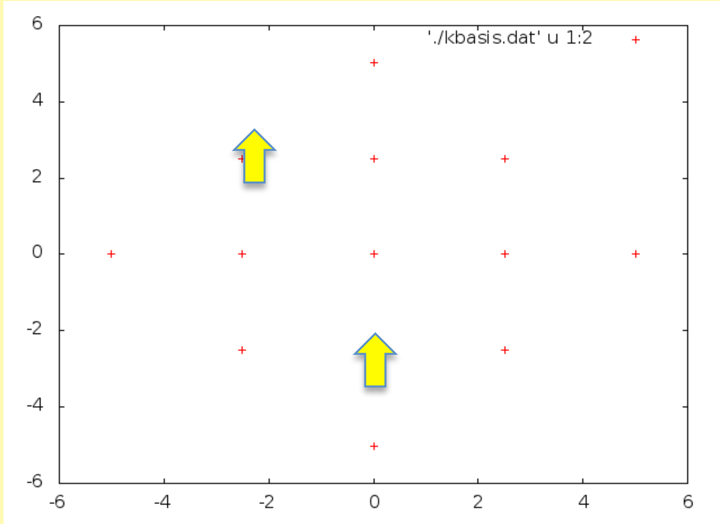
Spins $\uparrow,\downarrow$

13 plane waves as one particle basis

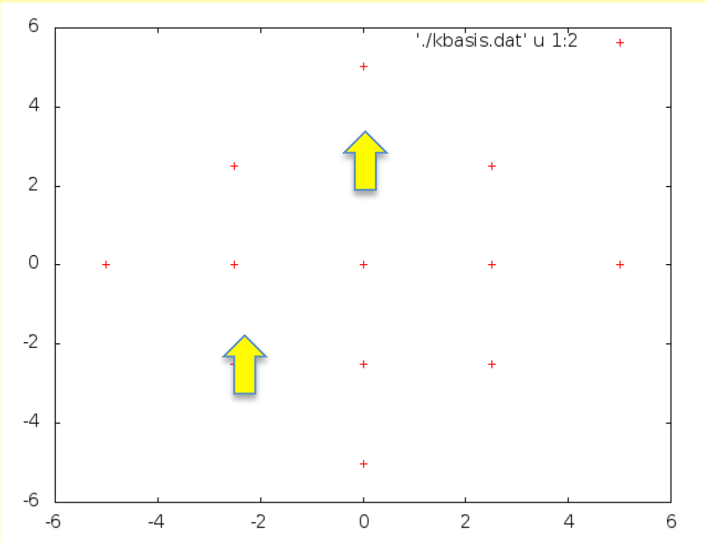
$$\left|\Psi_0^{(\vec{q})}\right\rangle = \alpha$$



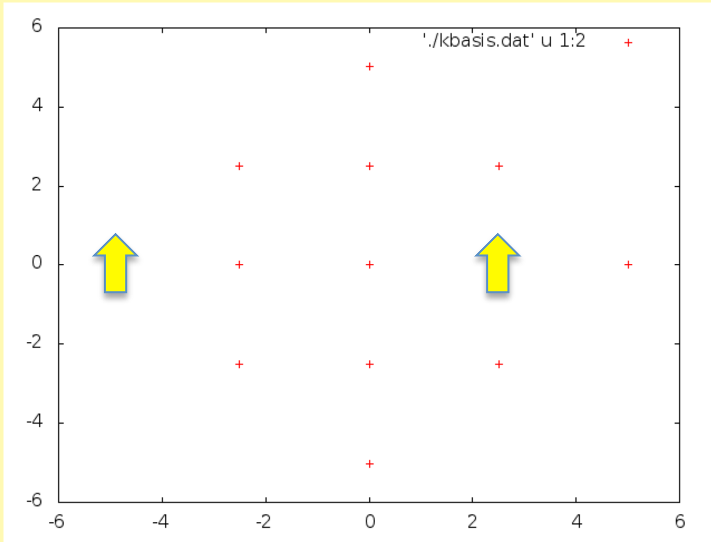
$$+\beta$$



$$+\gamma$$



$$+\delta$$

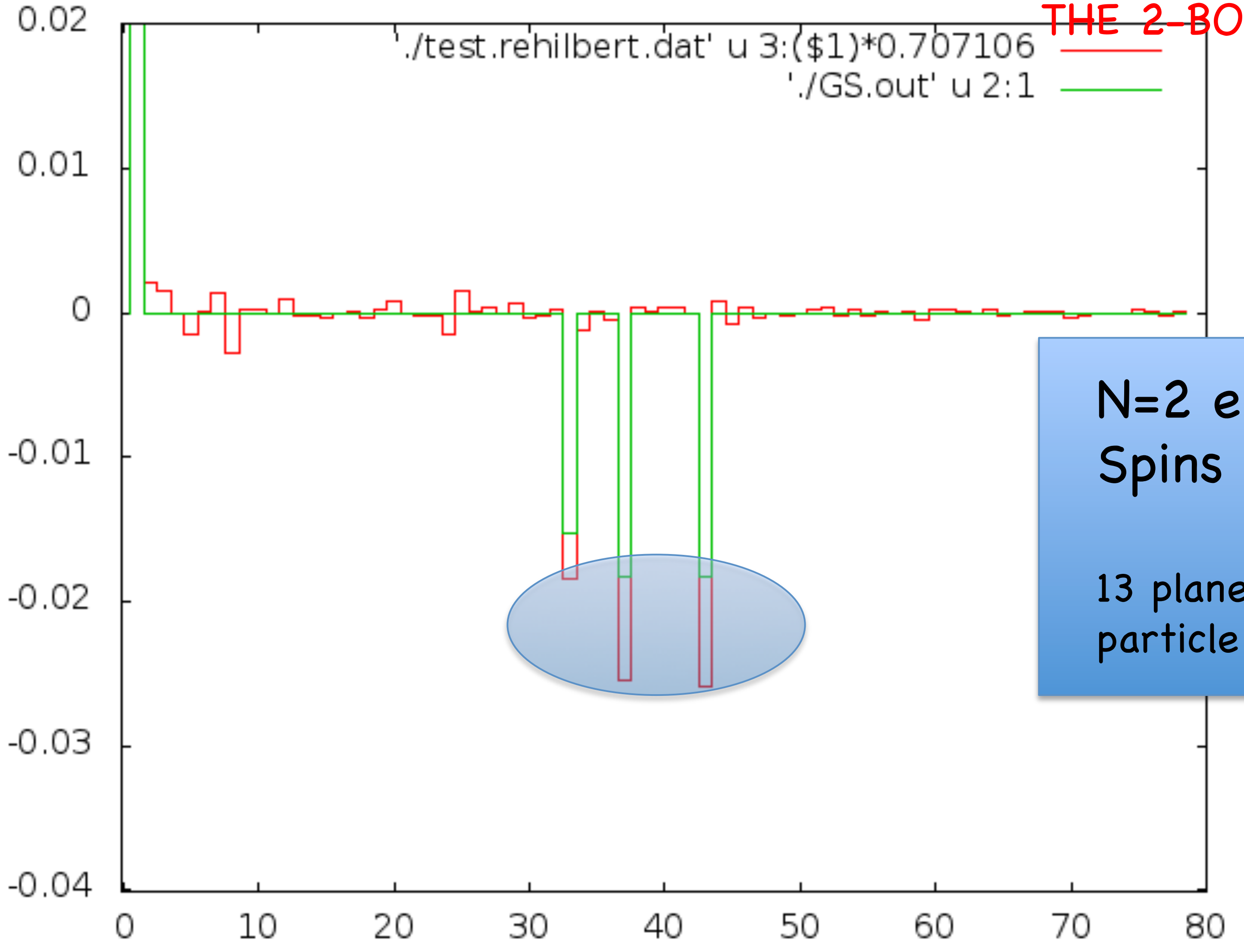


$\alpha \approx 0.999$ $\beta \approx -0.018$ $\gamma \approx -0.018$ $\delta \approx -0.015$

$$\left|\Psi_0\right\rangle \approx \frac{1}{N_W}\sum_{w=1}^{N_W} w^w_{L\delta\tau}\frac{\left|\Phi^w_{L\delta\tau}\right\rangle}{\left\langle\Psi_T\middle|\Phi^w_{L\delta\tau}\right\rangle}$$

$$\left\langle i_1\uparrow, i_2\uparrow\middle|\Psi_0\right\rangle$$

COMPONENTS OF THE GROUND STATE ON THE 2-BODY BASIS



N=2 electrons, rs=1

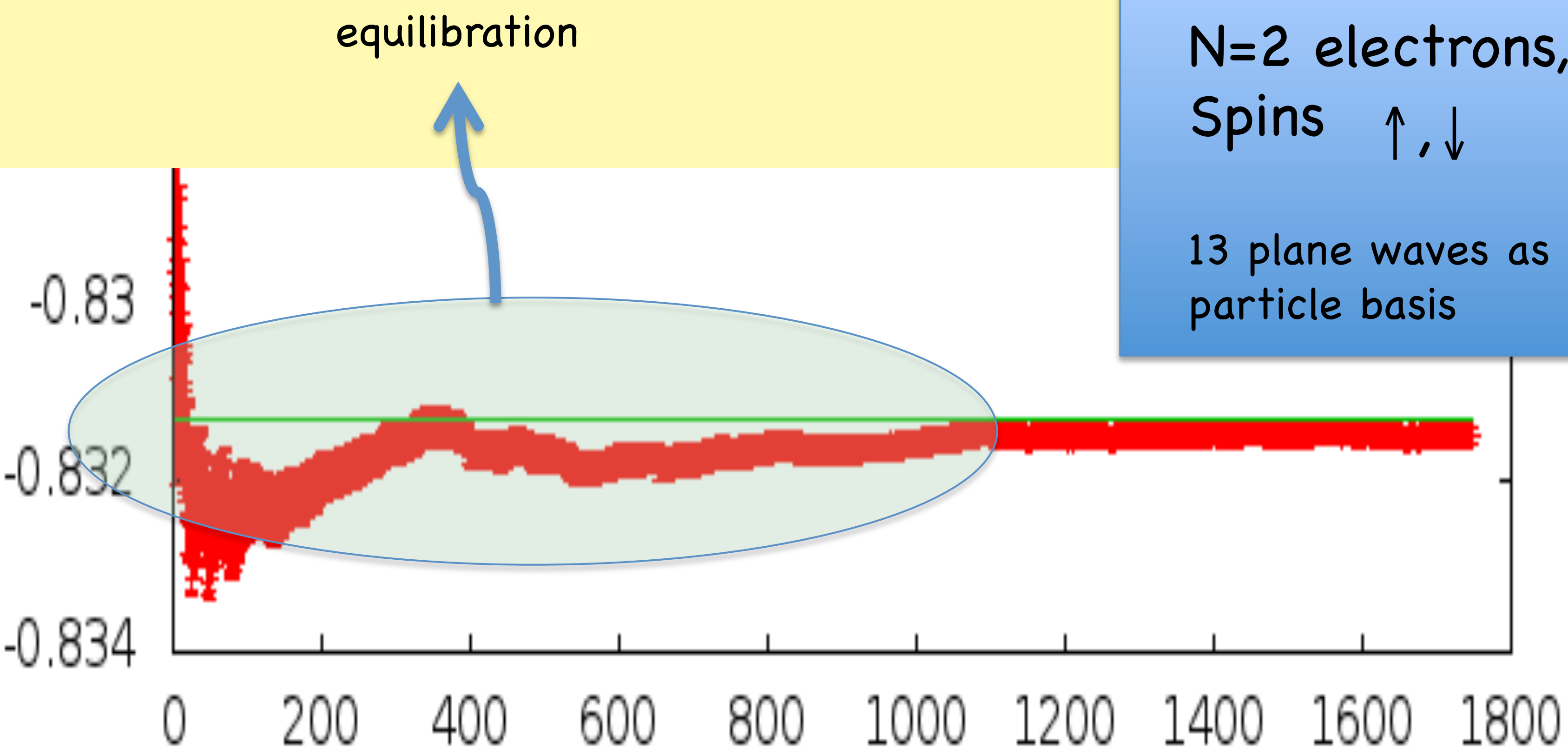
Spins $\uparrow,\uparrow$

13 plane waves as one particle basis

$$\left|\Psi_0\right\rangle \approx \frac{1}{N_W}\sum_{w=1}^{N_W} W_{L\delta\tau}^{w}\frac{\left|\Phi_{L\delta\tau}^{w}\right\rangle}{\left\langle\Psi_T\middle|\Phi_{L\delta\tau}^{w}\right\rangle}$$

$$\frac{\left\langle\Psi_T\middle|H\middle|\Psi_0\right\rangle}{\left\langle\Psi_T\middle|\Psi_0\right\rangle}$$

MIXED ESTIMATION
OF THE TOTAL ENERGY



N=2 electrons, rs=1
Spins ↑,↓

13 plane waves as one particle basis

$$|\Psi_0\rangle \approx \frac{1}{N_W}\sum_{w=1}^{N_W} w^{w}_{L\delta\tau}\,\frac{|\Phi^{w}_{L\delta\tau}\rangle}{\langle \Psi_T|\Phi^{w}_{L\delta\tau}\rangle}$$

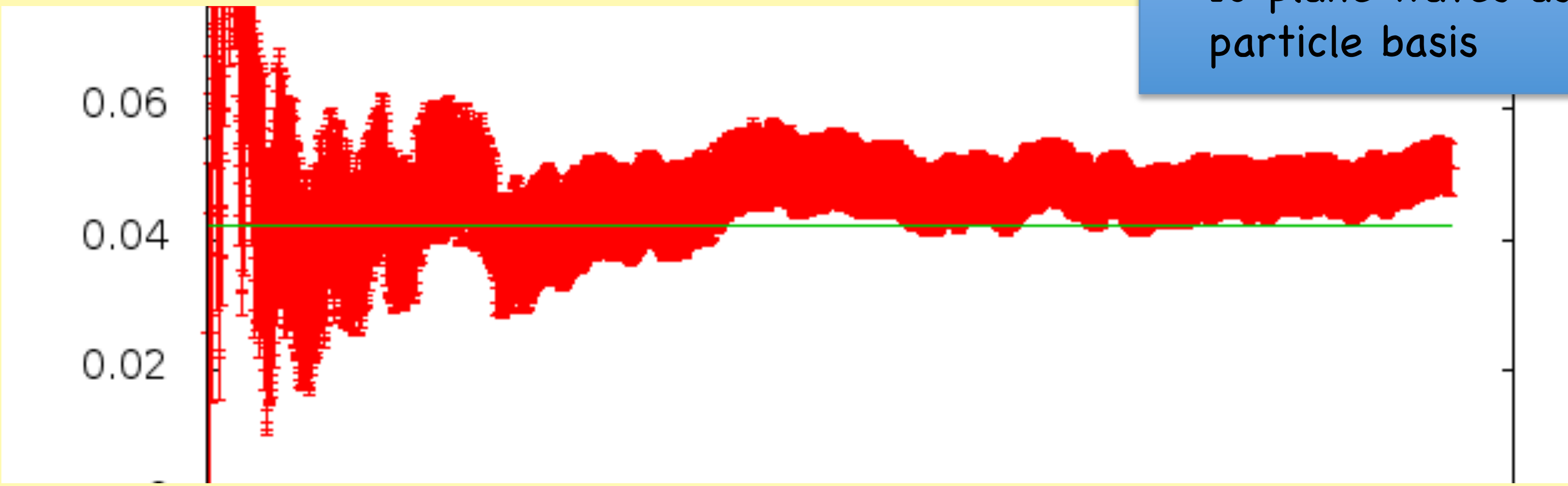
$$\frac{\langle\Psi_0|T|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle}$$

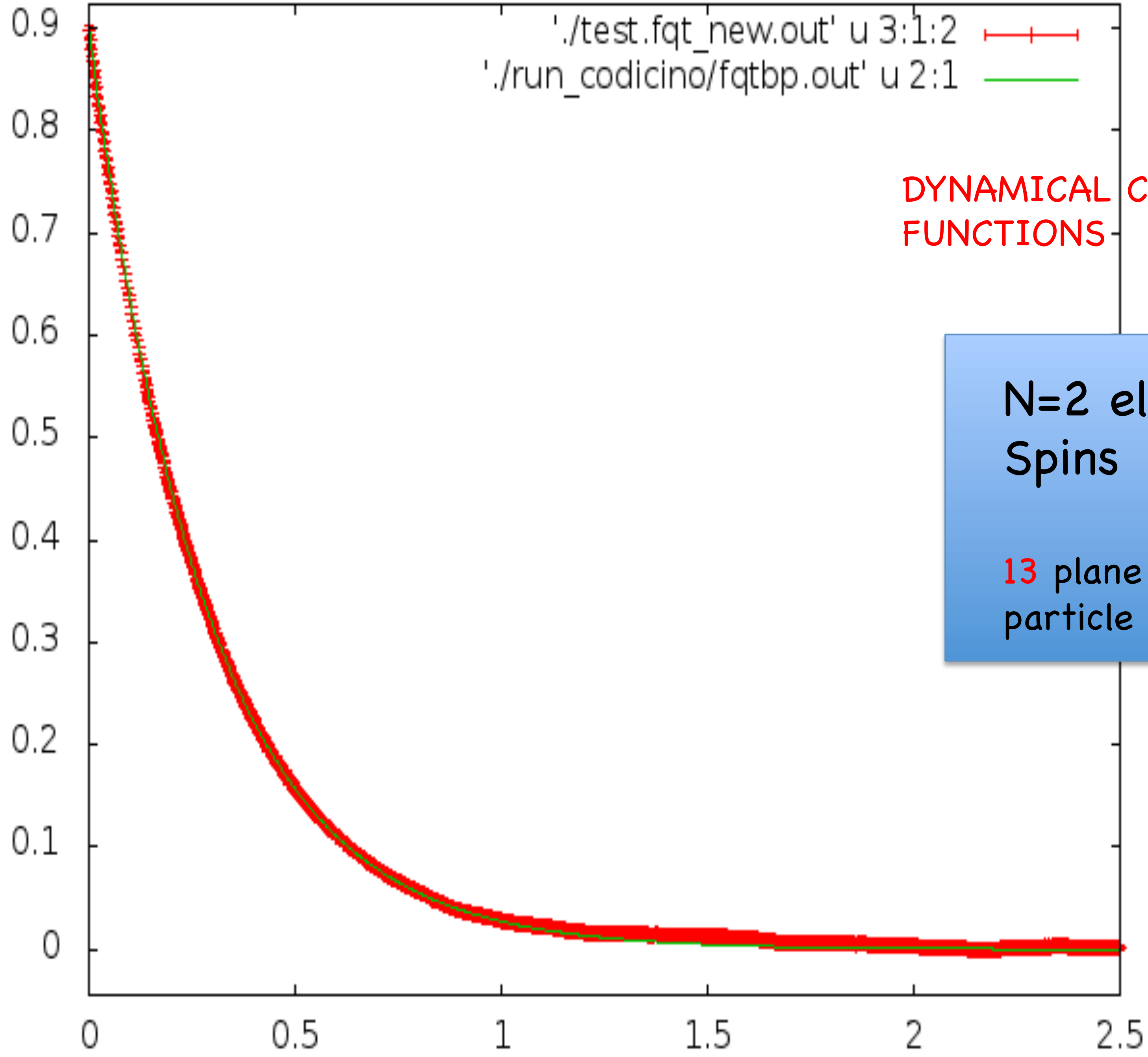
BACK-PROPAGATED ESTIMATION OF THE TOTAL ENERGY

N=2 electrons, rs=1

Spins ↑,↓

13 plane waves as one particle basis





$F(q,\tau)$

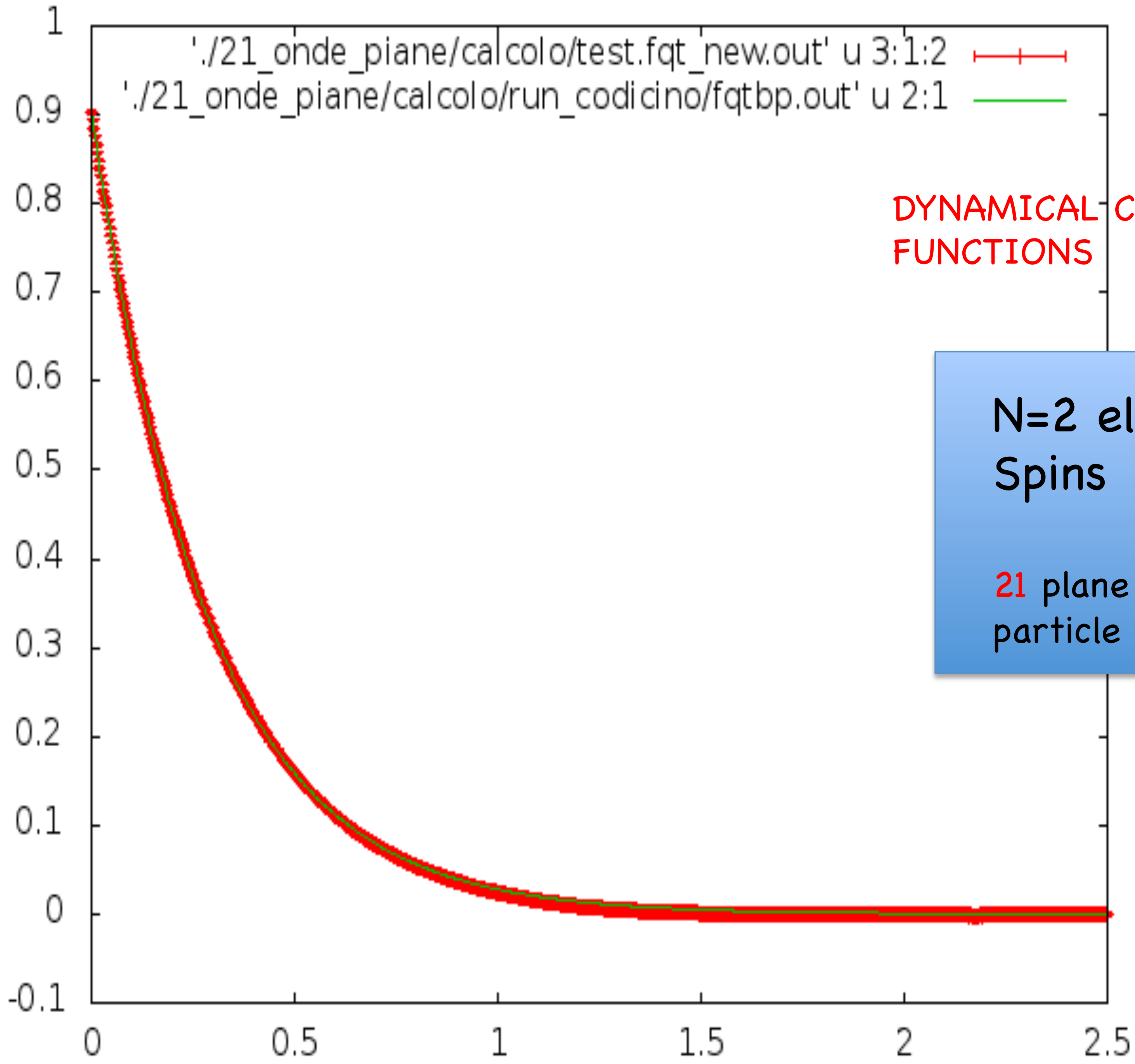
DYNAMICAL CORRELATION FUNCTIONS

N=2 electrons, rs=1

Spins ↑,↓

13 plane waves as one particle basis

$qa_0 = 2.507$



$F(q,\tau)$

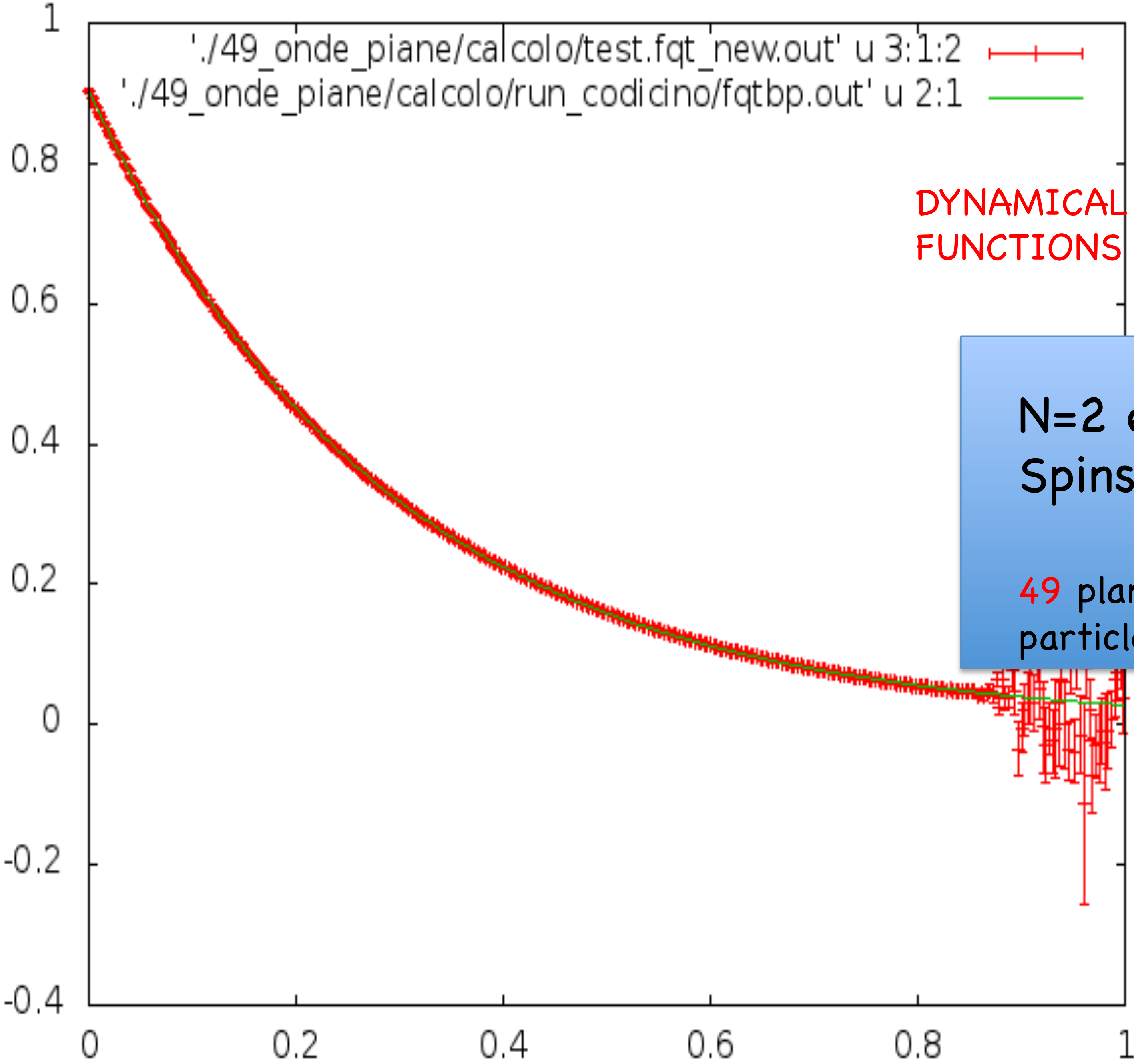
DYNAMICAL CORRELATION FUNCTIONS

N=2 electrons, rs=1

Spins $\uparrow,\downarrow$

21 plane waves as one particle basis

$qa_0 = 2.507$



$F(q,\tau)$

DYNAMICAL CORRELATION FUNCTIONS

N=2 electrons, rs=1

Spins $\uparrow,\downarrow$

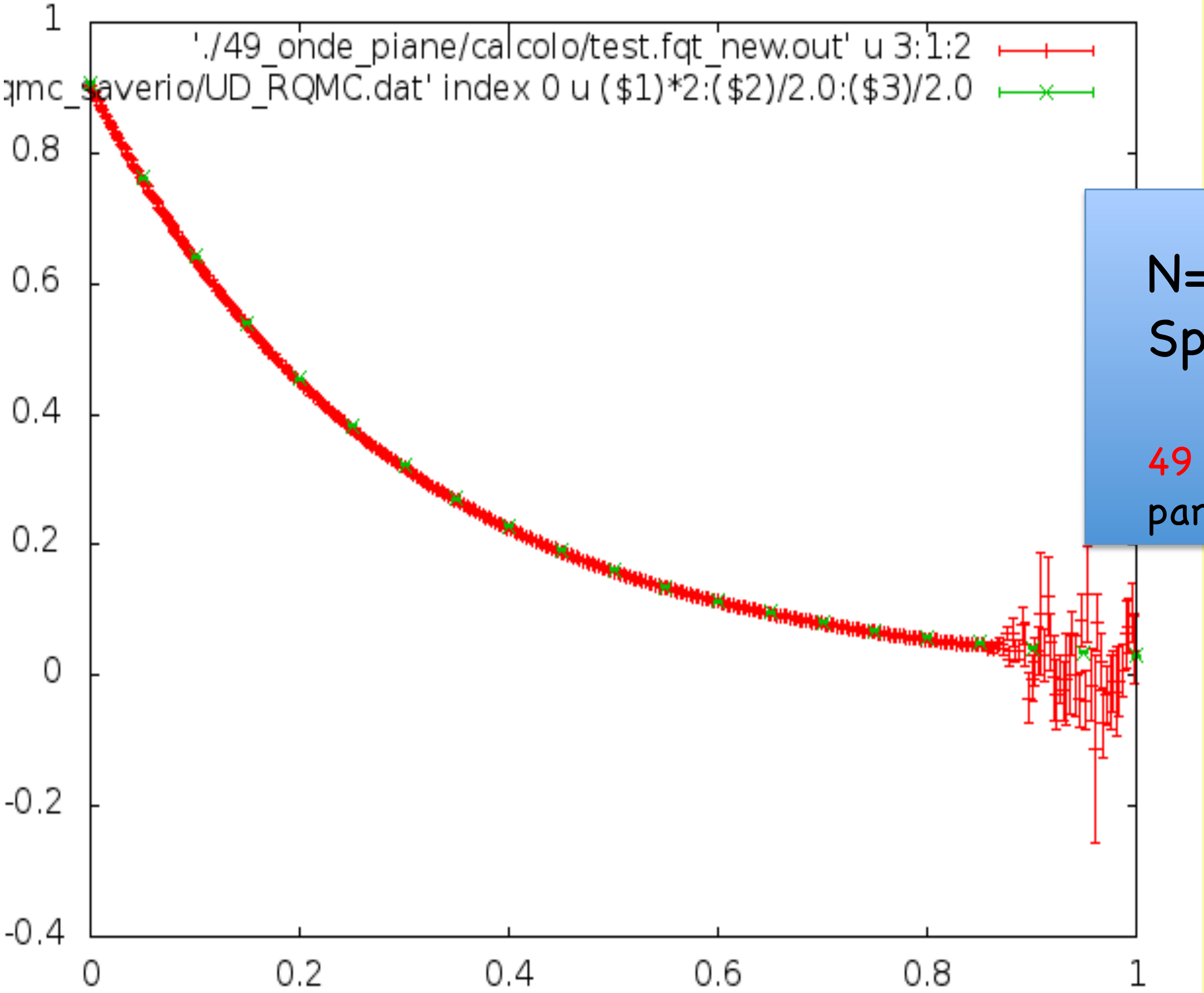
49 plane waves as one particle basis

$qa_0 = 2.507$

AFQMC vs PIGS

DYNAMICAL CORRELATION FUNCTIONS

$F(q,\tau)$



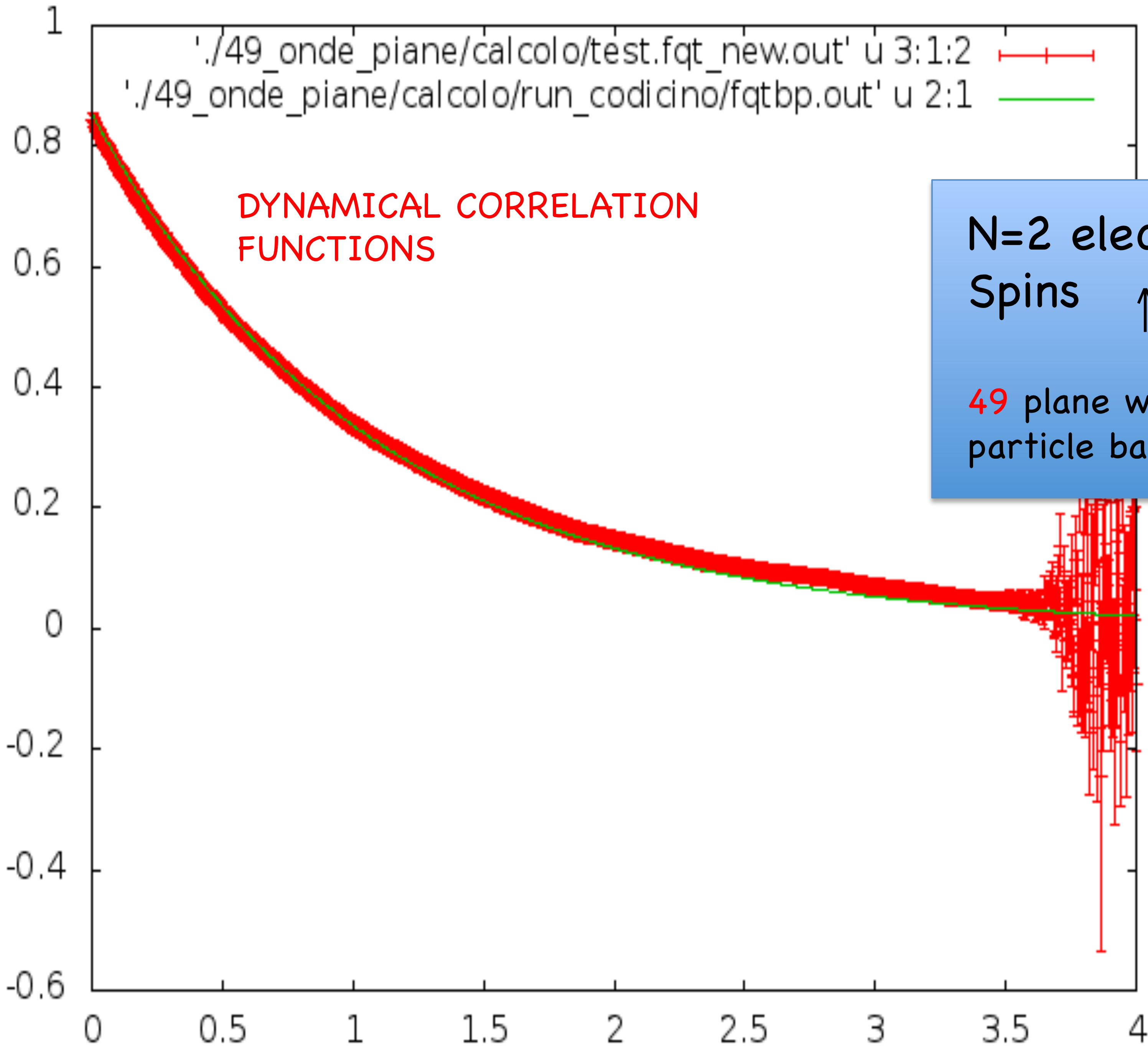
N=2 electrons, rs=1

Spins $\uparrow,\downarrow$

49 plane waves as one particle basis

$qa_0 = 2.507$

$F(q,\tau)$



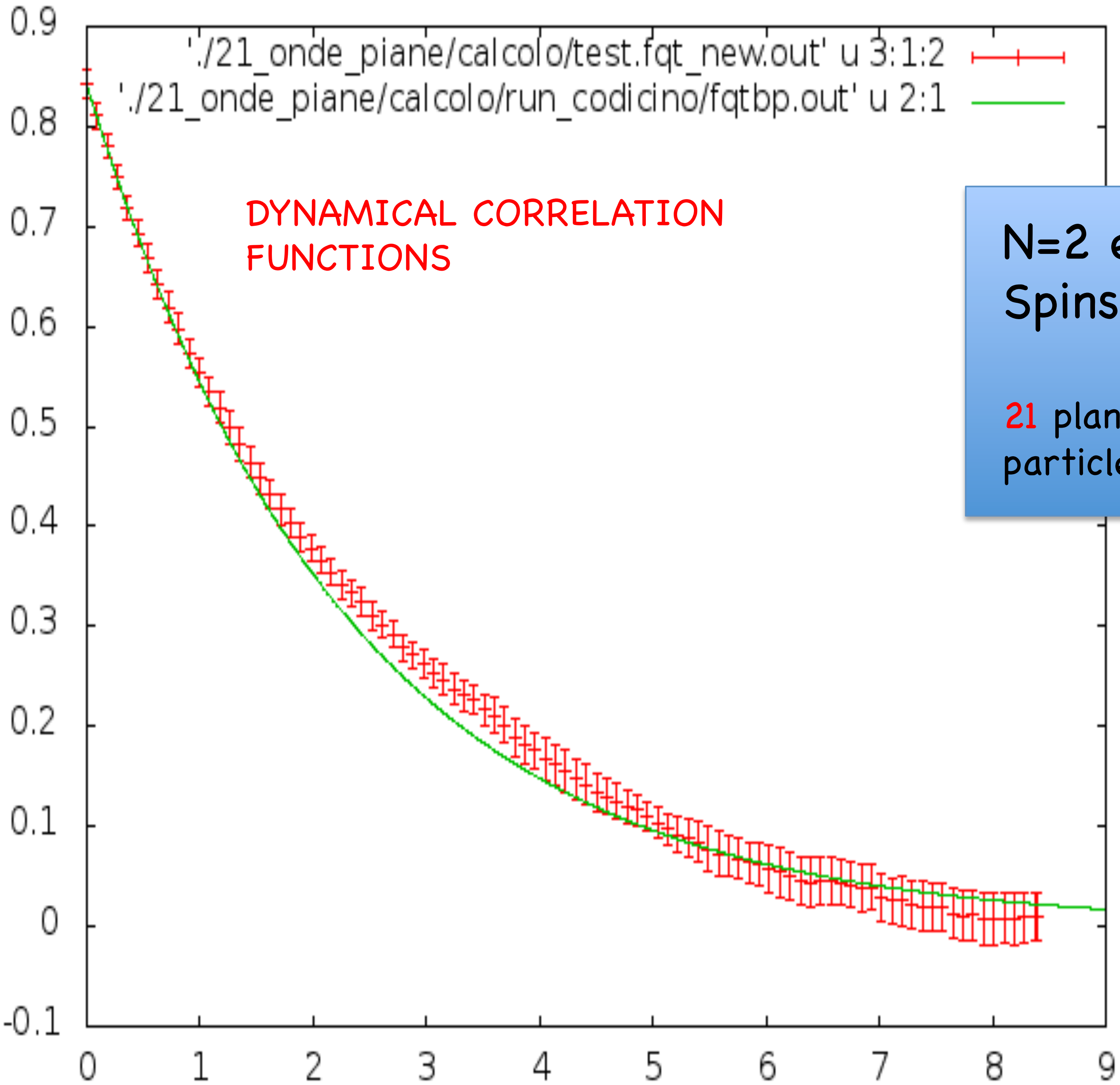
N=2 electrons, rs=2

Spins ↑,↓

49 plane waves as one particle basis

$qa_0 = 1.2533$

$F(q,\tau)$

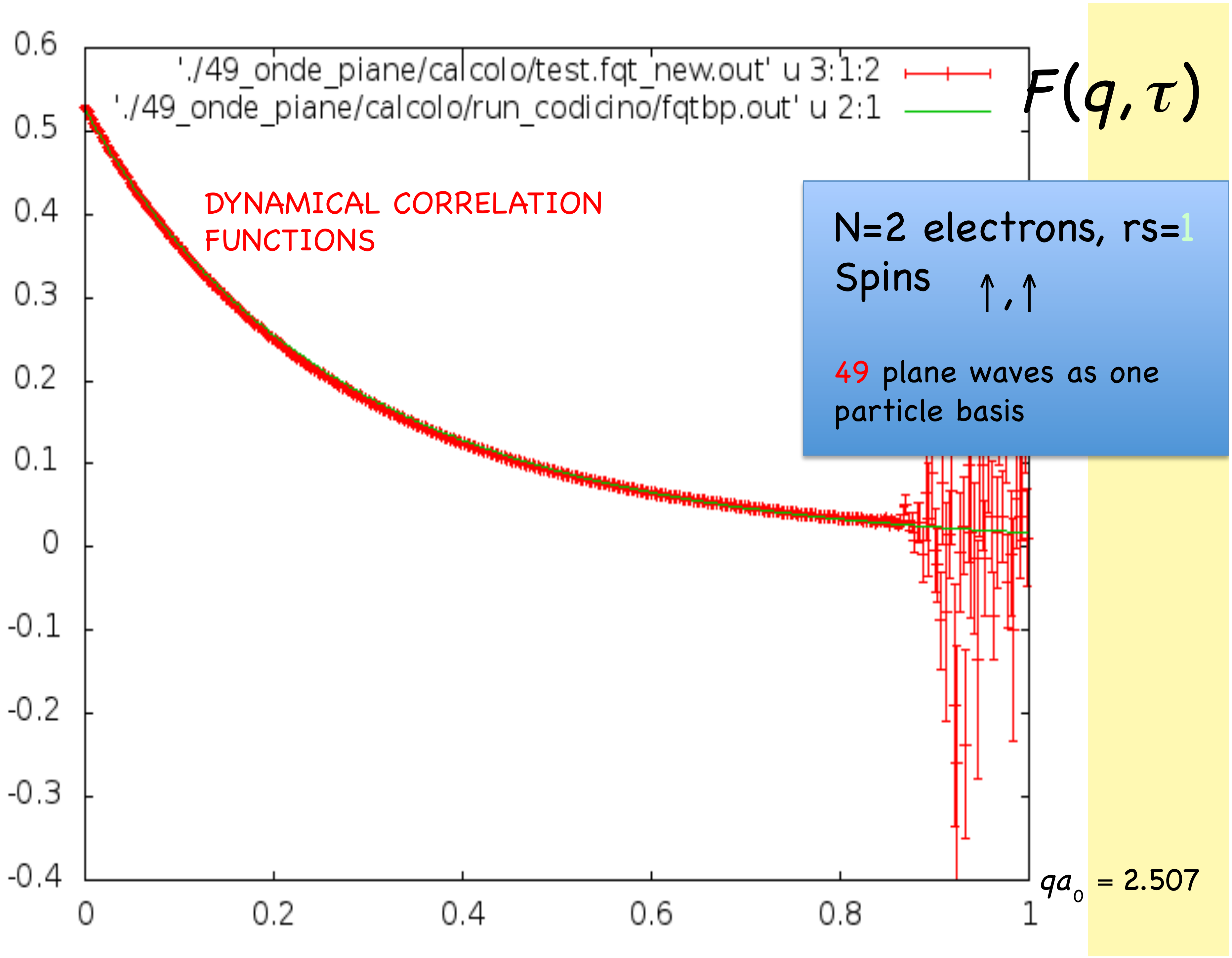


N=2 electrons, rs=3

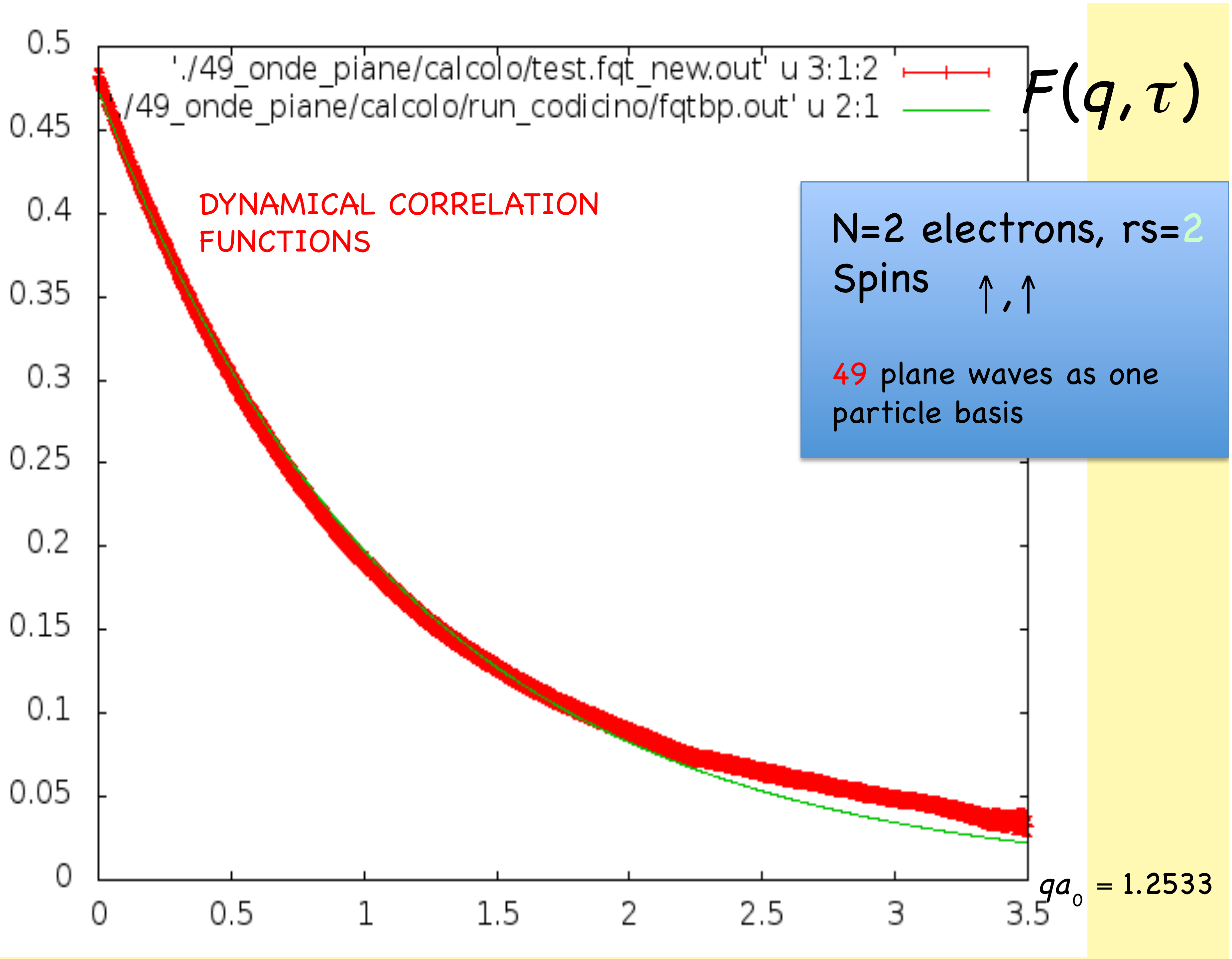
Spins ↑,↓

21 plane waves as one particle basis

$qa_0 = 0.8355$



'./49_onde_piane/calcolo/test.fqt_new.out' u 3:1:2
'./49_onde_piane/calcolo/run_codicino/fqtbp.out' u 2:1
DYNAMICAL CORRELATION
FUNCTIONS
$F(q,\tau)$
N=2 electrons, rs=1
Spins ↑,↑
49 plane waves as one particle basis
qa_0 = 2.507
0.6
0.5
0.4
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
-0.4
0
0.2
0.4
0.6
0.8
1

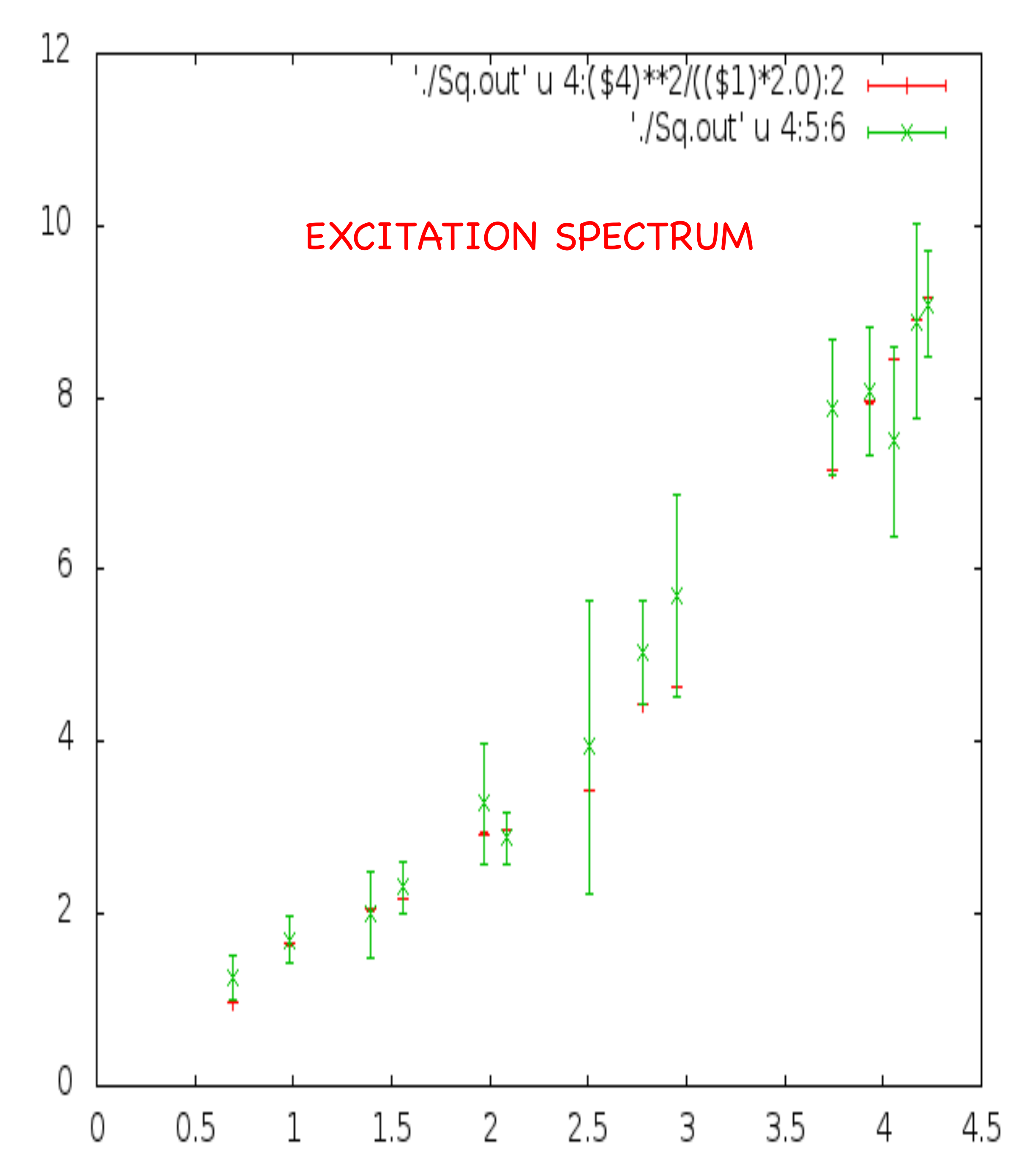


'./49_onde_piane/calcolo/test.fqt_new.out' u 3:1:2
'./49_onde_piane/calcolo/run_codicino/fqtbp.out' u 2:1
$F(q,\tau)$
DYNAMICAL CORRELATION
FUNCTIONS
N=2 electrons, rs=2
Spins ↑,↑
49 plane waves as one particle basis
qa_0 = 1.2533
0.5
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
0
0.5
1
1.5
2
2.5
3
3.5

The algorithm at work ...

A test case .... The 2D Jellium model

N = 26 electrons, rs = 1

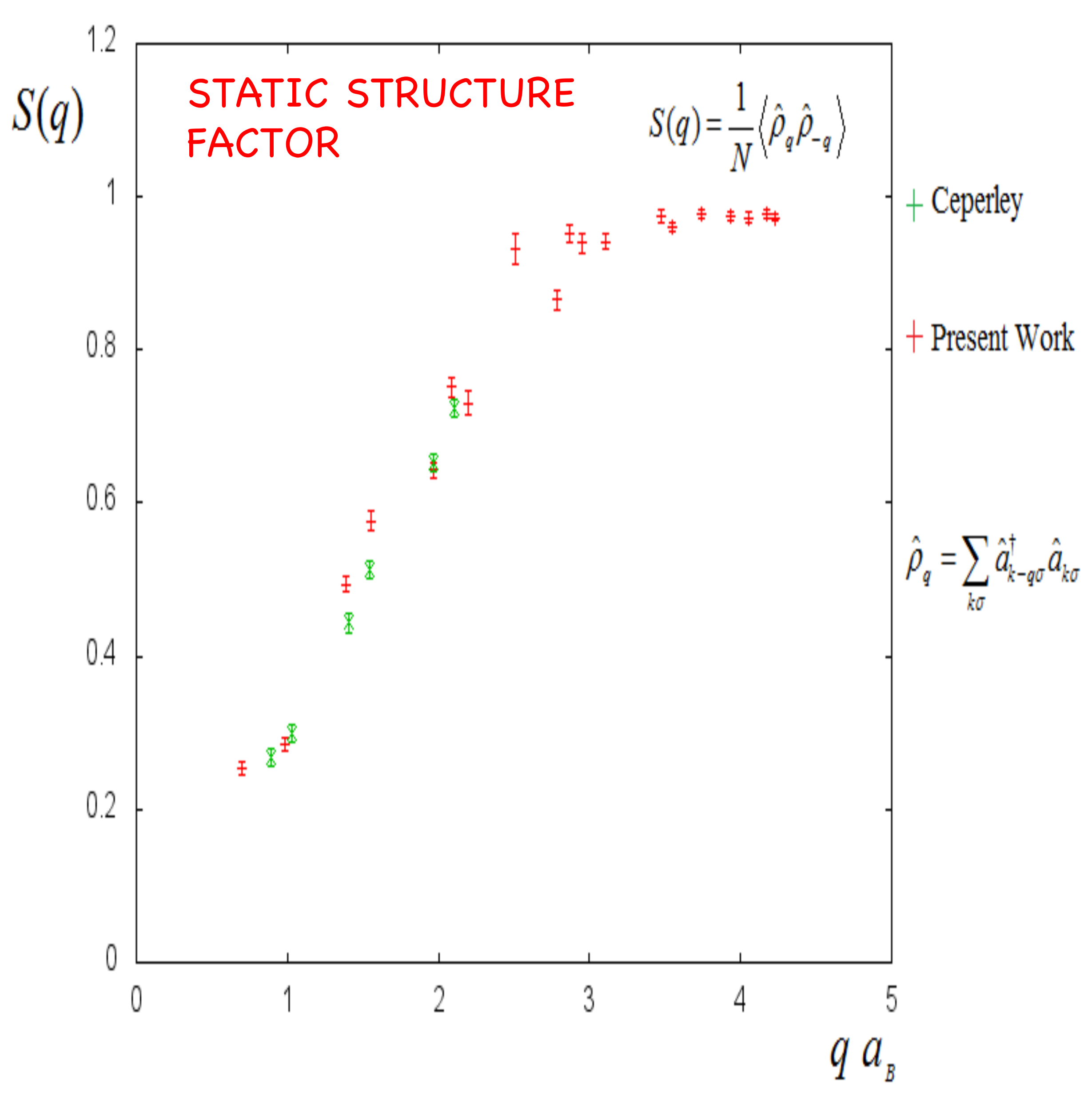


$\omega(q)$

N=26 electrons, rs=1
paramagnetic

213 plane waves as one particle basis

S(q)

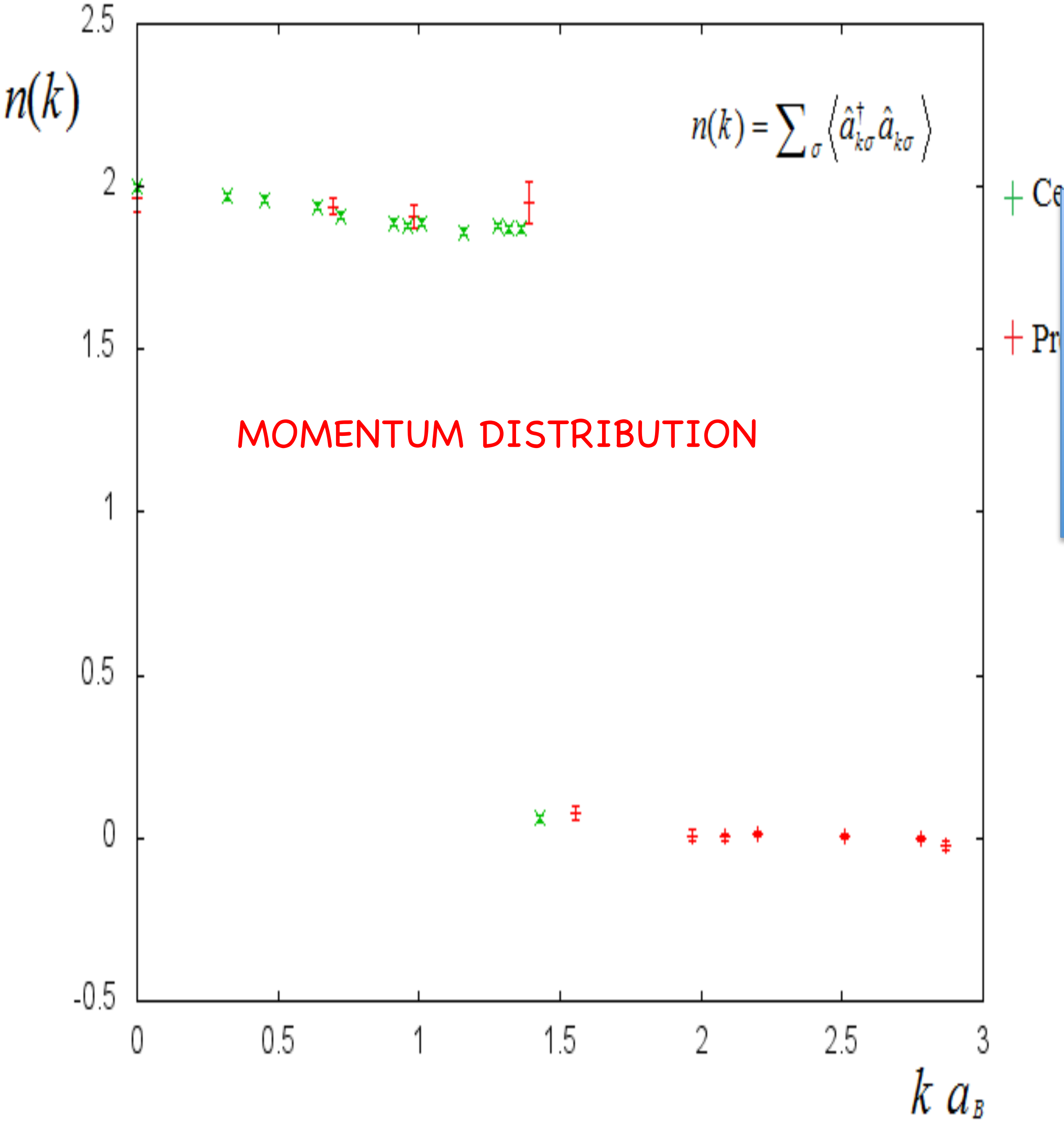


N=26 electrons, rs=1
paramagnetic

213 plane waves as one particle basis

B. Tanatar and D. M. Ceperley
PRB 39, 5005 (1989).

$n(k)$

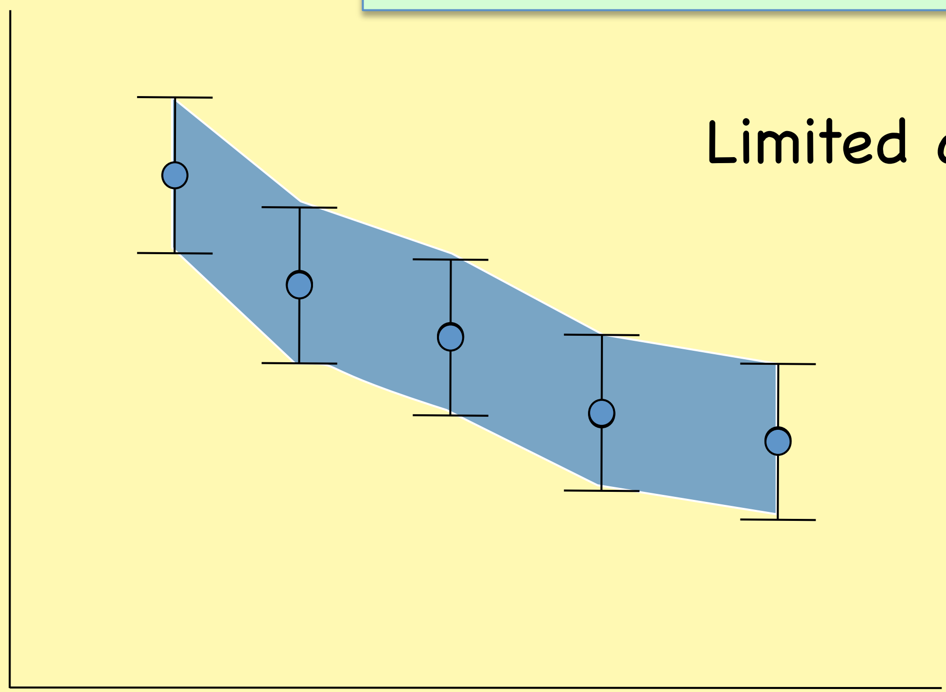


N=26 electrons, rs=1
paramagnetic

213 plane waves as one particle basis

B. Tanatar and D. M. Ceperley
PRB 39, 5005 (1989).

$$f(\tau) = \int_0^{+\infty} d\omega \exp(-\tau\omega)\, s(\omega)$$



Limited and noisy data for f:

$f_1,\dots,f_L$

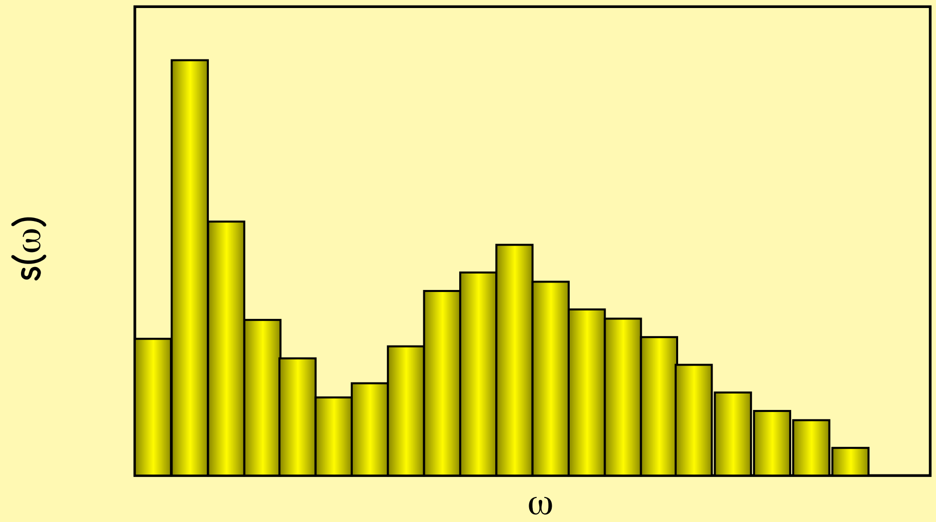
GENETIC
INVERSION
via FALSIFICATION
of THEORIES

How much information can we extract about s?

$$s(\omega) = \sum_{i=1}^{N_\omega} \frac{s_i}{M\,\Delta\omega}\,\underbrace{\chi_{[\omega_i,\omega_{i+1}]}}_{\text{characteristic function}}(\omega)$$

$$s_i \in \{0, 1, 2, \cdots\}$$

$$\int_0^{+\infty} d\omega\, s(\omega) = \frac{1}{M}\sum_{i=1}^{N_\omega} s_i = 1$$



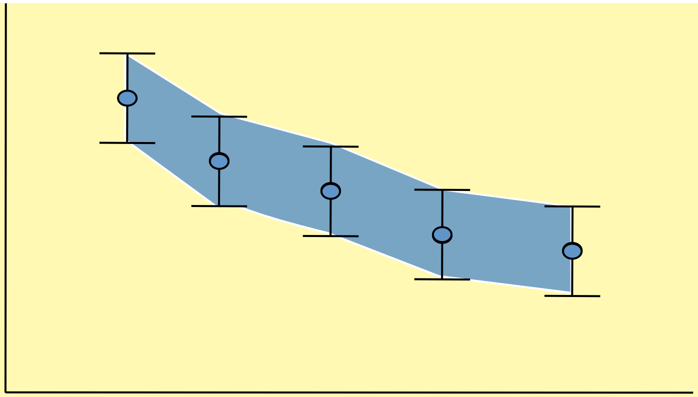
SPACE OF MODELS

Sometimes some a priori knowledge is available … e.g.

$$s(\omega) \geq 0, \qquad \int_0^{+\infty} d\omega\, s(\omega) = 1,$$

$$\int_0^{+\infty} d\omega\, \omega^n\, s(\omega) = c_n$$

GENETIC
INVERSION
via FALSIFICATION
of THEORIES



HOW GOOD IS A MODEL?

GENETIC
INVERSION
via FALSIFICATION
of THEORIES

the "fitness" of one particular $s(\omega)$ should be based on he noisy 'measured' set $\{f_l\}$.
Any set $\{f_l^*\}$
compatible with $\{f_l\}$ provides equivalent information to build a "fitness" function:

$$\varphi = -\alpha \sum_l \left[f_l^* - \int_0^{+\infty} d\omega\, e^{-\omega\tau_l} s(\omega) \right]^2 - \sum_n \gamma_n \left[c_n^* - \int_0^{+\infty} d\omega\, \omega^n s(\omega) \right]^2$$

adjustable parameters to make the two contributions of the same order of magnitude

For each "realization" f* .....

GENETIC DYNAMICS

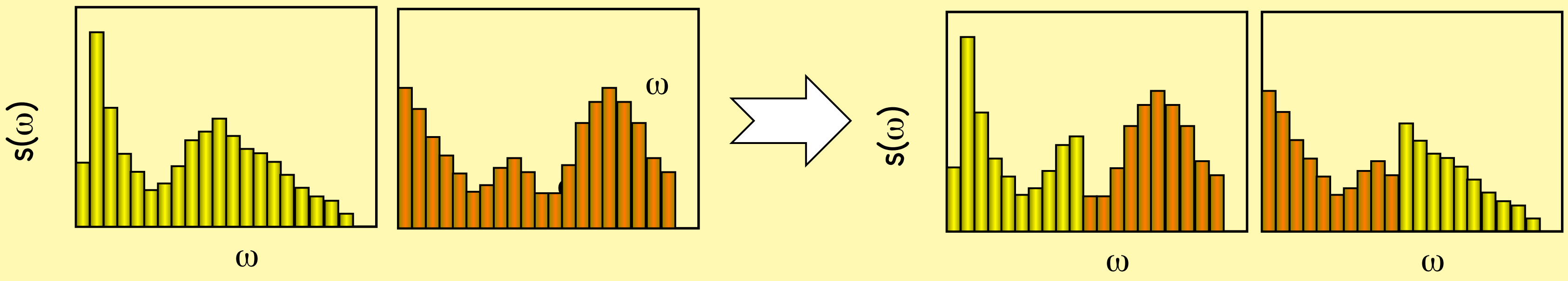
initial population: we construct a random collection of N>>1 models $s(\omega)$

generation: we replace the population with a new one in order to reach high fitness values.

We use biological like processes:

- selection: couples of individuals are selected for reproduction with a probability proportional to the fitness.
- crossover: a fixed amount of spectral weight, left in the original intervals, is exchanged between two selected $s(\omega)$
- mutation: shift of a fraction of spectral weight between two intervals

GENETIC INVERSION via FALSIFICATION of THEORIES



... at the end we average over the "realizations" f*

PHYSICAL REVIEW B **82**, 174510 (2010)

Ab initio low-energy dynamics of superfluid and solid ^{4}He

E. Vitali, M. Rossi, L. Reatto, and D. E. Galli
Dipartimento di Fisica, Università degli Studi di Milano, via Celoria 16, 20133 Milano, Italy

(Received 3 March 2010; revised manuscript received 28 September 2010; published 15 November 2010)

We have extracted information about real time dynamics of ^{4}He systems from noisy imaginary-time correlation functions $f(\tau)$ computed via quantum Monte Carlo (QMC): production and falsification of model spectral functions $s(\omega)$ are obtained via a survival-to-compatibility with $f(\tau)$ evolutionary process, based on genetic algorithms. Statistical uncertainty in $f(\tau)$ is promoted to be an asset via a sampling of equivalent $f(\tau)$ within the noise, which give rise to independent evolutionary processes. In the case of pure superfluid ^{4}He we have recovered from exact QMC simulations sharp quasiparticle excitations with spectral functions displaying also the multiphonon branch. As further applications, we have studied the impuriton branch of one ^{3}He atom in liquid ^{4}He and the vacancy-wave excitations in hcp solid ^{4}He finding an unexpected rotonlike feature.

DOI: 10.1103/PhysRevB.82.174510 PACS number(s): 67.25.dt, 02.30.Zz, 67.60.G–, 67.80.dj

GENETIC INVERSION via FALSIFICATION of THEORIES

I. INTRODUCTION

ıe development of *ab initio* theoretical descriptions of ɔw-energy dynamical behavior of quantum interacting ɛls is naturally a very important issue in a huge variety ysical studies, ranging from statistical physics to quanfield theory. In the realm of condensed-matter physics, equires to start from the Hamiltonian operator $\hat{H}$ of a -body system and to investigate dynamical properties ıe study of *spectral functions,*

$$s(\omega)=\int_{-\infty}^{+\infty}\frac{dt}{2\pi}e^{i\omega t}\langle e^{i\hat{H}t}\hat{A}e^{-i\hat{H}t}\hat{B}\rangle, \quad (1)$$

tual measurements on an ex in a QMC simulation it is st *observations*

$$\mathcal{F}\equiv\{f_0$$

which are estimations of in tions

$$f(\tau)=\langle e^{\hat{H}\tau}\hat{A}e^{-\hat{H}\tau}\hat{B}\rangle$$

in correspondence with a (unavoidably) finite numb imaginary-time values $\{0,\delta\tau,2\delta\tau,\ldots,l\delta\tau\}$, $\delta\tau$ bein time step of the QMC algorithm employed. In general

AB INITIO LOW-ENERGY DYNAMICS OF…

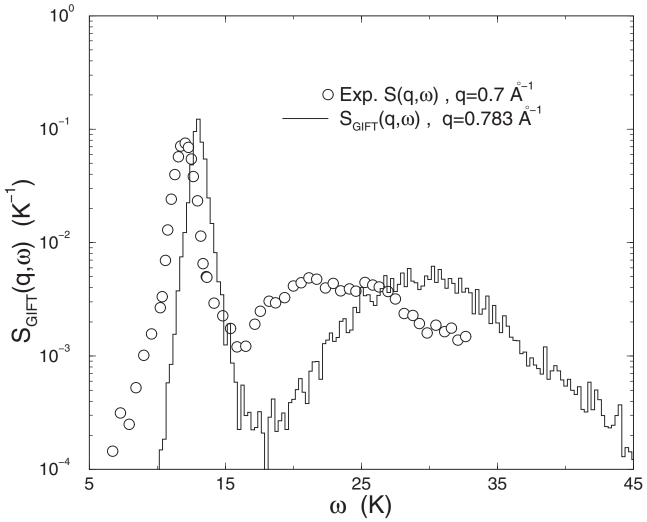
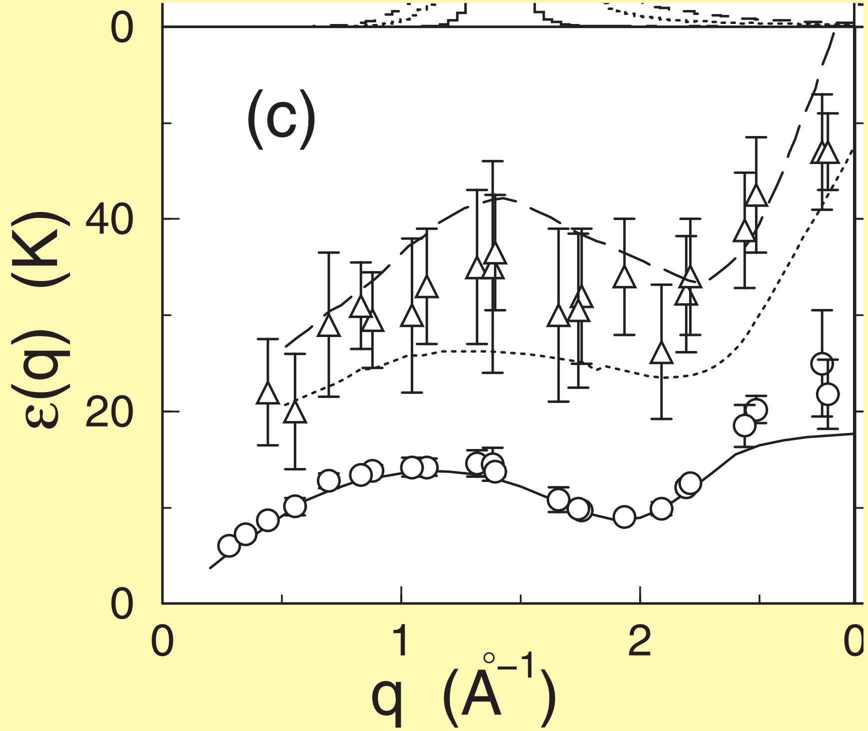


FIG. 1. (Line) $S_{\mathrm{GIFT}}(q,\omega)$ for $q=0.783$ Å^{-1} and $\rho=0.0218$ Å^{-3}; (open circles) observed (Ref. 24) dynamic structure factor $S(q,\omega)$ in liquid ^{4}He for $q=0.7$ Å^{-1} at saturated vapor pressure (SVP) and $T=1.3$ K. Notice the logarithmic scale. Notice also the difference between the wave vector of $S_{\mathrm{GIFT}}(q,\omega)$ and the one of the experimental available (Ref. 24) dynamic structure factor; the experimental single particle peak position is known to increase by about 0.8 K in moving from $q=0.7$ Å^{-1} to $q=0.783$ Å^{-1}.



Liquid ^{4}He at equilibrium density

GENETIC
INVERSION
via **F**ALSIFICATION
of **T**HEORIES

PHYSICAL REVIEW B **82**, 174510 (2010)

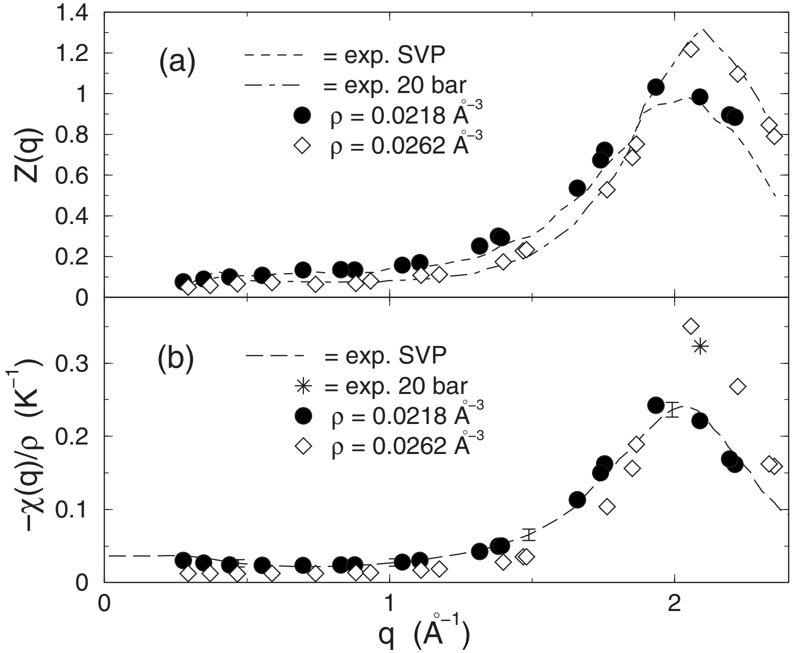


FIG. 5. (a) GIFT strength of the quasiparticle peak $Z(q)$ as function of q at two densities and experimental data (Ref. 27). (b) GIFT Static density response function $\chi(q)$ at two densities and experimental data (Refs. 25 and 28) Error bars of theoretical results are smaller than the symbol size.

Liquid ^{4}He: density response function and strength of the quasi-particle peak

GENETIC
INVERSION
via **F**ALSIFICATION
of **T**HEORIES

OTHER APPLICATIONS

Excitation spectrum in two-dimensional superfluid ^{4}He

F. Arrigoni, E. Vitali, D. E. Galli, and L. Reatto

Dipartimento di Fisica, Università degli Studi di Milano, via Celoria 16, 20133 Milano, Italy

(Dated: May 20, 2013)

In this work we perform an *ab-initio* study of an ideal two-dimensional sample of ^{4}He atoms, a model for ^{4}He films adsorbed on several kinds of substrates. Starting from a realistic hamiltonian we face the microscopic study of the excitation phonon-roton spectrum of the system at zero temperature. Our approach relies on Path

to evaluate ex-

e, and this gives

ning information

q,ω). The actual

orm in ill-posed

tion of Theories

] 17 May 2013

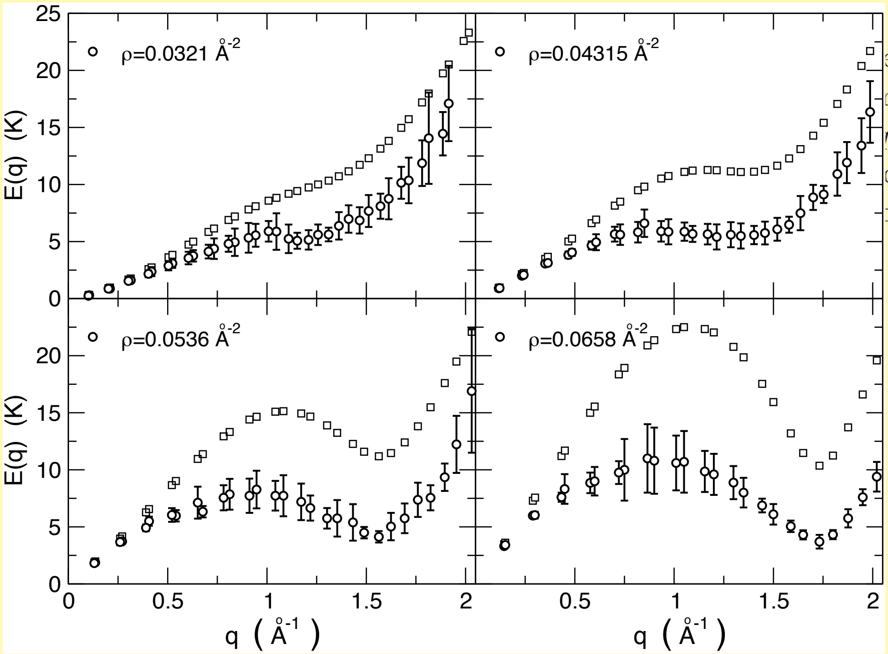


Figure 5: (circles) Excitation spectrum form GIFT reconstructions of SPIGS evaluations of imaginary time correlation functions in the liquid phase, together with Feynman spectrum (squares), at four densities as shown in the legends.

GENETIC
INVERSION
via **F**ALSIFICATION
of **T**HEORIES

OTHER APPLICATIONS: FERMIONIC EXCITED STATES

PHYSICAL REVIEW B **87**, 144506 (2013)

Dynamic structure factor for ^{3}He in two dimensions

M. Nava,[1] D. E. Galli,[1,*] S. Moroni,[2] and E. Vitali[1]

[1]*Dipartimento di Fisica, Università degli Studi di Milano, via Celoria 16, 20133 Milano, Italy*

[2]*IOM-CNR DEMOCRITOS National Simulation Center and SISSA, via Bonomea 265, 34136 Trieste, Italy*

(Received 7 February 2013; revised manuscript received 11 March 2013; published 12 April 2013)

Recent neutron scattering experiments on ^{3}He films have observed a zero-sound mode, its dispersion relation, and its merging with—and possibly emerging from—the particle-hole continuum [H. Godfrin *et al.*, Nature **483**, 576 (2012)]. Here we address the study of excitations in the system via quantum Monte Carlo methods: we suggest a practical scheme to calculate imaginary time correlation functions for moderate-size fermionic systems. Combined with an efficient method for analytic continuation, this scheme affords an extremely convincing description of the experimental findings.

DOI: 10.1103/PhysRevB.87.144506 PACS number(s): 67.30.ej, 67.30.em, 02.70.Ss

PHYSICAL REVIEW B **87**, 144506 (2013)

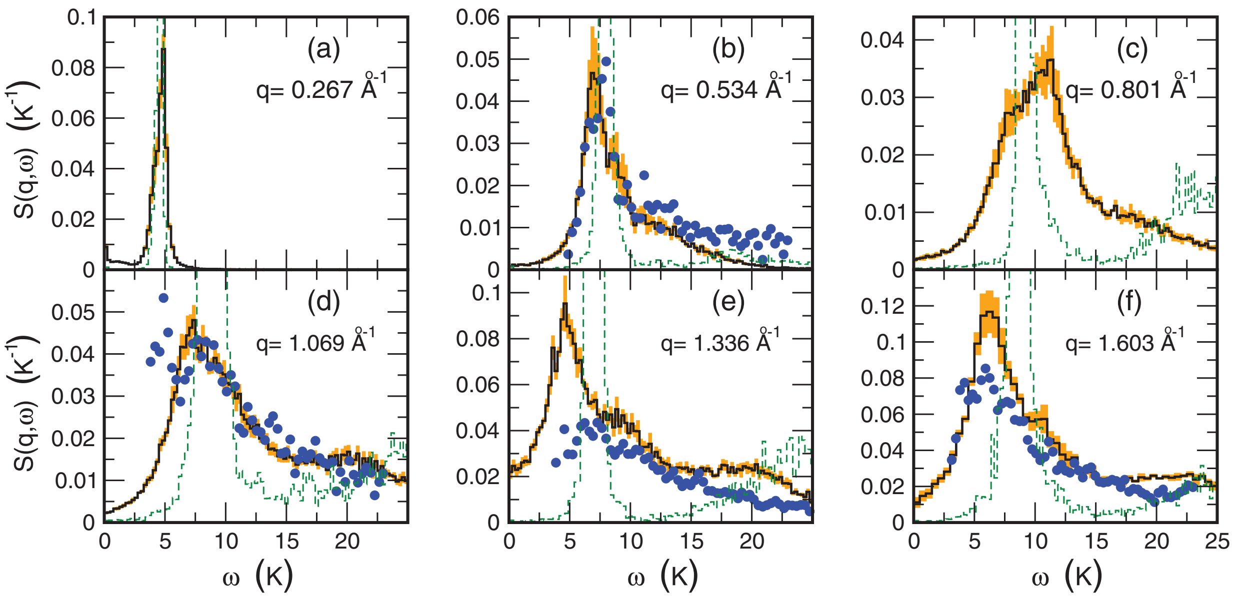


FIG. 2. (Color online) From left to right the coherent dynamic structure factor, obtained as an average of several independently extracted $S_1(q,\omega)$, for increasing wave vectors at $\rho = 0.047$ Å^{-2}. Orange shading represents statistical uncertainties and filled (blue) circles are the available experimental data from Refs. 3 and 4. The wave vectors shown are those accessible from our simulation; the experimental wave vectors are $q = 0.55$ Å^{-1} (b), $q = 1.15$ Å^{-1} (d), $q = 1.25$ Å^{-1} (e), and $q = 1.65$ Å^{-1} (f). We have used different scales in the panels to make the comparison with experimental data more easily visible. The dashed (green) line shows the dynamic structure factor of a fictitious system of bosons of mass m_3. The bosonic peaks in the roton region are five to nine times higher than the fermionic ones.

PHYSICAL REVIEW B **87**, 144506 (2013)

Dynamic structure factor for ^{3}He in two dimensions

M. Nava,[1] D. E. Galli,[1,*] S. Moroni,[2] and E. Vitali[1]
[1]*Dipartimento di Fisica, Università degli Studi di Milano, via Celoria 16, 20133 Milano, Italy*
[2]*IOM-CNR DEMOCRITOS National Simulation Center and SISSA, via Bonomea 265, 34136 Trieste, Italy*
(Received 7 February 2013; revised manuscript received 11 March 2013; published 12 April 2013)

Recent neutron scattering experiments on ^{3}He films have observed a zero-sound mode, its dispersion relation, and its merging with—and possibly emerging from—the particle-hole continuum [H. Godfrin *et al.*, Nature **483**, 576 (2012)]. Here we address the study of excitations in the system via quantum Monte Carlo methods: we suggest a practical scheme to calculate imaginary time correlation functions for moderate-size fermionic systems. Combined with an efficient method for analytic continuation, this scheme affords an extremely convincing description of the experimental findings.

DOI: 10.1103/PhysRevB.87.144506 PACS number(s): 67.30.ej, 67.30.em, 02.70.Ss

OTHER APPLICATIONS: FERMIONIC EXCITED STATES

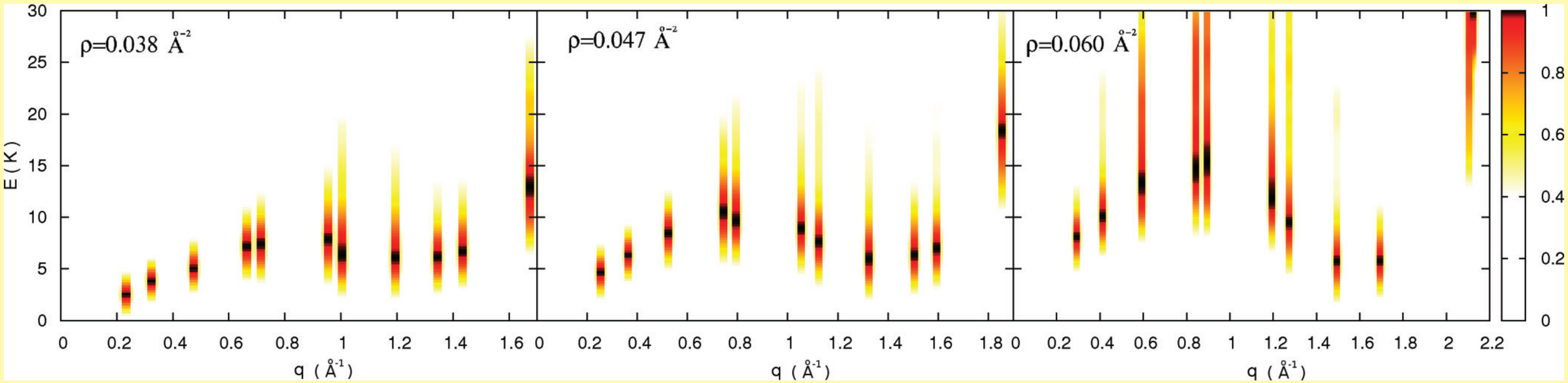


FIG. 3. (Color online) Color map of normalized $S_2(q,\omega)$ for many wave vectors q. For better visibility, each $S_2(q,\omega)$ for different q has been normalized in order to have their maximum value equal to 1. The vertical scale has been shifted by a quantity $E_0^B - E_0^F$, so that the excitation energies are measured with respect to the fermionic ground state.