University of Milan

Faculty of Mathematical, Physical and Natural Sciences

PhD School

Dynamical Properties of Many Fermion Systems

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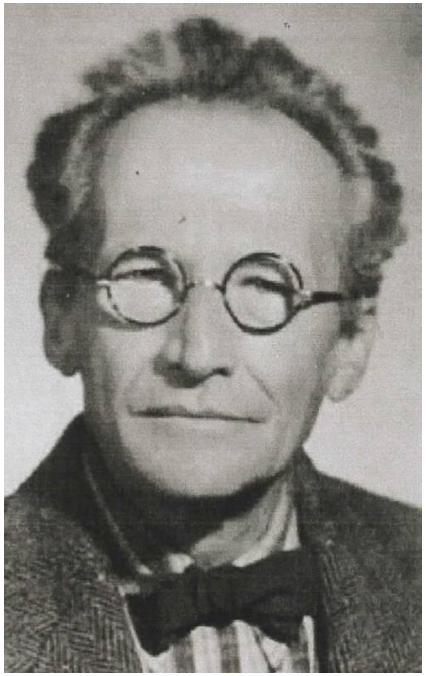
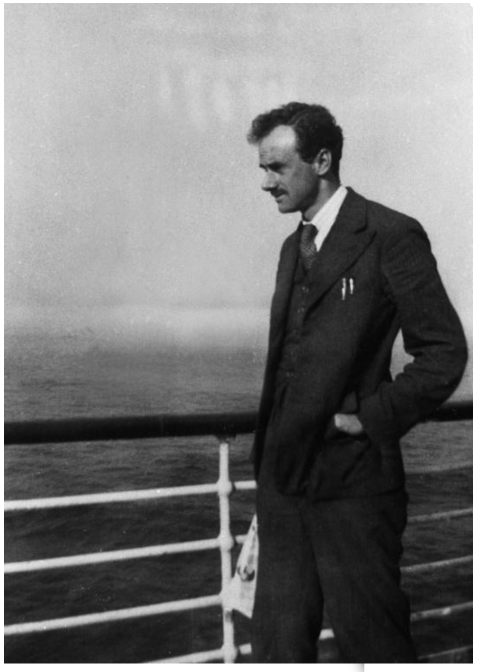
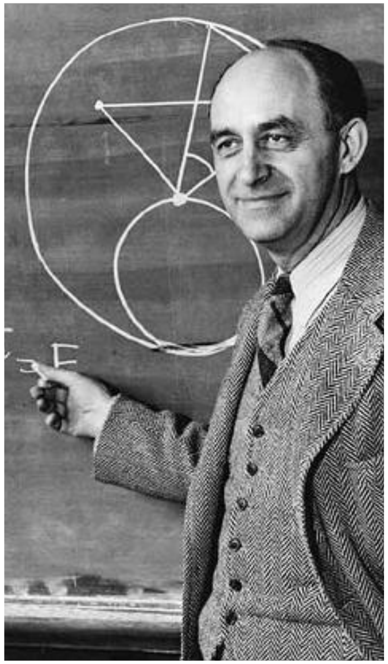
The N-body Problem in Quantum Mechanics

$$\left[-\frac{\hbar^2}{2m}\sum_{i=1}^{n}\Delta_i + \frac{1}{2}\sum_{i\neq j=1}^{n}\phi(x_i, x_j)\right]\Psi(x_1 \ldots x_n) = \varepsilon\,\Psi(x_1 \ldots x_n)$$

$$\Psi(x_1 \ldots x_i \ldots x_j \ldots x_n) = -\,\Psi(x_1 \ldots x_j \ldots x_i \ldots x_n)$$

The N-body Problem in Quantum Mechanics

$$\left[-\frac{\hbar^2}{2m} \sum_{i=1}^{n} \Delta_i + \frac{1}{2} \sum_{i \neq j=1}^{n} \phi(x_i, x_j) \right] \Psi(x_1 \ldots x_n) = \varepsilon \, \Psi(x_1 \ldots x_n)$$

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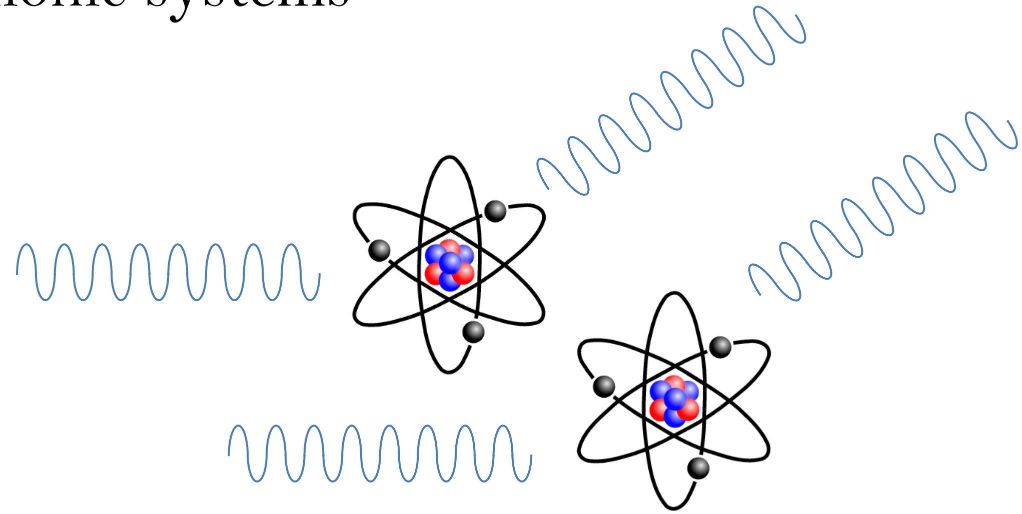
↓

static (ground state) and dynamic (excited state) properties of fermionic systems



The N-body Problem in Quantum Mechanics

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↓

static (ground state) and dynamic (excited state) properties
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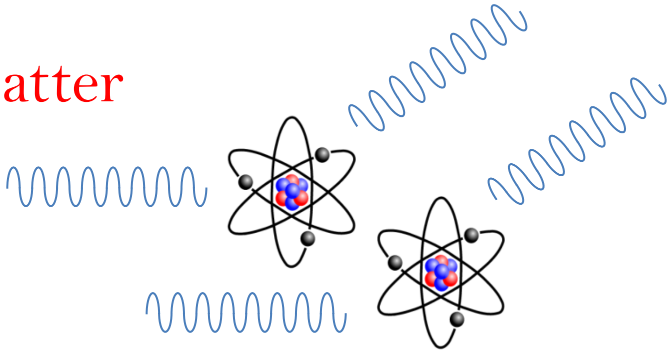
↓

understanding ordinary matter



A Really Difficult Problem

- analytic solution ➡ not for interacting systems

  - perturbative methods
  - approximate methods
  - modeling strategies

- simulations

computer experiments ➡ unknown quantities

⬇

averages of random variables

$$\sum_{i=1}^{n} \frac{X_i}{n} \approx E[X]$$

Imaginary Time Schrodinger Equation

$$i\hbar\,\partial_t \left|\Psi(t)\right\rangle = \hat{H}\left|\Psi(t)\right\rangle \qquad -\hbar\,\partial_\tau \left|\Psi(\tau)\right\rangle = \hat{H}\left|\Psi(\tau)\right\rangle$$

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Projection onto the Ground State (T=0 systems)

$$e^{-\tau\hat{H}}\left|\Psi(\tau)\right\rangle \xrightarrow[\tau\to\infty]{} \left|\Psi_0\right\rangle$$

static properties

Imaginary Time Correlation Functions + Analytic Continuation

$$F_{\hat{A}}(\tau) = \left\langle\Psi_0\right|\hat{A}^{+}e^{-\tau\hat{H}}\hat{A}\left|\Psi_0\right\rangle$$

dynamic properties

The Sign Problem

$$i\hbar\, \partial_t \left|\Psi(t)\right\rangle = \hat{H} \left|\Psi(t)\right\rangle \qquad -\hbar\, \partial_\tau \left|\Psi(\tau)\right\rangle = \hat{H} \left|\Psi(\tau)\right\rangle$$

↓

Path Integral → Stochastic Process in Coordinate Space

↓

Bose exact preditions

Fermi sign problem

$$antisymmetric\ \Psi \qquad \frac{mean}{variance} \propto e^{-\gamma N}$$

Auxiliary Fields Quantum Monte Carlo

$$e^{-\delta\tau\hat{H}} = \int d\eta \, g(\eta) \, \hat{G}(\eta) + O(\delta\tau)$$

↑ Interaction

↑ Fluctuating External Potential

S. Zhang, H. Krakauer et al: Comp. Phys. Comm. 169, 394 (2005)

M. Feldbacher and F. F. Assaad: Phys. Rev. B 63, 073105 (2001)

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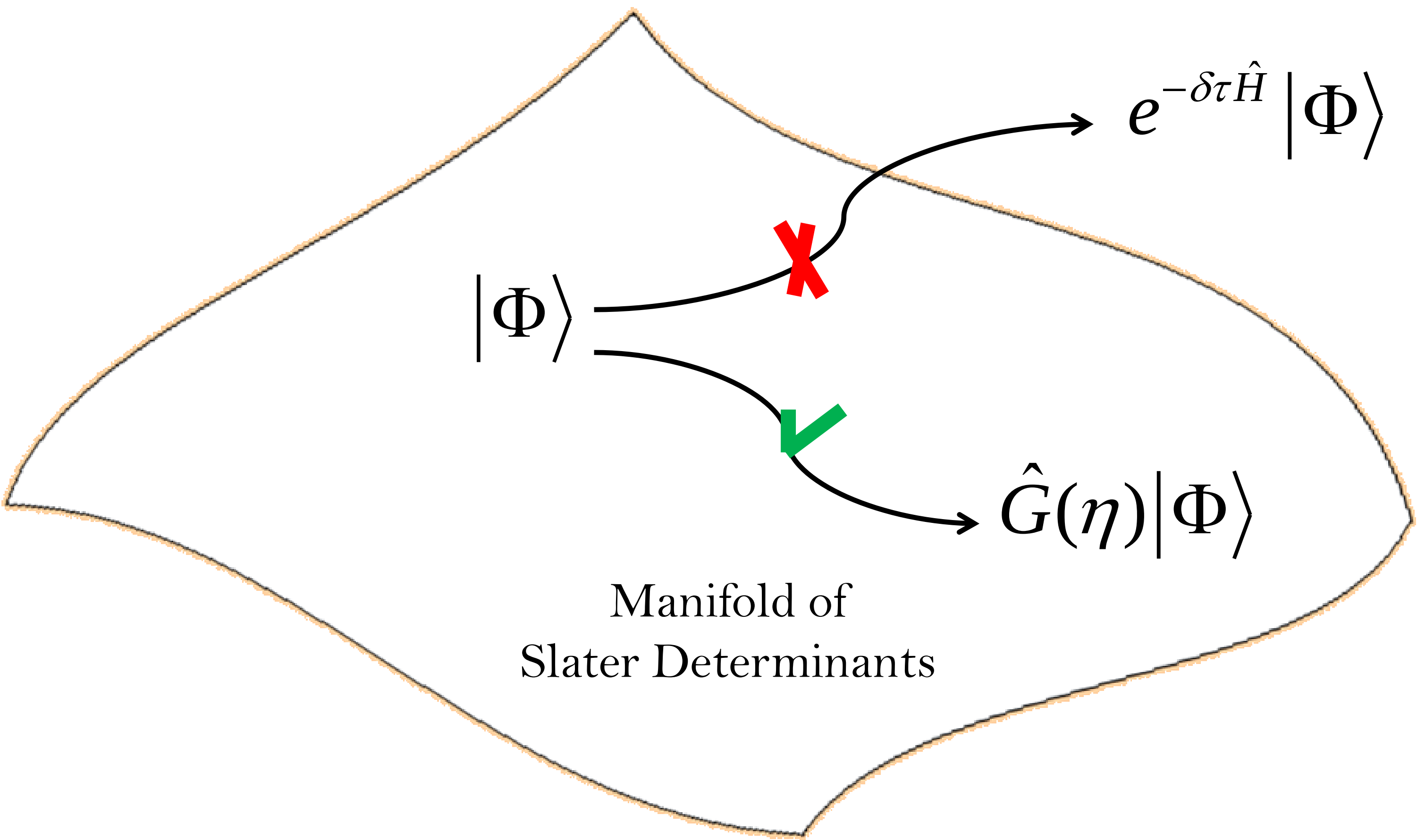
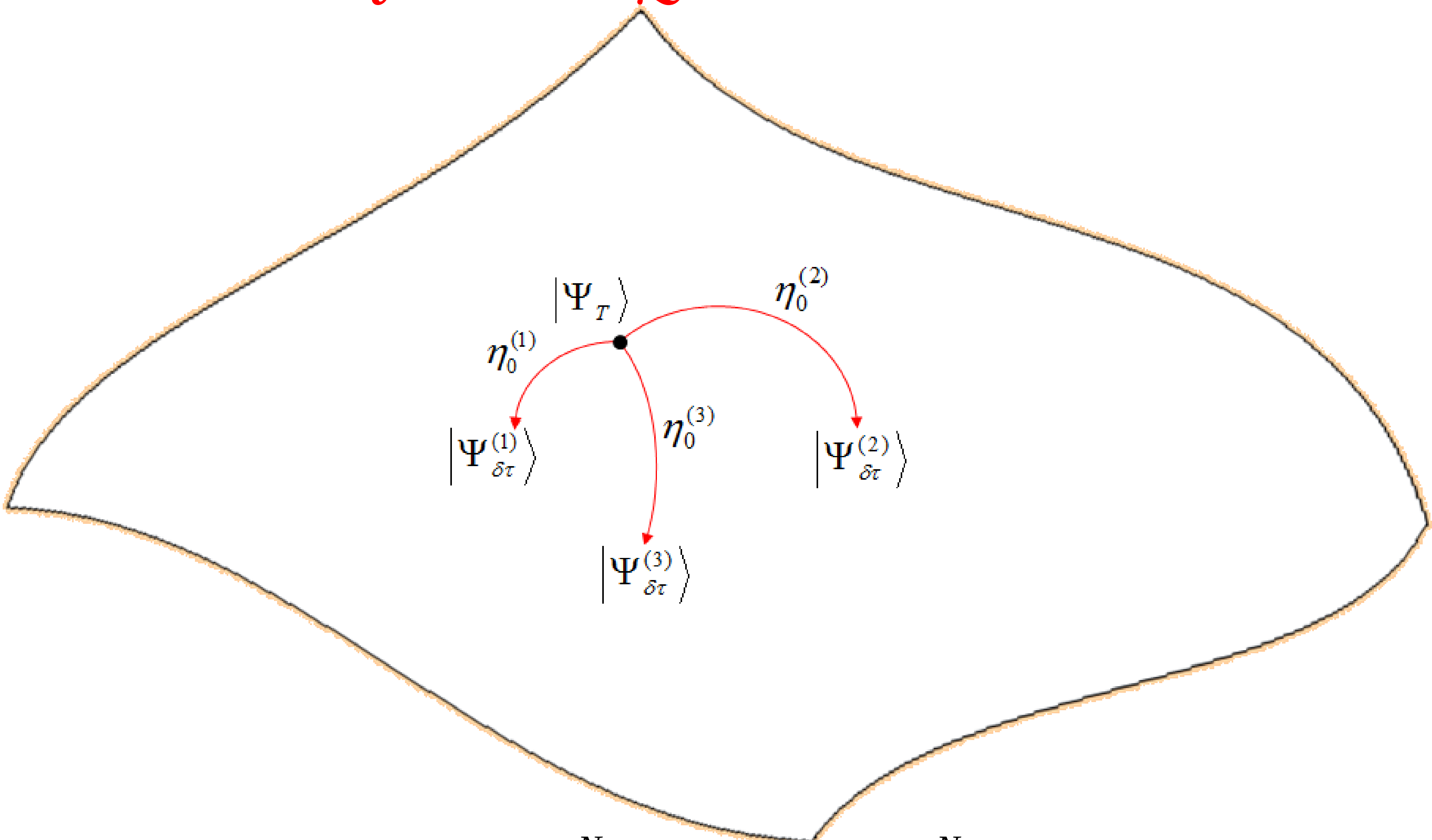
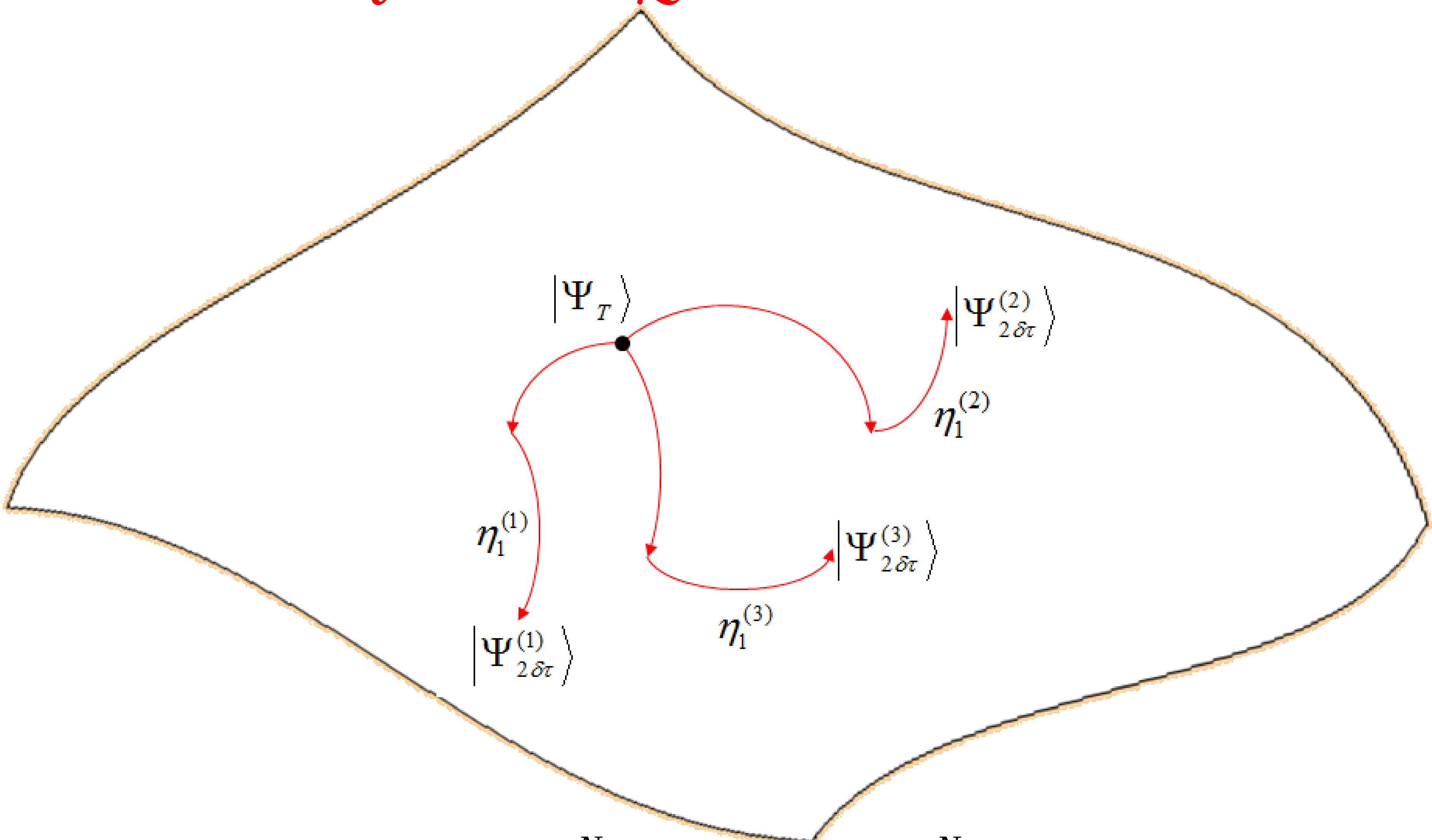


Auxiliary Fields Quantum Monte Carlo



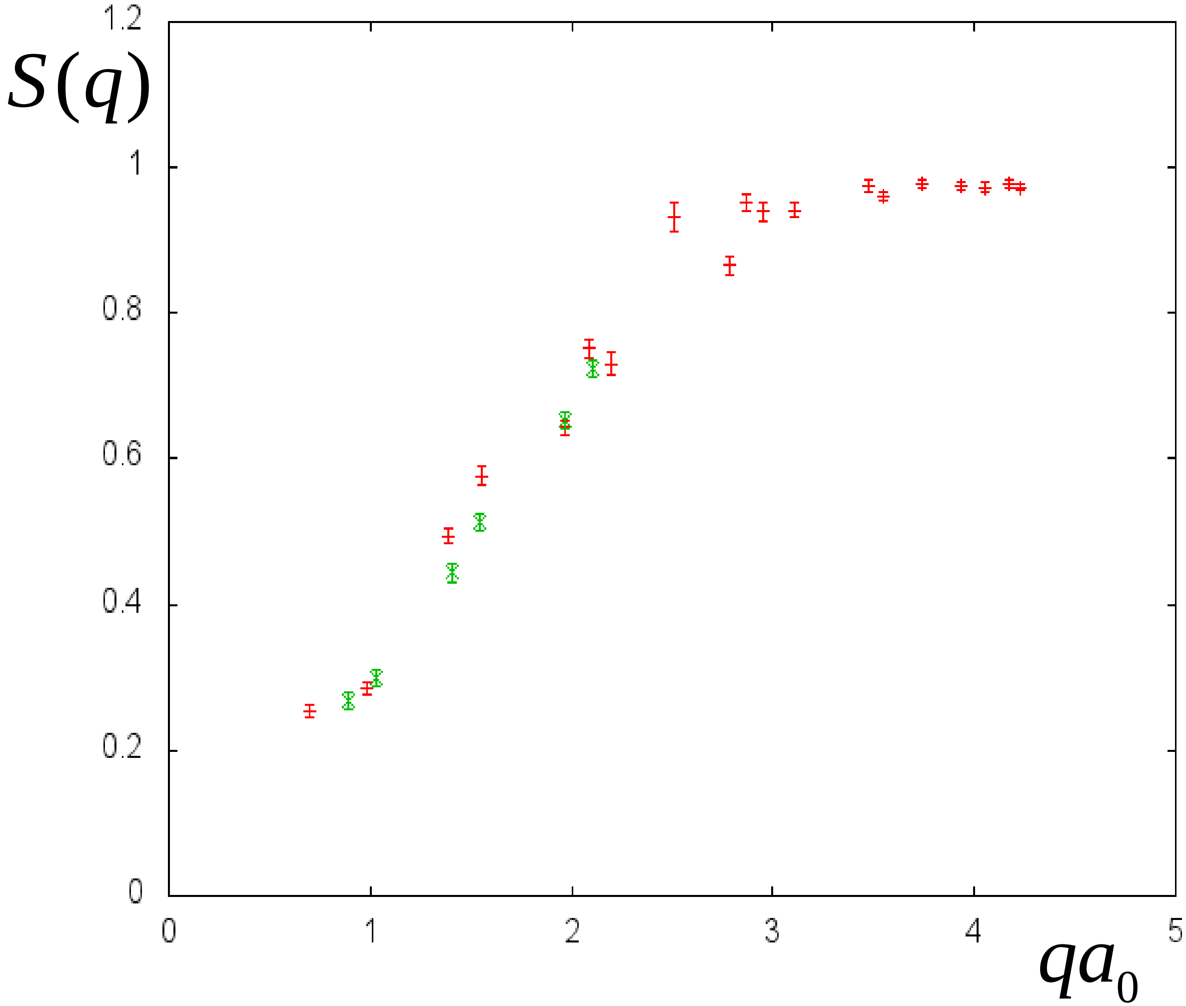
$$e^{-\delta\tau\hat{H}}\left|\Psi_T\right\rangle = \frac{1}{N_w}\sum_{i=1}^{N_w}\left|\Psi_{\delta\tau}^{(i)}\right\rangle = \frac{1}{N_w}\sum_{i=1}^{N_w}\hat{G}(\eta_0^{(i)})\left|\Psi_T\right\rangle$$

Auxiliary Fields Quantum Monte Carlo



$$e^{-\delta\tau\hat{H}}\left|\Psi_T\right\rangle = \frac{1}{N_w}\sum_{i=1}^{N_w}\left|\Psi^{(i)}_{\delta\tau}\right\rangle = \frac{1}{N_w}\sum_{i=1}^{N_w}\hat{G}(\eta^{(i)}_0)\left|\Psi_T\right\rangle$$

Application to the 2D Electron Gas



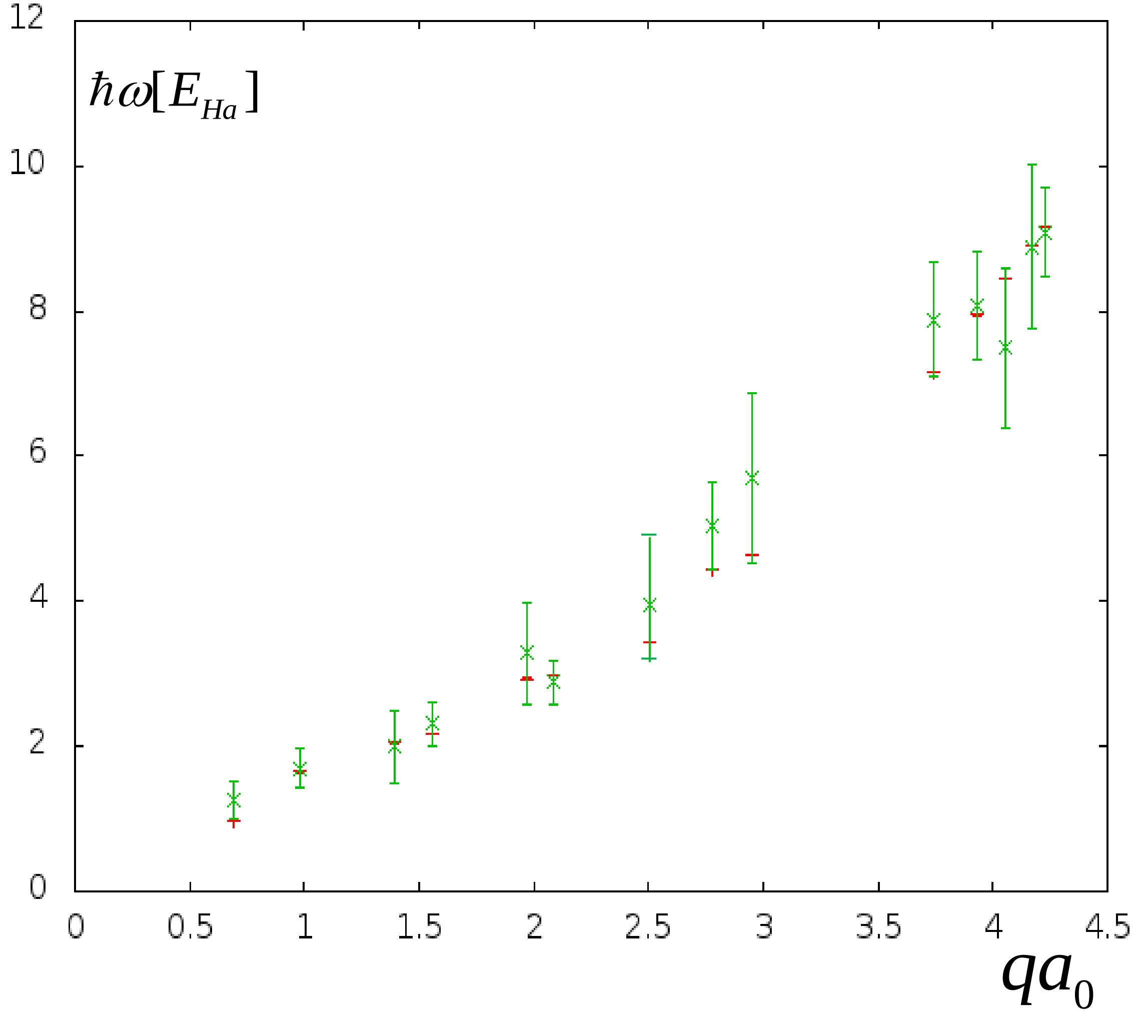
STATIC STRUCTURE FACTOR

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

N=26 electrons, rs=1
spin-unpolarized

213 plane waves

Application to the 2D Electron Gas



PLASMON SPECTRUM

$$\hbar\omega_{Feynman} = \frac{\hbar^2 q^2}{2m\,S(q)}$$

N=26 electrons, rs=1
spin-unpolarized

213 plane waves

Further Development

(1) Further tests and applications (Jellium, 1D systems, quantum dots)

(2) high-level code optimization (in collaboration with CINECA)

(3) access to supercomputing facilities (Fermi Supercomputer, CINECA)

Thank You

for your Attention!