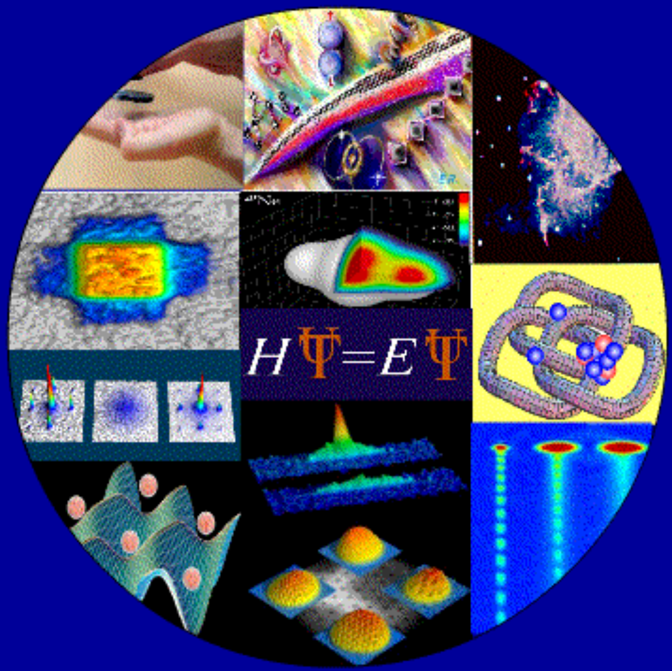
Stochastic wavefunction approach to Hubbard-like models



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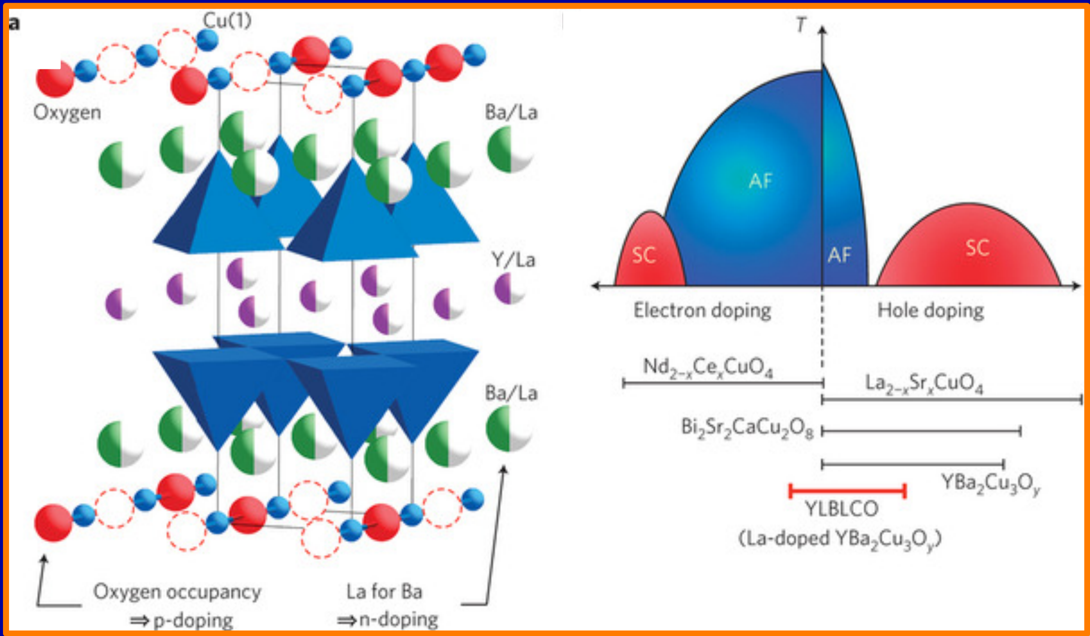
Hubbard-like models

$$\hat{H} = \sum_{\vec{k}} \varepsilon_{\vec{k}} \hat{\tilde{n}}_{\vec{k}} + U \sum_{\vec{r}} \hat{n}_{\vec{r}\uparrow} \hat{n}_{\vec{r}\downarrow} + \sum_{\vec{r}} V_{\vec{r}} \hat{n}_{\vec{r}}$$

Kinetic energy	On-site interactions	External potential

Cuprates oxides



2D repulsive Hubbard Hamiltonian with next-neighbour hopping

$$\varepsilon_{\vec{k}} = -2t\left[\cos(k_x) + \cos(k_y)\right]$$

$$U > 0, V_{\vec{r}} = 0$$

Low energy effective model of electrons in CuO_2 planes

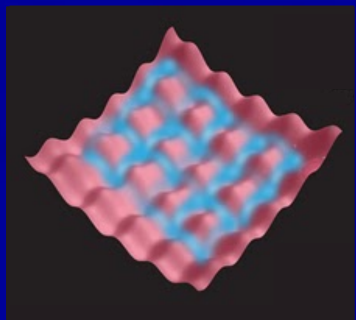
Hubbard-like models

$$\hat{H} = \sum_{\vec{k}} \varepsilon_{\vec{k}} \hat{\tilde{n}}_{\vec{k}} + U \sum_{\vec{r}} \hat{n}_{\vec{r}\uparrow} \hat{n}_{\vec{r}\downarrow} + \sum_{\vec{r}} V_{\vec{r}} \hat{n}_{\vec{r}}$$

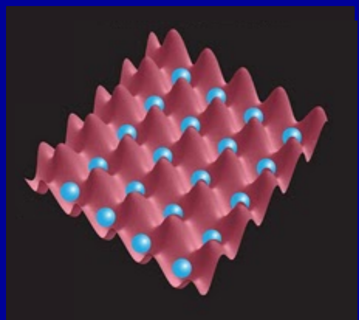
Fermionic atoms loaded in optical lattices

Delocalized states

$U = 0$

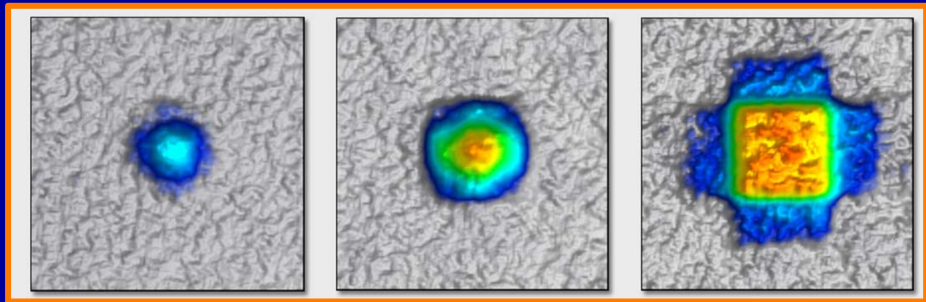


$U >> t$

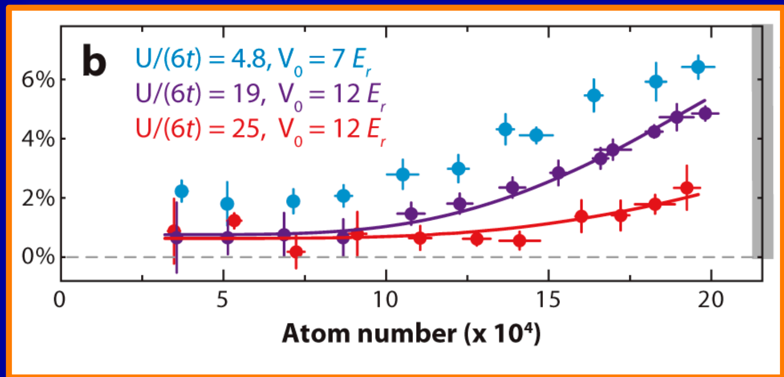


Mott insulator
One atom per site

M. Köhl & al, Phys. Rev. Lett. (2005)



R. Jördens & al, Nature (2008)

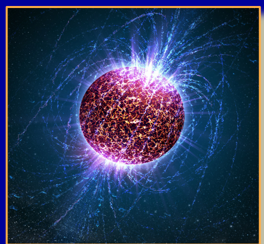


Hubbard-like models

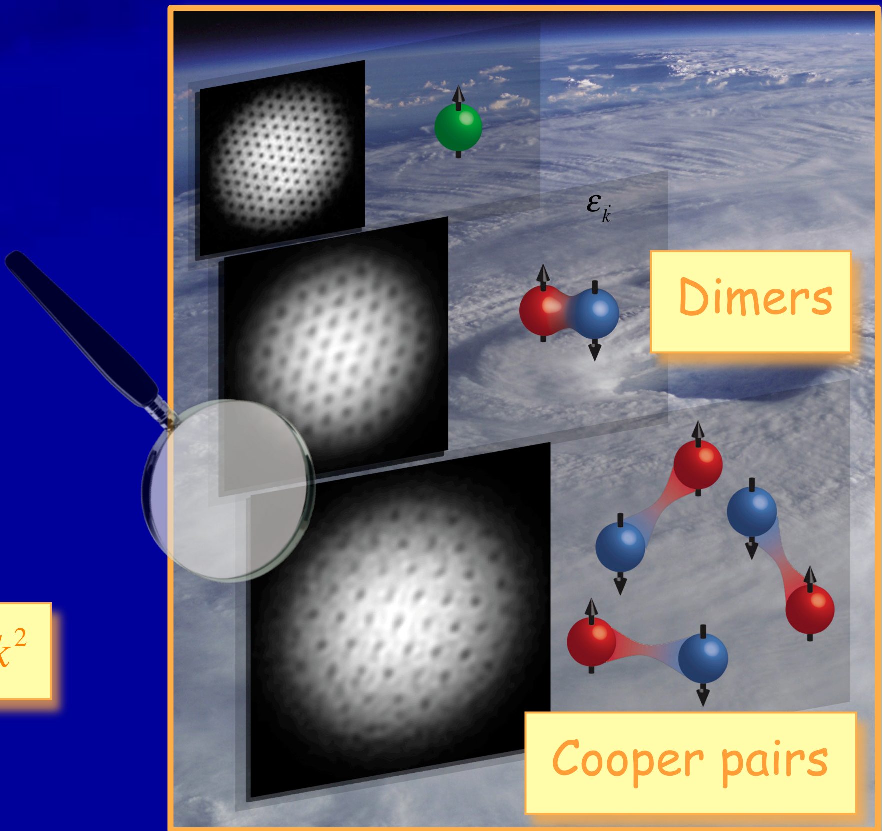
$$\hat{H} = \sum_{\vec{k}} \varepsilon_{\vec{k}} \hat{\tilde{n}}_{\vec{k}} + U \sum_{\vec{r}} \hat{n}_{\vec{r}\uparrow} \hat{n}_{\vec{r}\downarrow} + \sum_{\vec{r}} V_{\vec{r}} \hat{n}_{\vec{r}}$$

BEC-BCS crossover

Unitary limit



$$\sigma = \sigma_{\max} = 4\pi / k^2$$



The on-site coupling constant has to be tuned to reproduce low-energy scattering in continous space

Dilute limit

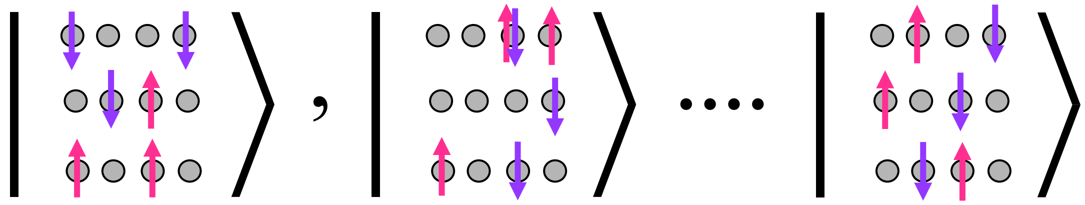
The stochastic wavefunction approach : an alternative to exact diagonalization

- Hamiltonian eigenproblem : exponential complexity $\dim(\mathcal{E}) \propto 4^{N_{\vec{r}}}$

$$\hat{D} = \sum_{\Phi^{(a)},\Phi^{(b)}} D_{\Phi^{(a)},\Phi^{(b)}} \left|\Phi^{(a)}\right\rangle\left\langle\Phi^{(b)}\right|$$

Orthonormal basis of independent particle states

$$\left.\begin{aligned} \left|\Phi^{(a)}\right\rangle &= \hat{c}^{+}_{\phi_1^{(a)}}\hat{c}^{+}_{\phi_2^{(a)}}\cdots\hat{c}^{+}_{\phi_N^{(a)}}\left|\ \right\rangle \\ \left|\Phi^{(b)}\right\rangle &= \hat{c}^{+}_{\phi_1^{(b)}}\hat{c}^{+}_{\phi_2^{(b)}}\cdots\hat{c}^{+}_{\phi_N^{(b)}}\left|\ \right\rangle \end{aligned}\right\} \in$$



- Other solution : use of unrestricted single-particle wavefunctions

Positive reals

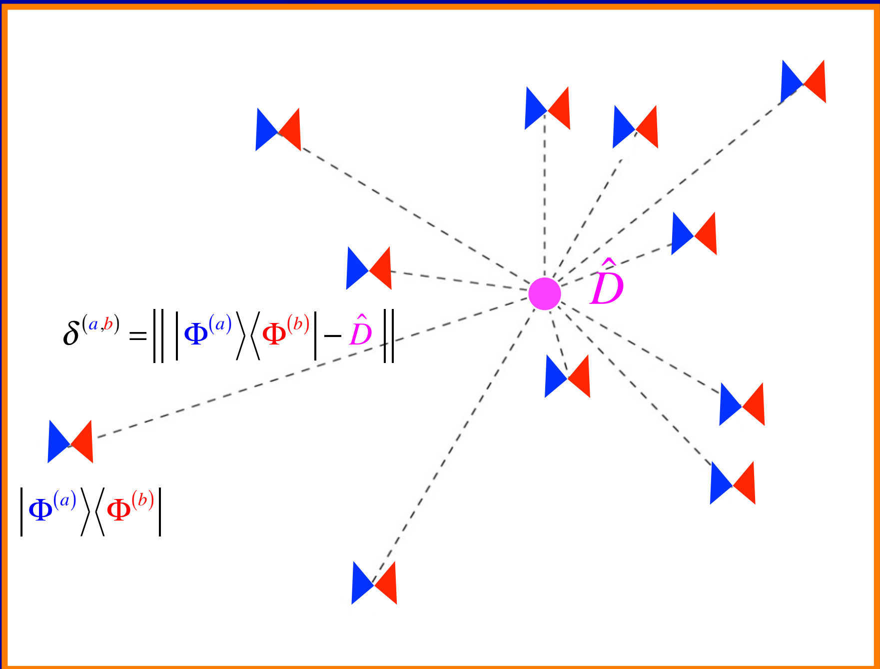
$$\hat{D} = \int_{\Phi^{(a)},\Phi^{(b)}} \mathscr{D}\Phi^{(a)}\,\mathscr{D}\Phi^{(b)}\, P\left(\Phi^{(a)},\Phi^{(b)}\right)\,\Omega^{(a,b)}\left|\Phi^{(a)}\right\rangle\left\langle\Phi^{(b)}\right|$$

$$= \mathbb{E}\left[\Omega^{(a,b)}\left|\Phi^{(a)}\right\rangle\left\langle\Phi^{(b)}\right|\right]$$

Weighted average of stochastic dyadics

The stochastic wavefunction approach : validity

The tail of the distribution for the norm of dyadics controls the statistical spread in the simulation



$$\mathbb{E}_\Omega\left[\delta^{(a,b)}\right] \geq \mathbb{E}_\Omega\left[\left\|\Phi^{(a)}\right\| \left\|\Phi^{(b)}\right\|\right] - \sqrt{Tr\left(\hat{D}^+\hat{D}\right)}$$

$$\mathbb{E}_\Omega\left[\left(\delta^{(a,b)}\right)^2\right] = \mathbb{E}_\Omega\left[\left\|\Phi^{(a)}\right\|^2\left\|\Phi^{(b)}\right\|^2\right] - Tr\left(\hat{D}^+\hat{D}\right)$$

Long tail scaling as $1/\left(\left\|\Phi^{(a)}\right\| \left\|\Phi^{(b)}\right\|\right)^{1+\mu}$ implies an infinite mean error for $\mu \leq 1$ and an infinite variance on the error if $\mu \leq 2$. Monte-Carlo sampling requires $\mu > 2$:

$$\left\langle\hat{O}\right\rangle = Tr\left(\hat{D}\hat{O}\right) = \mathbb{E}_\Omega\left[\left\langle\Phi^{(b)}\middle|\hat{O}\middle|\Phi^{(a)}\right\rangle\right]$$

$$\sigma_O^2 = \mathbb{E}_\Omega\left[\left\langle\Phi^{(b)}\middle|\hat{O}\middle|\Phi^{(a)}\right\rangle^2\right] - \left\langle\hat{O}\right\rangle^2$$

$$\leq \mathbb{E}_\Omega\left[\left\|\Phi^{(a)}\right\|^2\left\|\Phi^{(b)}\right\|^2\right] Tr\left(\hat{O}^2\right)$$

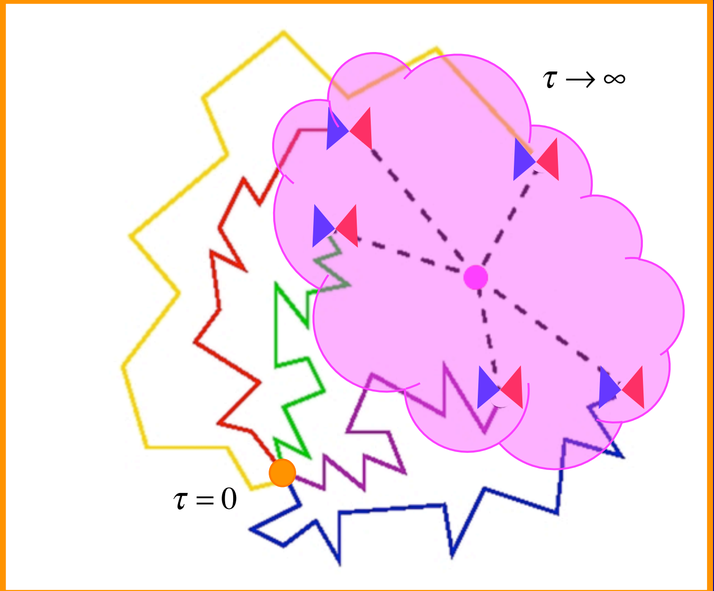
The stochastic wavefunction approach : Ground-state reconstruction

- Imaginary-time propagation method

$$\exp\left(-\tau\hat{H}/2\right)\left|\Phi_0^{(a)}\right\rangle\left\langle\Phi_0^{(b)}\right|\exp\left(-\tau\hat{H}/2\right)=\mathbb{E}\left[\Omega_\tau^{(a,b)}\left|\Phi_\tau^{(a)}\right\rangle\left\langle\Phi_\tau^{(b)}\right|\right]$$

$$\propto\left|\Psi_g\right\rangle \quad \text{as } \tau\to\infty$$

$$\Rightarrow\exp\left(-\tau E_g\right)\left\langle\Psi_g\middle|\Phi_0^{(a)}\right\rangle\left\langle\Phi_0^{(b)}\middle|\Psi_g\right\rangle\left|\Psi_g\right\rangle\left\langle\Psi_g\right|=\mathbb{E}\left[\Omega_\tau^{(a,b)}\left|\Phi_\tau^{(a)}\right\rangle\left\langle\Phi_\tau^{(b)}\right|\right]$$



$$\left\langle\hat{O}\right\rangle_{\Psi_g}\underset{\tau\to\infty}{=}\frac{\mathbb{E}\left[\Omega_\tau^{(a,b)}\left\langle\Phi_\tau^{(b)}\middle|\hat{O}\middle|\Phi_\tau^{(a)}\right\rangle\right]}{\mathbb{E}\left[\Omega_\tau^{(a,b)}\left\langle\Phi_\tau^{(b)}\middle|\Phi_\tau^{(a)}\right\rangle\right]}$$

Provided initial wavefunctions are not orthogonal to the ground state

The stochastic wavefunction approach : Brownian motion in imaginary-time

A toy model : two-sites Ising Hamiltonian $\hat{H}=\varepsilon\left(\hat{\sigma}_{1,z}+\hat{\sigma}_{2,z}\right)-J\ \hat{\sigma}_{1,z}\hat{\sigma}_{2,z}$

Imaginary-time dependent Schrödinger equation

$$\left(1-d\tau\hat{H}/2\right)\left|\Phi^{(a)}\right\rangle=\left|\phi_1^{(a)}\right\rangle\otimes\left|\phi_2^{(a)}\right\rangle -\frac{d\tau}{2}\left(\varepsilon\hat{\sigma}_z\left|\phi_1^{(a)}\right\rangle\right)\otimes\left|\phi_2^{(a)}\right\rangle-\frac{d\tau}{2}\left|\phi_1^{(a)}\right\rangle\otimes\left(\varepsilon\hat{\sigma}_z\left|\phi_2^{(a)}\right\rangle\right) +\frac{Jd\tau}{2}\left(\hat{\sigma}_z\left|\phi_1^{(a)}\right\rangle\right)\otimes\left(\hat{\sigma}_z\left|\phi_2^{(a)}\right\rangle\right)$$

Evolution of a non-interacting state

$$\left|\Phi^{(a)}+d\Phi^{(a)}\right\rangle=\left|\phi_1^{(a)}\right\rangle\otimes\left|\phi_2^{(a)}\right\rangle + \left|d\phi_1^{(a)}\right\rangle\otimes\left|\phi_2^{(a)}\right\rangle+\left|\phi_1^{(a)}\right\rangle\otimes\left|d\phi_2^{(a)}\right\rangle + \left|d\phi_1^{(a)}\right\rangle\otimes\left|d\phi_2^{(a)}\right\rangle$$

The exact dynamics can be recovered in average with single-particle Ito stochastic differential equations: $\left|d\phi_n^{(a)}\right\rangle=\left[\left(-\frac{d\tau}{2}\ \varepsilon+\sqrt{\frac{J}{2}}\,dW\right)\hat{\sigma}_z\ \right]\left|\phi_n^{(a)}\right\rangle$

Wiener increments over the step $d\tau$

$\mathbb{E}\left(dW\right)=0,\ dW^2=d\tau$

Fermion case –Hubbard model

$$\left|d\phi_n^{(a)}\right\rangle=\left[-\frac{d\tau}{2}\sum_{\vec{k}\sigma}\left|\vec{k}\sigma\right\rangle\varepsilon_{\vec{k}}\left\langle\vec{k}\sigma\right|+\sqrt{\frac{|U|}{2}}\sum_{\vec{r}\sigma}\left|\vec{r}\sigma\right\rangle\mathrm{sgn}(U)\,dW_{\vec{r}}^{(a)}\left\langle\vec{r}\sigma\right|\ \right]\left|\phi_n^{(a)}\right\rangle$$

Imaginary-time discretization → « Auxiliary-field /Determinantal QMC »

The stochastic meanfield scheme

The solution that minimises the growth of the error on the exact ground-state

O. Juillet, Ph. Chomaz, Phys. Rev. Lett. (2002)

- Non-linear Ito-stochastic differential equation with multiplicative noise

$$\left|d\phi_n^{(a)}\right\rangle = \left[-\frac{d\tau}{2} h_{HF}\left(\rho^{(a)}\right) + \left(1-\rho^{(a)}\right)\sqrt{\frac{|U|}{2}} \sum_{\vec{r}\sigma} |\vec{r}\sigma\rangle \operatorname{sgn}(U)\, dW_{\vec{r}}^{(a)} \langle \vec{r}\sigma| \right] \left|\phi_n^{(a)}\right\rangle$$

Hartree-Fock Hamiltonian

one-body density matrix of the Slater determinant

$$\rho^{(a)} = \sum_n \left|\phi_n^{(a)}\right\rangle \left(g^{-1}\right)_{nn'} \left\langle \phi_{n'}^{(a)}\right|$$

$$\left(g_{nn'} = \left\langle \phi_n^{(a)} \middle| \phi_{n'}^{(a)} \right\rangle\right)$$

- The distance between EACH realization and the exact solution is finite at any imaginary-time

$$\delta_\tau^{(ab)} \leq \left[1 + \exp\left(\frac{\tau N |U|}{2}\left(1 - \frac{1}{N_{\vec{r}}}\right)\right)\right] \exp\left(-\tau E_g\right)$$

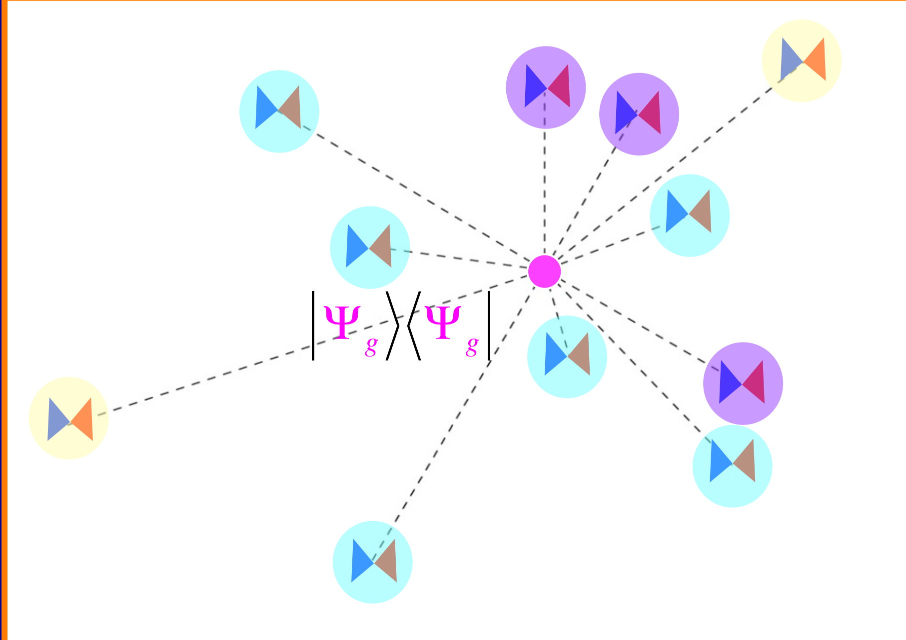
The stochastic wavefunction approach : Sign problem

Sign fluctuations in the overlap between walkers and the ground state strongly contaminate the sampling

$$\exp\left(-\Delta\tau E_g\right)\langle\Psi_g|\Phi^{(a)}_{\tau_o}\rangle\langle\Psi_g|\Phi^{(b)}_{\tau_o}\rangle\,|\Psi_g\rangle\langle\Psi_g| = \mathbb{E}\left[\Omega^{(a,b)}_{\tau_o+\Delta\tau}|\Phi^{(a)}_{\tau_o+\Delta\tau}\rangle\langle\Phi^{(b)}_{\tau_o+\Delta\tau}|\right],\quad \Delta\tau\to\infty$$

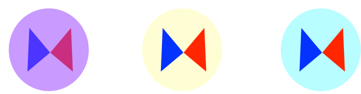
$$\Rightarrow \mathbb{E}\left[\Omega^{(a,b)}_{\tau_o+\Delta\tau}\langle\Phi^{(b)}_{\tau_o+\Delta\tau}|\Phi^{(a)}_{\tau_o+\Delta\tau}\rangle\right] > 0 \text{ as long as } \langle\Psi_g|\Phi^{(a)}_{\tau_o}\rangle\langle\Psi_g|\Phi^{(b)}_{\tau_o}\rangle > 0$$

⇒ Sign-problem in observables



$$\langle\hat{O}\rangle_{\Psi_g} \underset{\tau\to\infty}{=} \frac{\mathbb{E}\left[\Omega^{(a,b)}_{\tau}\langle\Phi^{(b)}_{\tau}|\hat{O}|\Phi^{(a)}_{\tau}\rangle\right]}{\mathbb{E}\left[\Omega^{(a,b)}_{\tau}\langle\Phi^{(b)}_{\tau}|\Phi^{(a)}_{\tau}\rangle\right]}$$

Balance between 3 contributions from previous populations :



$\langle\Psi_g|\Phi^{(a)}_{\tau_o}\rangle\langle\Psi_g|\Phi^{(b)}_{\tau_o}\rangle$ $-$ 0 $+$

The sign-free stochastic mean-field scheme

O. Juillet, New J. Phys (2007)

$$\exp\left(-\Delta\tau E_g\right)\left\langle \Psi_g \middle| \Phi_{\tau_o}^{(a)}\right\rangle \left\langle \Psi_g \middle| \Phi_{\tau_o}^{(b)}\right\rangle = \mathbb{E}\left[\Omega_{\tau_o+\Delta\tau}^{(a,b)} \left\langle \Phi_{\tau_o+\Delta\tau}^{(b)} \middle| \Phi_{\tau_o+\Delta\tau}^{(a)}\right\rangle\right], \quad \Delta\tau \to \infty$$

$$\left\langle \hat{O}\right\rangle_{\Psi_g} \underset{\tau\to\infty}{=} \frac{\mathbb{E}\left[\Omega_\tau^{(a,b)}\left\langle \Phi_\tau^{(b)} \middle| \hat{O} \middle| \Phi_\tau^{(a)}\right\rangle\right]}{\mathbb{E}\left[\Omega_\tau^{(a,b)}\left\langle \Phi_\tau^{(b)} \middle| \Phi_\tau^{(a)}\right\rangle\right]}$$

= 1 with biorthogonal wavefunctions $\left\langle \phi_n^{(b)} \middle| \phi_{n'}^{(a)}\right\rangle = \delta_{nn'}$

No sign problem

⇨ Non-linear Ito-stochastic differential equation with multiplicative noise

$$\left|d\phi_n^{(a)}\right\rangle = \left(1-\mathcal{R}^{(ab)}\right)\left[-\frac{d\tau}{2} h_{HF}\left(\mathcal{R}^{(ab)}\right) + \sqrt{\frac{|U|}{2}}\sum_{\vec{r}\sigma}\left|\vec{r}\sigma\right\rangle \mathrm{sgn}(U)\, dW_{\vec{r}}^{(a)} \left\langle \vec{r}\sigma\right|\right]\left|\phi_n^{(a)}\right\rangle, \quad d\Omega_\tau^{(a,b)} = -d\tau\ \Omega_\tau^{(a,b)}\left\langle \Phi_\tau^{(b)}\middle|\hat{H}\middle|\Phi_\tau^{(a)}\right\rangle$$

Interstate one-body density matrix

Hartree-Fock Hamiltonian

$$\mathcal{R}^{(ab)} = \sum_n \left|\phi_n^{(a)}\right\rangle\left\langle \phi_n^{(b)}\right|$$

(Semi-implicit Euler algorithm – Adaptive step with Brownian trees)

⇨ Zero-temperature and canonical version of the « Gaussian QMC » method

J. F. Corney, P.D. Drummond, Phys. Rev. Lett. (2004)

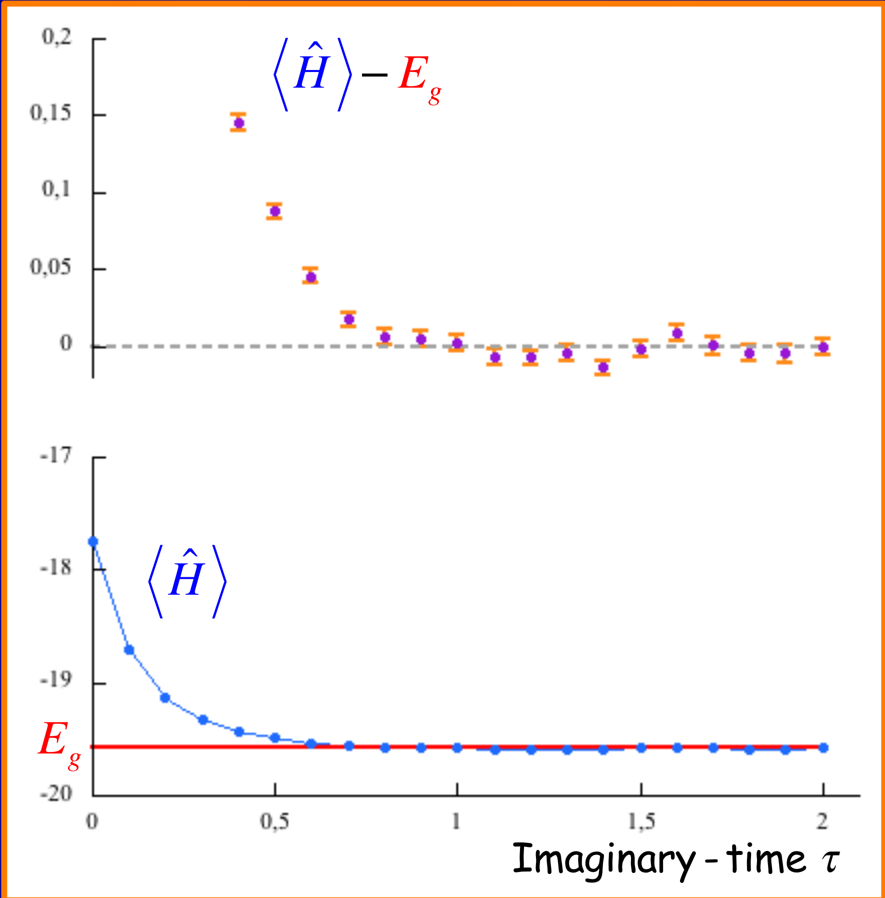
The sign-free stochastic mean-field scheme

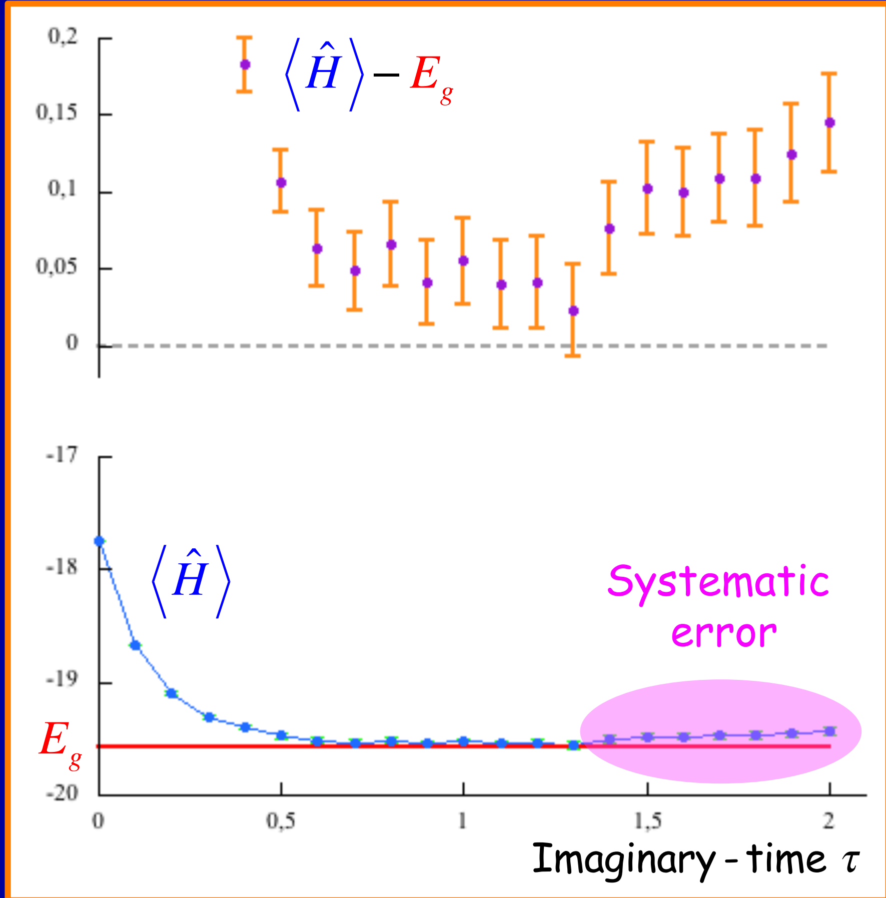
Fixed

$$\left|\Psi_g\right\rangle\left\langle\Phi_0^{(b)}\right| \underset{\tau\to\infty}{\propto} \mathbb{E}\left[\Omega_\tau^{(a,b)}\left|\Phi_\tau^{(a)}\right\rangle\left\langle\Phi_0^{(b)}\right|\right]$$

$$\left|\Psi_g\right\rangle\left\langle\Psi_g\right| \underset{\tau\to\infty}{\propto} \mathbb{E}\left[\Omega_\tau^{(a,b)}\left|\Phi_\tau^{(a)}\right\rangle\left\langle\Phi_\tau^{(b)}\right|\right]$$

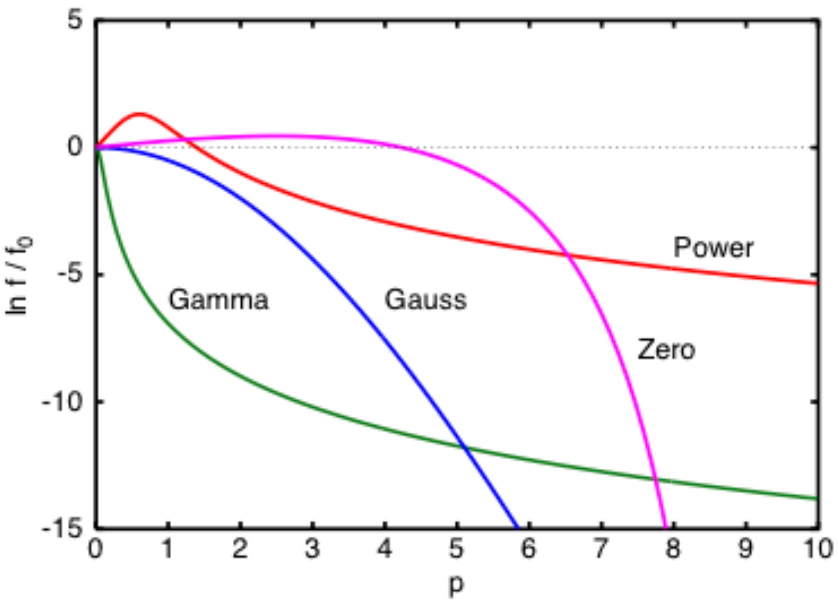
4*4 lattice – U=4 – t=1 – N=10 electrons





The sign-free stochastic mean-field scheme

Multiplicative noises generate power-law tail distribution



Langevin equation

$$dp = (p_o - \gamma p)dt + dW_1 - p dW_2$$

Drift term | Additive noise | Multiplicative noise

Stationary distributions

Gauss

$$dW_1^2 = 2Ddt,\ dW_2^2 = 0$$

Gamma distribution in 1/p

$$dW_1^2 = 0,\ dW_2^2 = 2Cdt$$

Power-law distribution

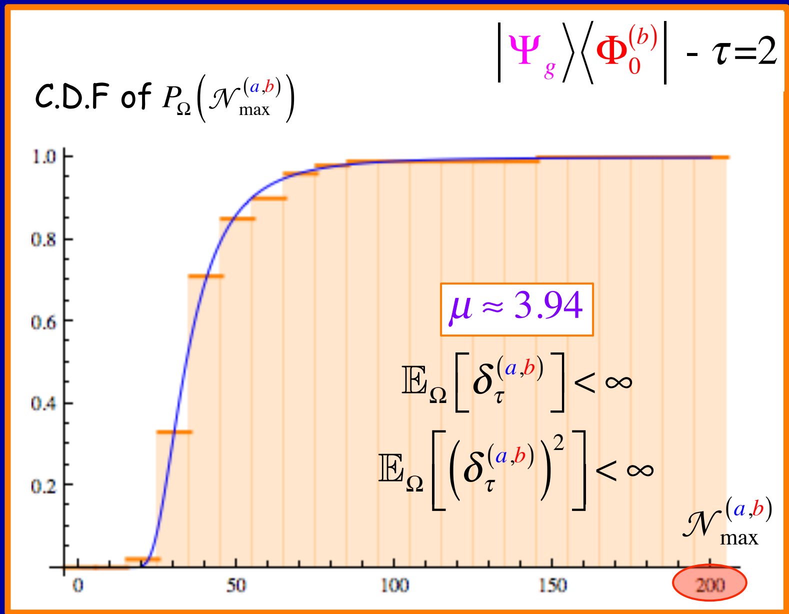
$$\gamma = 0,\ dW_1^2 = 2Ddt,\ dW_2^2 = 2Cdt$$

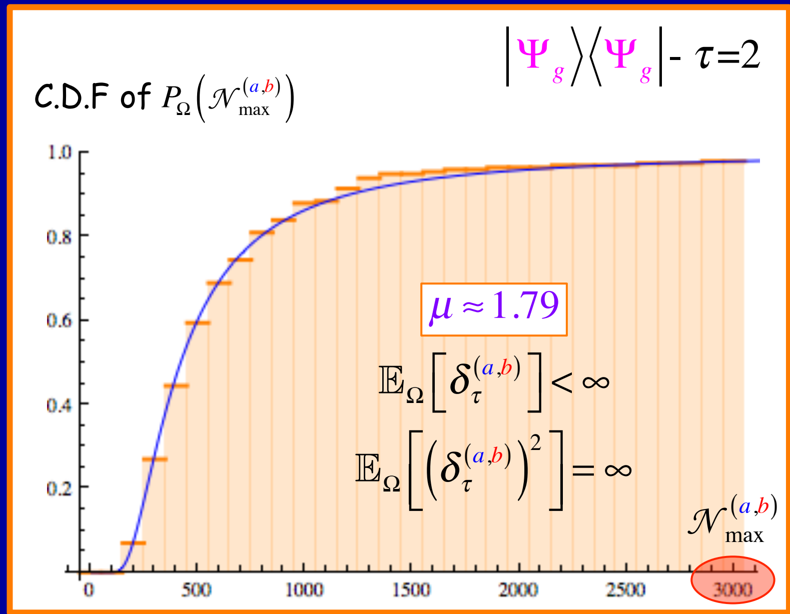
T.S. Biro, A. Jacovàk,
Phys. Rev. Letters (2004)

The sign-free stochastic mean-field scheme

Infinite moments of the error on the exact many-body state can be detected through extreme value analysis of dyadics' norm $\mathcal{N}^{(a,b)} = \left\| \left|\Phi^{(a)}\right\rangle\left\langle\Phi^{(b)}\right| \right\|$

If $P_\Omega\left(\mathcal{N}^{(a,b)}\right) \propto 1/\left(\mathcal{N}^{(a,b)}\right)^{1+\mu}$ for $\mathcal{N}^{(a,b)} \to \infty$, the distribution of the maximum $\mathcal{N}^{(a,b)}_{\max}$ over a sufficiently large sample is given by the Frechet distribution $\frac{\mu}{\left(\mathcal{N}^{(a,b)}_{\max}/\mathcal{N}_o\right)^{1+\mu}} \exp\left[\left(\mathcal{N}^{(a,b)}_{\max}/\mathcal{N}_o\right)^{-\mu}\right]$





The sign-free stochastic mean-field scheme

Distributions for the norm of projected dyadics on ground-state quantum-numbers $\Gamma = (\vec{K}, S, S_z, \cdots)$ decay much faster

Same idea used in Gaussian QMC : T. Aima, M. Imada , J. Phys. Soc. Jpn . (2007)

$$\exp(-\Delta\tau E_g)\langle\Psi_g|\Phi_0^{(a)}\rangle\langle\Psi_g|\Phi_0^{(b)}\rangle\hat{P}^{(\Gamma)}|\Psi_g\rangle\langle\Psi_g|\hat{P}^{(\Gamma)} \underset{\tau\to\infty}{=} \mathbb{E}\left[\Omega_\tau^{(a,b)}\hat{P}^{(\Gamma)}|\Phi_\tau^{(a)}\rangle\langle\Phi_\tau^{(b)}|\hat{P}^{(\Gamma)}\right]$$

Projection operator

$$\underset{\tau\to\infty}{=} \mathbb{E}\left[\Omega_\tau^{(a,b)}\left|\langle\Phi_\tau^{(b)}|\hat{P}^{(\Gamma)}|\Phi_\tau^{(a)}\rangle\right|\frac{\hat{P}^{(\Gamma)}|\Phi_\tau^{(a)}\rangle\langle\Phi_\tau^{(b)}|\hat{P}^{(\Gamma)}}{\left|\langle\Phi_\tau^{(b)}|\hat{P}^{(\Gamma)}|\Phi_\tau^{(a)}\rangle\right|}\right]$$

Importance sampling

$$\underset{\tau\to\infty}{=} \mathbb{E}_{\tilde{\Omega}}\left[\frac{\hat{P}^{(\Gamma)}|\Phi_\tau^{(a)}\rangle\langle\Phi_\tau^{(b)}|\hat{P}^{(\Gamma)}}{\left|\langle\Phi_\tau^{(b)}|\hat{P}^{(\Gamma)}|\Phi_\tau^{(a)}\rangle\right|}\right]$$

Sign problem in observables, but less severe :

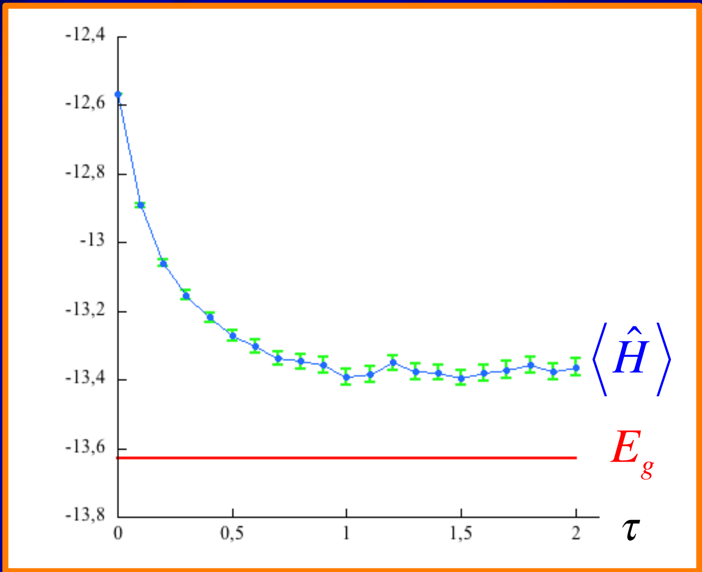
Any walker leads to a positive-sign population in the $\tau\to\infty$ limit

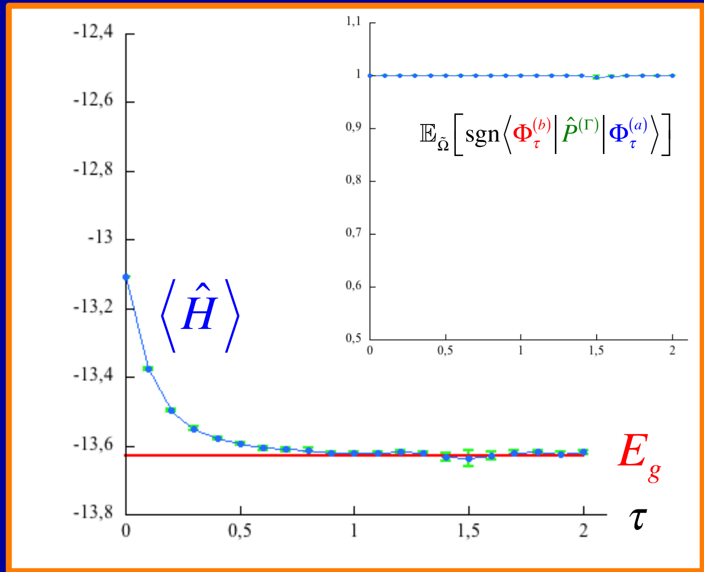
$$\exp(-\Delta\tau E_g)\underbrace{\langle\Psi_g|\Phi_{\tau_0}^{(a)}\rangle\langle\Psi_g|\Phi_{\tau_0}^{(b)}\rangle}_{>0} \underset{\Delta\tau\to\infty}{=} \mathbb{E}_{\tilde{\Omega}}\left[\frac{\langle\Phi_{\tau_0+\Delta\tau}^{(b)}|\hat{P}^{(\Gamma)}|\Phi_{\tau_0+\Delta\tau}^{(a)}\rangle}{\left|\langle\Phi_{\tau_0+\Delta\tau}^{(b)}|\hat{P}^{(\Gamma)}|\Phi_{\tau_0+\Delta\tau}^{(a)}\rangle\right|}\right]$$

The sign-free stochastic Hartree-Fock scheme

$$|\Psi_g\rangle\langle\Psi_g| \underset{\tau\to\infty}{\propto} \mathbb{E}_\Omega\left[|\Phi_\tau^{(a)}\rangle\langle\Phi_\tau^{(b)}|\right]$$

$$|\Psi_g\rangle\langle\Psi_g| \underset{\tau\to\infty}{\propto} \mathbb{E}_{\tilde{\Omega}}\left[\frac{\hat{P}^{(\Gamma)}|\Phi_\tau^{(a)}\rangle\langle\Phi_\tau^{(b)}|\hat{P}^{(\Gamma)}}{\left|\langle\Phi_\tau^{(b)}|\hat{P}^{(\Gamma)}|\Phi_\tau^{(a)}\rangle\right|}\right]$$





	$\langle \hat{T} \rangle$	$S_m = \frac{1}{3}\sum_{\vec{r}}(-1)^{x+y}\langle\hat{\vec{\sigma}}_{\vec{0}}.\hat{\vec{\sigma}}_{\vec{r}}\rangle$	$S_c = \sum_{\vec{r}}(-1)^{x+y}\langle\hat{n}_{\vec{0}}.\hat{n}_{\vec{r}}\rangle$
Ex. Diag.	−20.989	3.64	0.385
QMC – No projection	−20.85(3)	3.35(1)	0.385(1)
QMC – projection	−21.00(2)	3.66(1)	0.386(1)

4*4 lattice
U=4 - t=1
N=16 electrons

The sign-free stochastic mean-field scheme

$$|\Psi_g\rangle\langle\Psi_g| \underset{\tau\to\infty}{\propto} \mathbb{E}_\Omega\left[\,|\Phi_\tau^{(a)}\rangle\langle\Phi_\tau^{(b)}|\,\right]$$

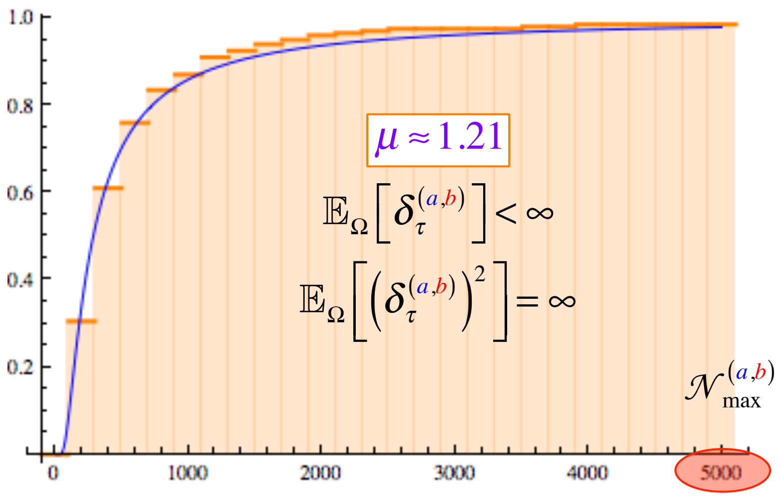
Norm $\mathcal{N}^{(a,b)}$

$$|\Psi_g\rangle\langle\Psi_g| \underset{\tau\to\infty}{\propto} \mathbb{E}_{\tilde\Omega}\left[\frac{\hat P^{(\Gamma)}|\Phi_\tau^{(a)}\rangle\langle\Phi_\tau^{(b)}|\hat P^{(\Gamma)}}{\left|\langle\Phi_\tau^{(b)}|\hat P^{(\Gamma)}|\Phi_\tau^{(a)}\rangle\right|}\right]$$

Norm $\tilde{\mathcal{N}}^{(a,b)}$

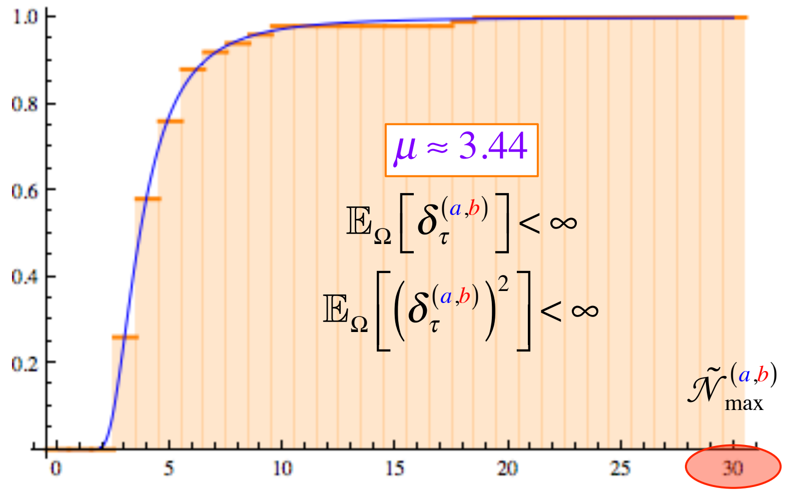
$\tau=2$

C.D.F of $P_\Omega\left(\mathcal{N}_{\max}^{(a,b)}\right)$



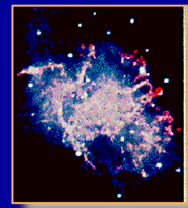
$\tau=2$

C.D.F of $P_{\tilde\Omega}\left(\tilde{\mathcal{N}}_{\max}^{(a,b)}\right)$



Hubbard model at unitarity

- Ideal regime of strong interaction where the cross-section saturates the limit imposed by unitarity : $\sigma = \sigma_{\max} = 4\pi / k^2$



Bertsch many-body X challenge, Seattle, 1999

- Scale invariance $E_{unitarity}(N) = \xi \, E_{Free}(N)$

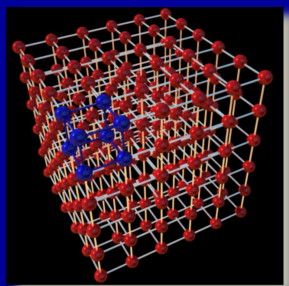
$$\xi_{\exp} = \begin{cases} 0.376(5) & \text{M.J.H. Ku \& al (2011)} \\ 0.41(1) & \text{N. Navon \& al, Science (2011)} \end{cases}$$

$$\xi_{QMC} \begin{cases} \leq 0.383(1) & \text{M. Forbes \& al, Phys. Rev. Lett. (2011)} \\ = 0.372(5) & \text{J. Carlson \& al (2011)} \end{cases}$$

- OK with Hubbard-like models in the dilute limit

$$k \sim k_F = \left(3\pi^2 \rho\right)^{1/3} \underset{\rho \to 0}{\longrightarrow} 0$$

$$\sigma \underset{k \to 0}{\sim} \frac{4\pi}{\left| a^{-1} + ik - r_e k^2 / 2 + \cdots \right|^2}$$



3D cubic lattice with period b

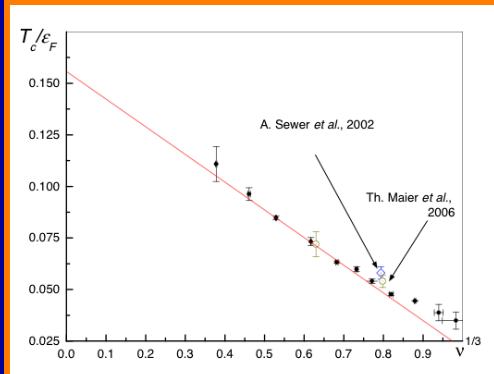
Scattering length $a = a(\varepsilon_{\vec{k}}, U)$

Effective range $r_e = r_e(\varepsilon_{\vec{k}})$

Divergence for finite U<0

→ Pairing correlations

E. Burovski & al, Phys. Rev. Lett. (2006)



Lattice modeling of the unitary gas :
Sign-free stochastic mean-field with BCS states

O. Juillet, to be published (2011)

Fixed

$$\left|\Psi_g\right\rangle\left\langle\Phi_0^{(b)}\right| \underset{\tau\to\infty}{\propto} \mathbb{E}\left[\Omega_\tau^{(a,b)}\left|\Phi_\tau^{(a)}\right\rangle\left\langle\Phi_0^{(b)}\right|\right]$$

$$\left\langle\Phi_0^{(b)}\middle|\Phi_\tau^{(a)}\right\rangle=1$$

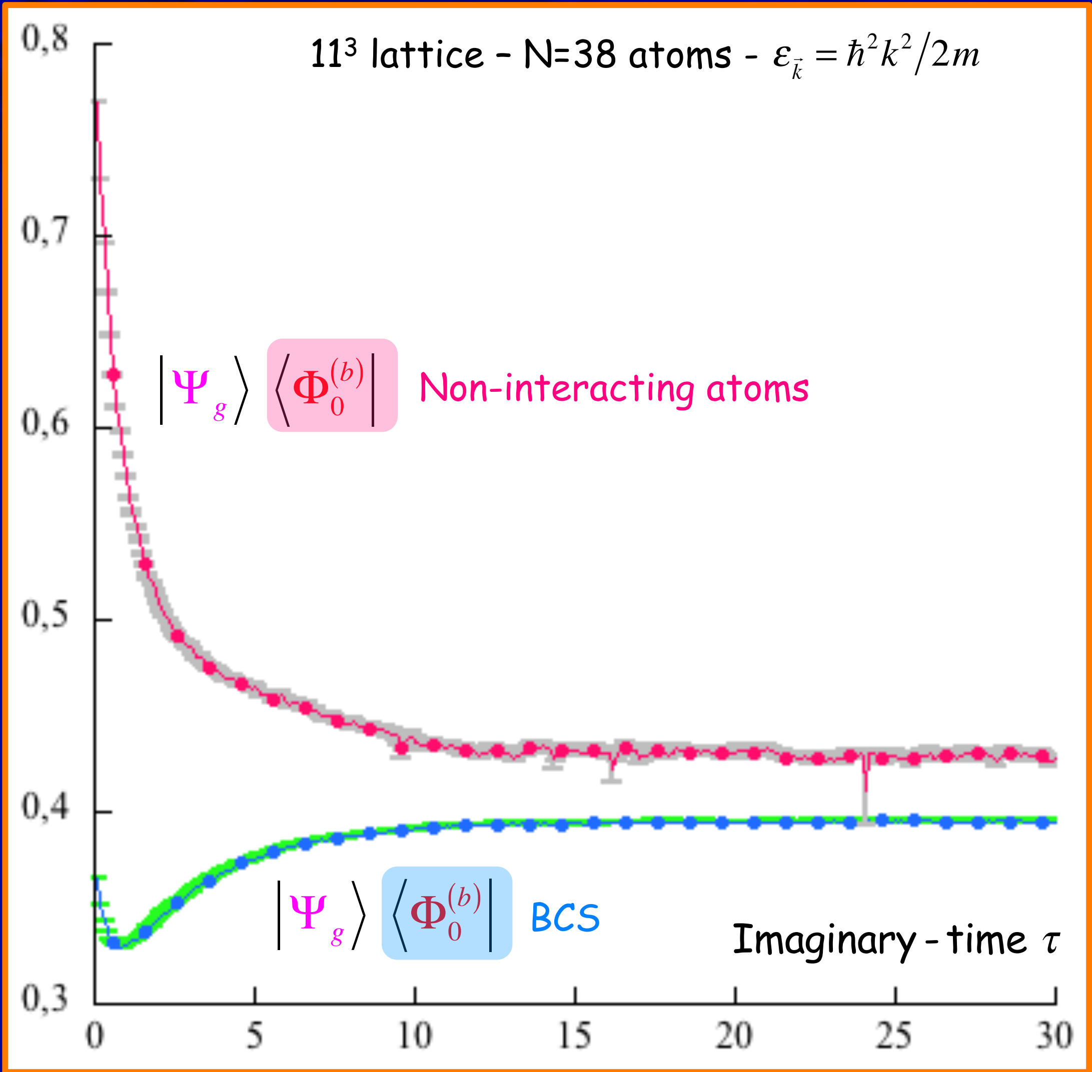
$$\begin{cases}\left|\Phi^{(a)}\right\rangle=\hat{c}^+_{\phi_1^{(a)},\uparrow}\cdots\hat{c}^+_{\phi_{N/2}^{(a)},\uparrow}\hat{c}^+_{\phi_1^{(a)},\downarrow}\cdots\hat{c}^+_{\phi_{N/2}^{(a)},\downarrow}\left|\ \right\rangle \\ \left|\Phi^{(b)}\right\rangle\propto\exp\left[\sum_{\vec{k}} f_{\vec{k}}^{(b)} c^+_{\vec{k}\uparrow}c^+_{\vec{k}\downarrow}\right]\left|\ \right\rangle\end{cases}$$

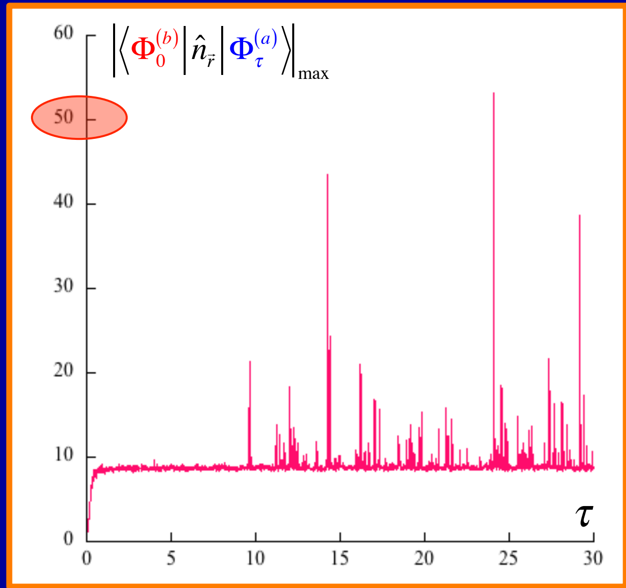
$$\left|d\phi_n^{(a)}\right\rangle=\left(1-\mathcal{R}^{(ab)}\right)\left[-d\tau\ h_{HF}\left(\mathcal{R}^{(ab)}\right)+\sqrt{|U|}\sum_{\vec{r}}\left|\vec{r}\right\rangle dW_{\vec{r}}^{(a)}\left\langle\vec{r}\right|\right]\left|\phi_n^{(a)}\right\rangle$$
$$+\left[\frac{Ud\tau}{2N}\sum_{\vec{r}}\left\langle\Phi_0^{(b)}\middle|\hat{n}_{\vec{r}\uparrow}\hat{n}_{\vec{r}\downarrow}\middle|\Phi_\tau^{(a)}\right\rangle-\left\langle\Phi_0^{(b)}\middle|\hat{n}_{\vec{r}\uparrow}\middle|\Phi_\tau^{(a)}\right\rangle\left\langle\Phi_0^{(b)}\middle|\hat{n}_{\vec{r}\downarrow}\middle|\Phi_\tau^{(a)}\right\rangle\right]\mathcal{R}^{(ab)}\left|\phi_n^{(a)}\right\rangle$$

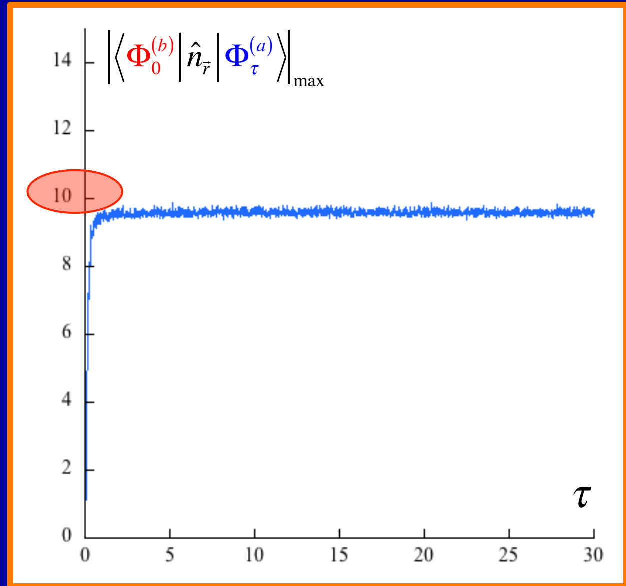
$$d\Omega_\tau^{(a,b)}=-d\tau\ \Omega_\tau^{(a,b)}\left\langle\Phi_0^{(b)}\middle|\hat{H}\middle|\Phi_\tau^{(a)}\right\rangle$$

$$\mathcal{R}^{(ab)}=\sum_{n,n'}\left|\phi_n^{(a)}\right\rangle\left(g^{-1}\right)_{nn'}\left\langle\phi_{n'}^{(a)}\right| \quad \text{with} \quad g_{nn'}=\left\langle\phi_n^{(a)}\middle|f^{(b)}\middle|\phi_{n'}^{(a)}\right\rangle$$

Hubbard-like model at unitarity

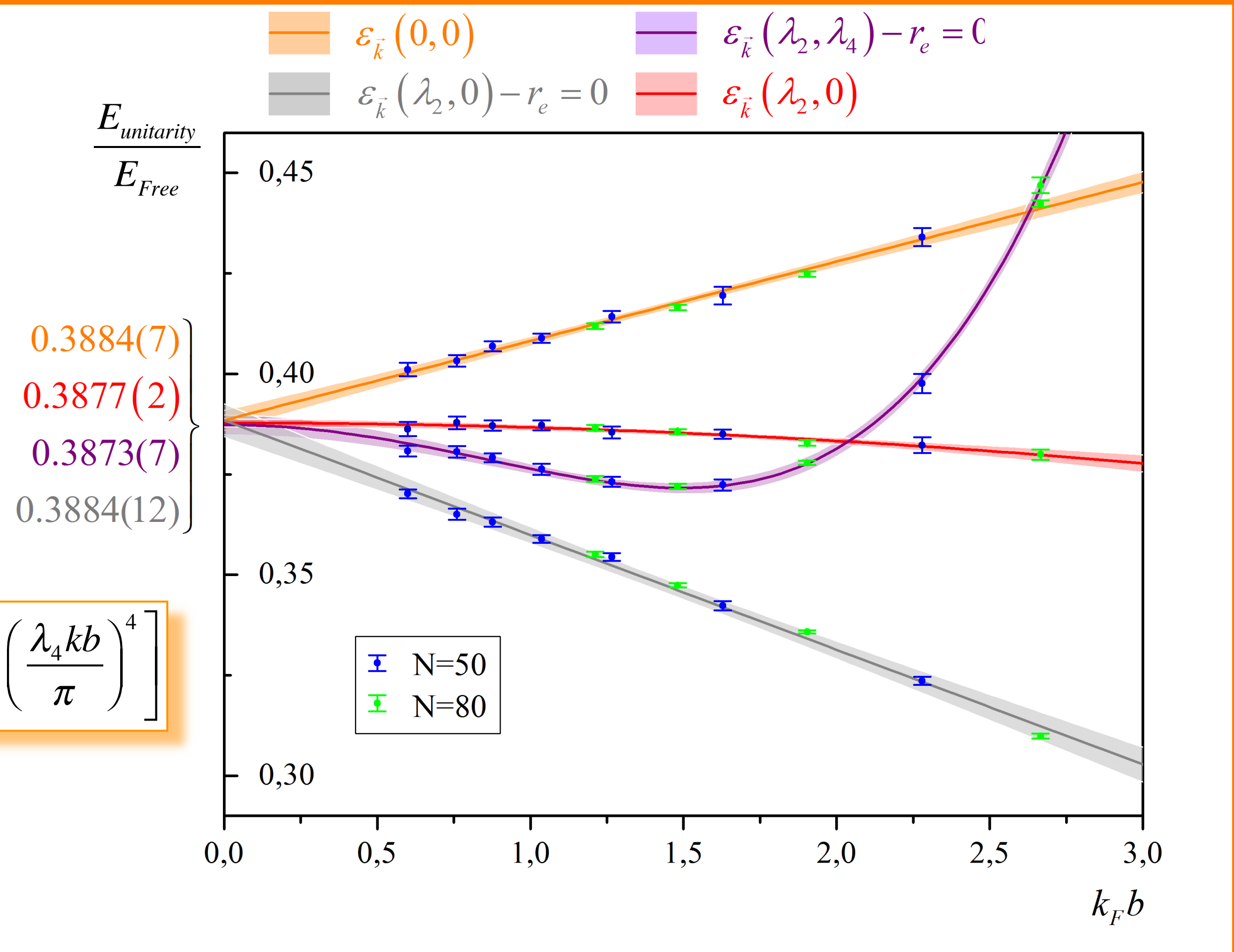






Lattice modeling of the unitary gas : Sign-free stochastic mean-field with BCS states

Different dispersion relations must give the same universal parameter ξ in the vanishing lattice filling limit



$$\varepsilon_{\vec{k}} = \frac{\hbar^2 k^2}{2m}\left[1 - \left(\frac{\lambda_2 k b}{\pi}\right)^2 + \left(\frac{\lambda_4 k b}{\pi}\right)^4\right]$$

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Stochastic wavefunction approach to Hubbard-like models

The Hubbard-model can be investigated with stochastic wavefunctions undergoing a Brownian motion in imaginary-time that ensures positive weigths in any regime

Positive weights in Quantum Monte-Carlo methods are NOT sufficient to obtain exact results

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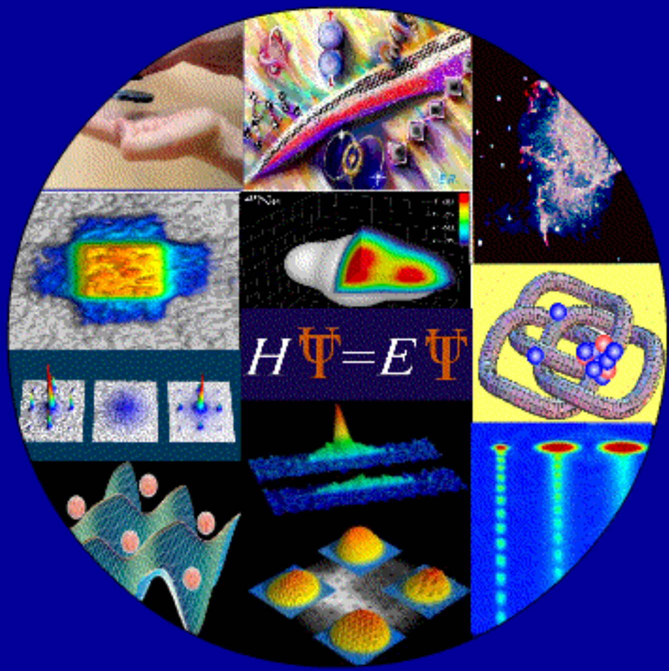
Stochastic wavefunction approach to Hubbard-like models



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