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Stochastic mean-field approach to strongly correlated phases of ultracold fermions.

Olivier Juillet

LPC/ENSICAEN, Boulevard du Maréchal Juin, F-14050 Caen Cedex, France

We propose a new projector quantum Monte-Carlo method to investigate the ground state of ultracold fermionic atoms modeled by a lattice Hamiltonian with an on-site interaction. The many-body state is reconstructed from Slater determinants that evolve in imaginary-time according to a stochastic mean-field motion without explicit sign problems. The method is applied to calculate ground-state energies and correlation functions of the repulsive two-dimensional Hubbard model. Numerical results for the unitary Fermi gas validate simulations with nodal constraints.

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Since the experimental achievement of Fermi degeneracy¹ with an atomic vapor, a considerable attention has been attracted by the physics of dilute ultracold fermions. The ability to tune many parameters, such as temperature, density or inter-particle interactions, makes atomic Fermi gases ideal candidates to understand a wealth of phenomena relevant for physical systems ranging from nuclear matter to high-temperature superconductors. Of particular interest is the strongly interacting regime in the transition from Bardeen-Cooper-Schrieffer (BCS) superfluidity of Cooper pairs to Bose-Einstein condensation (BEC) of atomic dimers. In the crossover region, Fermi condensates have been observed on both the BCS and the BEC sides of a magnetically controlled Feshbach resonance². The unitary regime, where the scattering length diverges, is particularly studied³ to investigate the universal features of the fermionic quantum many-body problem. With the help of several standing laser beams, ultracold atoms can also be loaded in optical lattices where they experience all the strong many-body correlations associated to the Hubbard model of solid-state physics⁴. Optical lattice setups may allow for engineering quantum spin models⁵, fractional quantum Hall effect⁶, non-Abelian gauge potentials⁷ or quantum information processing⁸.

In this letter, we investigate a new Monte-Carlo scheme to study strongly correlated ground states of ultracold fermions interacting on a lattice. The projection onto the ground state is performed through a reformulation of the imaginary-time Schrödinger equation in terms of Slater determinants undergoing a Brownian motion driven by the Hartree-Fock Hamiltonian. Such exact stochastic extensions of the mean-field approaches have been recently proposed for boson systems with a boson condensate ansatz and a Gutzwiller wave-function⁹. Up to now, the fermionic counterpart uses Slater determinants whose orbitals evolve under their own mean-field, supplemented with a stochastic one-particle-one-hole excitation¹⁰. Unfortunately, the sampling generally

suffers from negative weight trajectories that cause an exponential decay of the signal-to-noise ratio, which is known as the sign problem. The convergence issue of such a Monte-Carlo calculation plagued by negative “probabilities” belongs to the class of NP hard problems and a polynomial complexity solution can be probably ruled out¹¹. Here, we extend the stochastic Hartree-Fock approach to remove negative weight paths in the Monte-Carlo calculation of any observable.

For a system of fermions interacting through a binary potential, we first introduce a set of hermitian one-body operators \hat{A}_s ($s=0,1,\dots$) allowing to rewrite the model Hamiltonian \hat{H} in a quadratic form:

$$\hat{H} = \hat{A}_0 - \sum_{s \geq 1} \omega_s \hat{A}_s^2 \quad (1)$$

In what follows, we will adopt the second quantization formalism, so that $\hat{A}_s = \sum_{i,j} (A_s)_{ij} \hat{a}_i^+ \hat{a}_j$ where \hat{a}_i^+, \hat{a}_i are the Fermi creation and annihilation operator in a single-particle mode $|i\rangle$. Let us now consider two N -particle Slater determinants $|\psi\rangle, |\varphi\rangle$ of orbitals satisfying the biorthogonality relations $\langle \psi_n | \varphi_p \rangle = \delta_{n,p}$. Any matrix element $\langle \psi | \hat{A} | \varphi \rangle$ can then be evaluated by using Wick’s theorem with the set of contractions $\mathcal{R}_{ij} = \langle \psi | \hat{a}_j^+ \hat{a}_i | \varphi \rangle = \sum_n \langle i | \varphi_n \rangle \langle \psi_n | j \rangle$. The non-hermitian one-body density matrix \mathcal{R} is

linked to the usual Hartree-Fock single-particle Hamiltonian h by $h_{ij}(\mathcal{R}) = \frac{\partial \mathcal{H}}{\partial \mathcal{R}_{ji}}$, where

$\mathcal{H}(\mathcal{R}) = \langle \psi | \hat{H} | \varphi \rangle$ is the matrix element of the Hamiltonian. Under the Hamiltonian (1), it can be shown that the Slater determinant $|\varphi\rangle$ transforms according to:

$$\hat{H} |\varphi\rangle = \mathcal{H} |\varphi\rangle + \hat{h}_{0,1} |\varphi\rangle - \sum_{s \geq 1} \omega_s \hat{A}_{s,0,1}^2 |\varphi\rangle \quad (2)$$

$\hat{h}_{0,1}$ is defined by $\hat{h}_{0,1} = \sum_{i,j} [(1 - \mathcal{R})h\mathcal{R}]_{ij} \hat{a}_i^+ \hat{a}_j$ and $\hat{A}_{s,0,1}$ is given by a similar expression:

$\hat{A}_{s,0,1} = \sum_{i,j} [(1 - \mathcal{R})A_s\mathcal{R}]_{ij} \hat{a}_i^+ \hat{a}_j$. Note that if the two Slater determinants $|\psi\rangle, |\varphi\rangle$ are

identical, $\hat{h}_{0,1}$ and $\hat{A}_{s,0,1}^2$ physically represent one-particle-one-hole and two-particle-two-holes excitations. After an infinitesimal “time” step $d\tau$, during which $|\varphi\rangle$ evolves to $\exp(-d\tau\hat{H})|\varphi\rangle$, the last term of the expansion (2) causes departures from the Slater determinant manifold. Introducing random fields according to the Hubbard-Stratonovich transform¹², the dynamics can be linearized and the exact imaginary-time propagation of the Slater determinant $|\psi\rangle$ is obtained through a stochastic motion of its biorthogonal partner $|\varphi\rangle$:

$$\exp(-\tau\hat{H})|\psi\rangle = E \left[\exp(S(\tau)) |\varphi(\tau)\rangle \right] \quad (3)$$

where $E(\dots)$ is the statistical average over a random functional; S and the orbitals $|\varphi_n\rangle$ evolve according to the following equations in the Ito sense:

$$dS = -d\tau \mathcal{H}(\mathcal{R}), \quad S(0) = 0 \quad (4)$$

$$d|\varphi_n\rangle = (1 - \mathcal{R}) \left(-d\tau h(\mathcal{R}) + \sum_{s \geq 1} dW_s \sqrt{2\omega_s} A_s \right) |\varphi_n\rangle, \quad |\varphi_n(0)\rangle = |\psi_n\rangle \quad (5)$$

The dW_s are infinitesimal increments of independent Wiener processes: $E(dW_s) = 0$, $dW_s dW_{s'} = d\tau \delta_{s,s'}$. We emphasize that the dynamics (5) exactly preserves the biorthogonality properties between the two Slater determinants $|\psi\rangle, |\varphi\rangle$: indeed, the left-eigenvalue relation $\langle \psi_n | \mathcal{R} = \langle \psi_n |$ implies $\langle \psi_n | \varphi_p + d\varphi_p \rangle = \delta_{np}$ and therefore $\langle \psi | \varphi \rangle = 1$ at any ‘‘time’’. Provided that the trial state $|\psi\rangle$ is not orthogonal to the ground state $|\Psi_g\rangle$, the representation (4) then allows to compute the ground-state energy E_g according to

$$E_g = \lim_{\tau \rightarrow \infty} \frac{\langle \psi | \hat{H} \exp(-\tau \hat{H}) | \psi \rangle}{\langle \psi | \exp(-\tau \hat{H}) | \psi \rangle} = \lim_{\tau \rightarrow \infty} \frac{E[\exp(S(\tau)) \langle \psi | \hat{H} | \varphi(\tau) \rangle]}{E[\exp(S(\tau))]} \quad (6)$$

As long as $S(\tau)$ remain real during the imaginary-time motion, the weight $\exp(S(\tau))$ of each stochastic path is positive and one can perform an exact Monte-Carlo calculation without explicit sign problems. Moreover, if the Slater determinant ansatz $|\psi\rangle$ and the ground state share a common symmetry, the stochastic paths are automatically projected onto this symmetry sector in the estimate (6). Otherwise, the sampling can be improved by projection techniques¹³. These conclusions also hold for any observable commuting with the Hamiltonian. In other cases, one obtains an approximate ground-state expectation value, known as the mixed estimate¹⁴. It can be corrected by the following extrapolated estimate¹⁴ that is one order better in the difference $|\psi\rangle - |\Psi_g\rangle$:

$$\langle \hat{O} \rangle_{extrap.} = 2 \langle \hat{O} \rangle_{mixed} - \langle \psi | \hat{O} | \psi \rangle, \quad \langle \hat{O} \rangle_{mixed} = \lim_{\tau \rightarrow \infty} \frac{E[\exp(S(\tau)) \langle \psi | \hat{O} | \varphi(\tau) \rangle]}{E[\exp(S(\tau))]} \quad (7)$$

The exact expectation value would require obtaining the ground-state density matrix by a double propagation in imaginary-time¹⁵: $|\Psi_g\rangle \langle \Psi_g| \propto \lim_{\tau \rightarrow \infty} \exp\left(-\frac{\tau}{2} \hat{H}\right) |\psi\rangle \langle \psi| \exp\left(-\frac{\tau}{2} \hat{H}\right)$.

We now turn to applications in the field of ultracold atomic Fermi gases. First, we concentrate on the single-band $SU(2)$ Hubbard model that describes the low-energy physics of two-component ultracold fermions trapped in optical lattices:

$$\hat{H} = -t \sum_{\langle \vec{r}, \vec{r}' \rangle, \sigma = \uparrow, \downarrow} \hat{a}_{\vec{r}, \sigma}^+ \hat{a}_{\vec{r}', \sigma} + U \sum_{\vec{r}} \hat{n}_{\vec{r}, \uparrow} \hat{n}_{\vec{r}, \downarrow} \quad (8)$$

Here $\hat{a}_{\vec{r}, \sigma}^+$ creates one atom at site \vec{r} in the internal state $|\sigma\rangle = |\uparrow\rangle, |\downarrow\rangle$ and $\hat{n}_{\vec{r}, \sigma} = \hat{a}_{\vec{r}, \sigma}^+ \hat{a}_{\vec{r}, \sigma}$ is the corresponding number operator; t is the hopping matrix element between nearest neighboring sites $\langle \vec{r}, \vec{r}' \rangle$; U is the amplitude of the on-site interaction between two atoms. Analytical solutions only exist in one dimension. For higher dimensional problems, standard quantum Monte-Carlo calculations are limited to the repulsive model at half filling and to the attractive model with symmetric populations in the two spin channels $|\uparrow\rangle, |\downarrow\rangle$. In other cases, one experiences severe sign problems that practically prohibit studying large lattices, strongly interacting systems or open shells configurations. In contrast, our improved stochastic Hartree-Fock scheme does not manifest explicit sign problems regardless of the lattice topology, band filling and sign of the interaction. Indeed, a quadratic form (1) can be recovered from the Hamiltonian (8) by using the local density or magnetization depending on the sign of the interaction parameter U :

$$\hat{H} = -t \sum_{\langle \vec{r}, \vec{r}' \rangle, \sigma = \uparrow, \downarrow} \hat{a}_{\vec{r}, \sigma}^+ \hat{a}_{\vec{r}', \sigma} - \frac{|U|}{2} \sum_{\vec{r}} (\hat{n}_{\vec{r}, \uparrow} + \text{sgn}(U) \hat{n}_{\vec{r}, \downarrow})^2 \quad (9)$$

where we have omitted a constant term proportional to the total number of particles. All the one-body operators \hat{A}_s defined by Eq. (9) are real in the representation $|\vec{r}, \sigma\rangle$. If the orbitals of the trial Slater determinant $|\psi\rangle$ are real in this same basis, their biorthogonal partners $|\varphi_n\rangle$, stochastically propagated by the dynamics (5), will be real at any imaginary-time. Therefore, $\mathcal{H}(\mathcal{R})$ and $S(\tau)$ are also real, so that positive weights trajectories are guaranteed. In practice, the ansatz $|\psi\rangle$ is a spin-singlet Slater determinant for free-fermions or an antiferromagnetic Hartree-Fock mean-field solution. Fig. 1 displays the convergence to the ground-state energy for the positive- U Hubbard model on two-dimensional lattices corresponding to a hole doping $\delta = 0.125$ from half-filling. This density generates the most important sign problem in conventional auxiliary-field Monte-Carlo approaches. As in fixed-node methods¹⁶, the accuracy of the stochastic Hartree-Fock scheme depends on the quality of the trial Slater determinant $|\psi\rangle$. For instance, the imaginary-time propagation of the free-atom wave-function does not achieve to filter out all the excited states. The antiferromagnetic mean-field state is far more efficient and the exact ground-state energy of the 4×4 lattice is recovered to within less than 0.2% if the sampling is improved by projecting onto the spin-singlet sector. At half-filling, our calculations confirm the emergence of an antiferromagnetic phase¹⁷, as shown in Fig. 2 through the extrapolated estimate (7) of the space spin-spin correlation function $\langle \hat{S}_0 \cdot \hat{S}_{\vec{r}} \rangle$. We also reproduce the destruction of antiferromagnetic order by hole doping or by a geometrical frustration induced via a large next-nearest neighbor hopping¹⁷ (see Fig.2). The extrapolated values (7) of the magnetic and charge structure factors, defined by

$$S_m(\vec{q}) = \frac{4}{3} \sum_{\vec{r}} e^{i\vec{q}\cdot\vec{r}} \left\langle \hat{S}_0 \cdot \hat{S}_{\vec{r}} \right\rangle, \quad S_c(\vec{q}) = \sum_{\vec{r}} e^{i\vec{q}\cdot\vec{r}} \left\langle \hat{n}_0 \hat{n}_{\vec{r}} \right\rangle, \quad (11)$$

are in agreement with the diagonalization results for the 4×4 lattice¹⁸: at the corner $\vec{q} = (\pi, \pi)$ of the Brillouin zone, one obtains $S_m = 3.681(4)$, $S_c = 0.3872(6)$ and $S_m = 2.254(1)$, $S_c = 0.4236(1)$ compared to the exact values $S_m = 3.64$, $S_c = 0.385$ and $S_m = 2.18$, $S_c = 0.424$ for a doping $\delta = 0$ (half-filling) and $\delta = 0.125$, respectively.

We finally address the unitary Fermi gas limit. In this ideal regime of strong interaction via a two-body potential of zero range and infinite scattering length, fermions are among the most intriguing physical systems since they are believed to exhibit universal many-body states. For instance, at zero temperature, the energy must be a universal fraction η of the Fermi energy that is the only relevant energy scale in the system. From experiments with trapped atomic gases³, the measured values for this ratio η vary from 0.32_{-13}^{+10} to $0.51(4)$. We model a spatially homogeneous Fermi gas by a lattice Hamiltonian with a two-body discrete delta potential whose coupling constant is adjusted to reproduce the physical scattering length a ¹⁹:

$$\hat{H} = \sum_{\vec{r}, \vec{r}', \sigma = \uparrow, \downarrow} T_{\vec{r}, \vec{r}'} \hat{a}_{\vec{r}, \sigma}^+ \hat{a}_{\vec{r}', \sigma} + \frac{4\pi\hbar^2}{Ml^3} \frac{a}{1 - Ka/l} \sum_{\vec{r}} \hat{n}_{\vec{r}, \uparrow} \hat{n}_{\vec{r}, \downarrow} \quad (12)$$

Here periodic boundary conditions are assumed in each direction; $T_{\vec{r}, \vec{r}'}$ are the matrix elements of the single-particle kinetic energy operator in the representation position; M is the atomic mass, l denotes the grid spacing and $K = 2.44275\dots$ is a numerical constant. In the unitary limit, $|a|$ goes to infinity but the coupling constant on the lattice remains finite and negative, so that the gas clearly experiences attraction. Our sign-free simulation method with the model Hamiltonian (12), transformed as in Eq. (9), has been checked from the known solutions of the two- and three-body problem in an harmonic trap at the unitarity point²⁰: in all cases, the discrepancy does not exceed one percent. For different systems, up to $N = 42$ atoms on a $8 \times 8 \times 8$ lattice, we plot in Fig. 3 the convergence of the ratio $\eta(\tau)$ between the mean energy $\langle \hat{H} \rangle(\tau)$ of the unitary gas at the imaginary-time τ and the non-interacting ground-state energy $E_{g,0}$ on the lattice. In the limit of large τ , all the results essentially concentrate around the same value and the emergence of a universal regime thus clearly appears. By fitting $\langle \hat{H} \rangle(\tau)$ to the form $\langle \hat{H} \rangle(\tau) = E_{g,\infty} + \kappa e^{-\omega\tau}$, we estimate the ground-state energy $E_{g,\infty}$ at unitarity and find, for even particle number, $\eta = E_{g,\infty}/E_{g,0} \approx 0.449(9)$ from the numerical values of Table 1. This is consistent with fixed-node Green's function Monte-Carlo calculations that predict $\eta \approx 0.44(1)$ in the region $10 \leq N \leq 40$ and $\eta \approx 0.42(1)$ for larger systems²¹. For odd particle number, we obtain similarly $E_{g,\infty} = 0.44(4)E_{g,0} + 0.442(3)\varepsilon_F$ where ε_F is the Fermi level. Therefore, the empirical gap $\delta(N) = E_{g,\infty}(N) - (E_{g,\infty}(N-1) + E_{g,\infty}(N+1))/2$ displays the odd-even staggering characteristic of a superfluid. The odd- N value of δ ,

i.e. $0.442(3) \varepsilon_F$, gives an estimate of the pairing gap that is also of the same order as the fixed node result ($0.54 \varepsilon_F$).

In summary, we have introduced a new exact stochastic Hartree-Fock scheme that allows quantum Monte-Carlo ground-state calculations of interacting fermions. For a wide class of ultracold fermions models, including the repulsive Hubbard model, positive weights trajectories are guaranteed and the sampling does not exhibit explicit sign problems. Up to now, we do not obtain an upper bound to the statistical error on the exact many-body state and divergent realizations could occur as an indirect manifestation of the sign problem. However, the actual numerical simulations are very encouraging and accurate results have been obtained in situations that traditionally experience severe convergence problems. Further investigation on unbalanced resonant Fermi gases and doped Mott insulators are under development to provide new insights into the physics of strongly correlated fermions.

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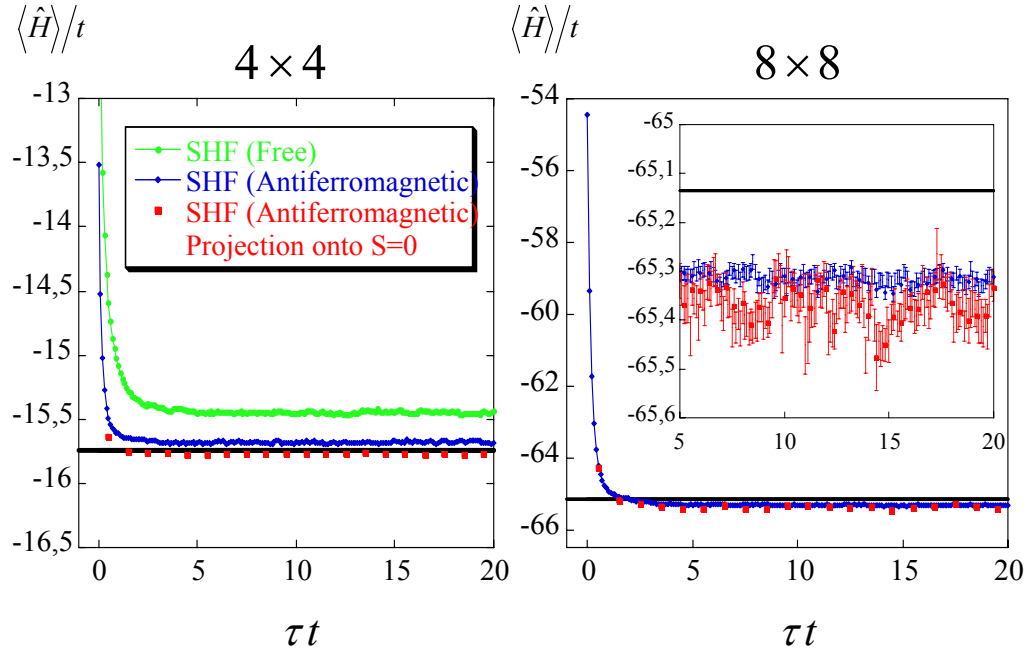


Fig. 1: Estimate (6) of the energy as a function of the imaginary-time τ for the two-dimensional Hubbard model with a hole doping $\delta=0.125$ from half-filling and an interaction parameter $U=4t$. The trial Slater determinant for stochastic Hartree-Fock calculations (SHF) is indicated in parentheses. The results have been averaged over several hundred of runs of 100 trajectories. The black line gives on the left the exact ground-state energy¹⁸ and on the right the constrained-path Monte-Carlo result¹².

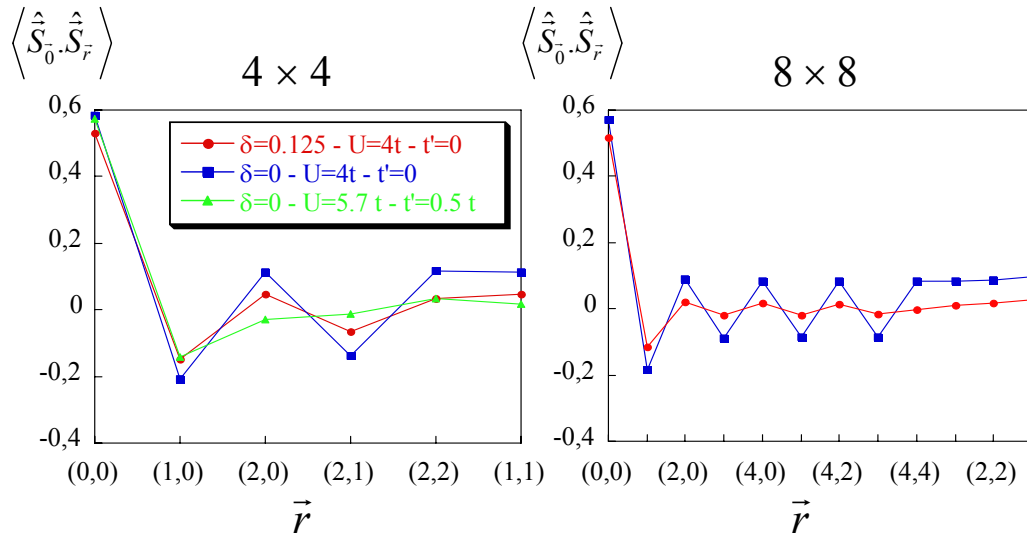


Fig. 2: Extrapolated estimate (7) of the real space spin-spin correlation function for the 4×4 Hubbard model. δ is the hole doping and t' denotes a next-to-nearest hopping. An antiferromagnetic mean-field solution was used as trial wave-function in all cases. Stochastic paths have been projected onto the spin-singlet sector. We averaged quantum Monte-Carlo results at the imaginary-time $\tau = 20/t$ with 100 trajectories over several hundred of runs. Statistical error bars are smaller than the size of the points.

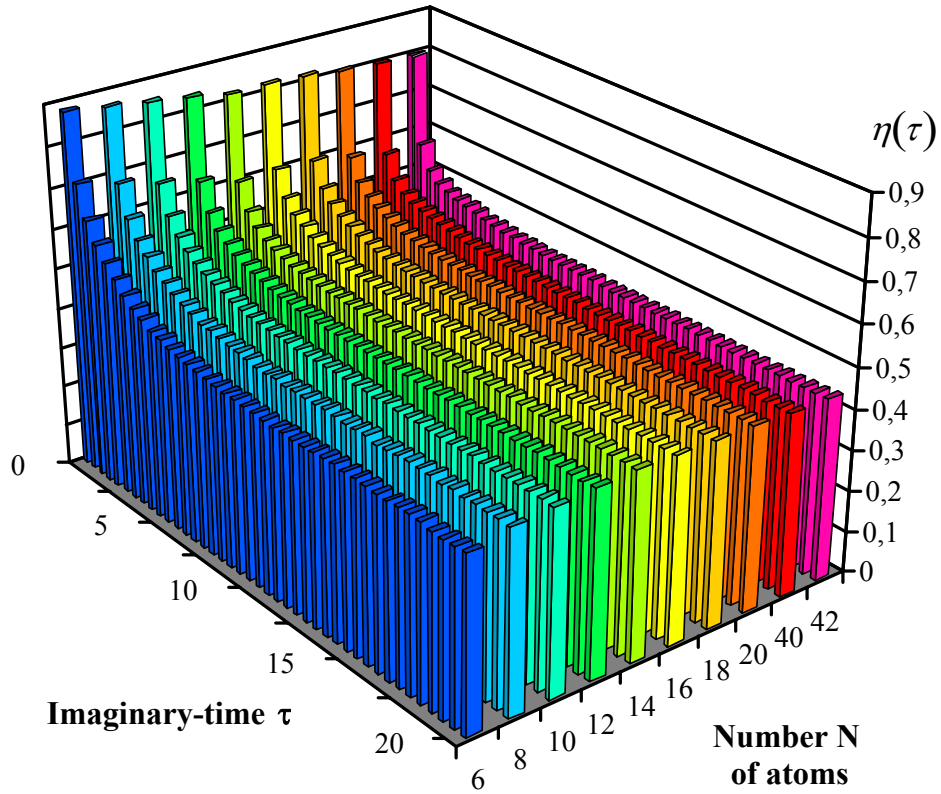


Fig. 3: Stochastic Hartree-Fock calculations of the ground-state energy of a unitary Fermi gas with $N_{\uparrow} = N_{\downarrow} = N/2$ atoms in each spin state. $\eta(\tau)$ is the ratio between the mean-energy of at “time” τ and the ground-state energy of the non-interacting gas on the lattice. The trial state is a spin-singlet Slater determinant for the free gas. We show the average result over many runs of 100 paths. We use a $6 \times 6 \times 6$ lattice, except for $N \geq 40$ where the calculations were performed on a $8 \times 8 \times 8$ grid. l is the lattice spacing.

N	η	N	η
6	0.42551	16	0.45473
8	0.44382	18	0.45273
10	0.45316	20	0.45211
12	0.45717	40	0.44691
14	0.46012	42	0.446

Table 1: Numerical values of the ratio $\eta = E_{g,\infty}/E_{g,0}$ for N interacting fermions in the unitarity limit. $E_{g,a}$ is the ground-state energy corresponding to a physical scattering length a .

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