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NUMERICAL SIMULATION OF FERMI SYSTEMS

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Abstract

We present a simple and effective method of Monte-Carlo simulation of fermions in quantum mechanics, based on Parisi-Klauder algorithm for complex action. As an illustration of the method properties we consider a gas of fermions in the oscillator potential and simple model of alpha clustering of nucleons in nuclei.

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INTRODUCTION. Path integral Monte-Carlo (MC) simulation is a good way to study any quantum system starting directly with first principles. In lattice field theories it results in a great activity (for a recent review, see, e.g. [1]). However, its applications to quantum mechanical problems [2] are not so extensive, although the method looks fruitful if applied to manybody systems like nuclei, neutron and quark matter, etc. The problem is that well elaborated ways of simulation based on the original Feynman path integral [3] ignore quantum statistics of particles, while interesting physical systems consist of identical bosons or fermions.

Recently [4] a system of identical bosons has been simulated using explicit symmetrization of the integrand in the corresponding path integral with respect to permutations of particles. Positivity of the symmetrized integrand allows to simulate a system of bossons using standard MC algorithms (like Metropolis or heat bath method). However, for a system of identical fermions the integrand should be antisymmetrized [2,4] and is not positively defined. Its "probabilistic" interpretation is invalid, and standard MC algorithms fail in fermion case.

In this letter a first successful attempt to simulate fermion systems starting directly with first principles is presented. It based on the Parisi-Klauder algorithm for path integration with complex action [5]. Although the reliability of the algorithm is not well understood [6], in our case it works well.

TWO IDENTICAL PARTICLES. The Feynman path integral for one-particle amplitude of transition from point x_i to x_f during time interval t is [3]:

$$U(x_i, x_f; t) = \langle x_f | \exp\{-i H t\} | x_i \rangle = \tag{1}$$

$$= \int \mathcal{D}x \exp\left\{ i \int dt' \left(\frac{m\dot{x}^2}{2} - V(x) \right) \right\}$$

where m is the mass of particle and V(x) is the potential. Numerical simulation requires Wick rotation from "Minkowsky" to "Eucleadian" time $t \to i\tau$. Slicing the time interval into N

steps: $\Delta\tau = \tau/N$ we turn the path integral into finite order one:

$$U(x_i, x_f; \tau) =$$

$$= \int dx_1 \dots dx_{N-1}\, U(x_i, x_1; \Delta\tau) \cdot U(x_1, x_2; \Delta\tau) \dots U(x_{N-1}, x_f; \Delta\tau) \tag{2}$$

where $U(x_k, x_{k+1}, \Delta\tau)$ is a transition amplitude for small time interval $\Delta\tau$:

$$U(x_k, x_{k+1}; \Delta\tau) \equiv \quad x_k \text{——} x_{k+1} \quad \simeq \tag{3}$$

$$\simeq C \cdot \exp\left\{ - \frac{m(x_{k+1} - x_k)^2}{2\Delta\tau} - \Delta\tau \cdot V\left(\frac{x_k + x_{k+1}}{2}\right) \right\}$$

(C is here normalization factor). For two distinguishable particles the transition amplitude is

$$U^{(d)}(x_k, y_k; x_{k+1}, y_{k+1}; \Delta\tau) \equiv \begin{array}{l} x_k \text{——} x_{k+1} \\ y_k \text{——} y_{k+1} \end{array} \simeq \tag{4}$$

$$\simeq C^2 \cdot \exp\left\{ - S^{(d)} \right\}$$

where

$$S^{(d)} = \frac{m(x_{k+1} - x_k)^2}{2\Delta\tau} + \frac{m(y_{k+1} - y_k)^2}{2\Delta\tau} + \tag{5}$$

$$+ \Delta\tau \cdot V\left(\frac{x_{k+1} + x_k}{2}, \frac{y_{k+1} + y_k}{2}\right)$$

is the usual action for two particles. If they are identical, the amplitude should be (anti) symmetrized:

$$U^{(id)}(x_k, y_k; x_{k+1}, y_{k+1}; \Delta\tau) = \tag{6}$$

$$= \begin{pmatrix} x_k \text{——} x_{k+1} \\ y_k \text{——} y_{k+1} \end{pmatrix} + \eta \cdot \begin{pmatrix} x_k \times x_{k+1} \\ y_k \quad\quad y_{k+1} \end{pmatrix}$$

with a factor $\eta = +/- 1$ for bosons and fermions, respectively. Exponentiation of eq.(6) gives

$$U^{(id)} = \exp\left\{ - S^{(id)}_{eff} \right\} \tag{7}$$

$$S_{eff}^{(id)} = -\ln\left(\rightrightarrows + \eta \times \right) \qquad (8)$$

where $S_{eff}^{(id)}$ is the "effective action" for a pair of identical particles. Permutations of particles in initial or final state leave the boson action unchanged, but in the fermion case the action is shifted by $i\pi$: $S_{eff}^{(id)} \rightarrow S_{eff}^{(id)} + i\pi$.

Following Parisi and Klauder [5], in our simulations of path integral we use Langevin equation:

$$\frac{dx_\kappa}{d\lambda} = -\frac{\partial S_{eff}^{(id)}}{\partial x_\kappa} + \xi_{x,\kappa}(\lambda) \qquad (9)$$

$$\frac{dy_\kappa}{d\lambda} = -\frac{\partial S_{eff}^{(id)}}{\partial y_\kappa} + \xi_{y,\kappa}(\lambda)$$

$$\kappa = 1,\ldots,N$$

where λ is a fictitious "langevin time", coordinate variables x_k, y_k are now complex-valued, while $\xi_{z,\kappa}(\lambda)$ is a real gaussian random noise, normalized by condition:

$$\langle \xi_{z,\kappa}(\lambda)\ \xi_{z',\kappa'}(\lambda) \rangle = 2\cdot\delta(\lambda-\lambda')\cdot\delta_{\kappa,\kappa'}\delta_{z,z'} \qquad (10)$$

If one starts with a real valued path, one never leaves the real axis (for real x_k, y_k the right hand sides of eqs.(9) are real). Moreover, one never passes through the pole at real axis, arising when indentical fermions are met. To avoid this problem we shift poles into the complex plane replacing $\eta = -1$ in eq.(8) by $\eta = -1 + i\varepsilon$, where $\varepsilon \sim 0.01$-0.1 is a small number (in fact, the path encemble is practically independent of ε).

Integration of Langevin equations gives for any Langevin time the paths $x_k(\lambda)$, $y_k(\lambda)$, k=1,...,N. To find mean value of physical observables one should make an analytic continuation of the corresponding operator and average it over the path ensemble:

$$\langle O \rangle = \Lambda^{-1} \int_0^\Lambda d\lambda\ O(x(\lambda), y(\lambda)) \qquad (11)$$

Although the coordinates are complex, the average of any observable should be real (in our calculations its imaginary part does not exceed several per cent of the real one).

The algorithm we use for integration of Langevin equation is specific, because of the pole in r.h.s. Updating one of the coordinates, say x_k, we find some "intermediate" point $\tilde{x}_k$:

$$\tilde{x}_\kappa = x_\kappa^{(old)} - \Delta\lambda \cdot \frac{\partial S^{(d)}}{\partial x_\kappa} + \xi\cdot\Delta\lambda \qquad (12)$$

where $x_k^{(old)}$ is an "old" point, and $S^{(d)}$ is the action for two distinguishable particles defined by eq.(5), and ξ is current value of random gauss noise. Then we calculate the "new" point, using the same value of ξ and final difference estimation of the derivative

$$x_\kappa^{(new)} = x^{(old)} - \Delta\lambda\cdot\left(\frac{\Delta S_{eff}^{(id)}}{\Delta x}\right) + \xi\cdot\Delta\lambda$$

$$\left(\frac{\Delta S_{eff}^{(id)}}{\Delta x}\right) \equiv \frac{S_{eff}^{(id)}(\tilde{x}_\kappa) - S_{eff}^{(id)}(x_\kappa^{(old)})}{\tilde{x}_\kappa - x_\kappa^{(old)}} \qquad (13)$$

Thus the derivative $\frac{\partial S_{eff}^{(id)}}{\partial x_\kappa}$ in r.h.s. of eq.(9) taken at some point is replaced by its value averaged over the interval $(x_k^{(old)}, \tilde{x}_k)$, which makes the integration procedure more accurate and stable. To stabilize it more for larger steps in λ we cut also the derivative near the pole, replacing

$$\left(\frac{\Delta S}{\Delta x}\right) \longrightarrow M \cdot \left(\frac{\Delta S}{\Delta x}\right) \Big/ \left|\frac{\Delta S}{\Delta x}\right| , \qquad (14)$$

$$if \quad \left|\frac{\Delta S}{\Delta x}\right| > M.$$

Let us present results of our simulations for two particles of mass m=1 moving in oscillator potential $V(x,y) = \left(\frac{x^2 + y^2}{2}\right)$ With periodical boundary conditions

$$x_f = x_i \ , \qquad y_f = y_i \qquad (15)$$

our quantum system propagating during the interval of eucledian time τ is equivalent to a statistical system with a temperature $T = 1/\tau$ [2]. Our numerical results for average energy of particles E(T) plotted in fig.1 are in a good agreement with analytical solution

$$E(T) = 2 + \frac{2}{e^{1/T} - 1} + \frac{1}{e^{1/T} + 1} \qquad (16)$$

Typical step in Langevin time in these runs is order of $\Delta\lambda$ = = 0.01-0.05, the number of steps in eucleadian time N=10.

n IDENTICAL PARTICLES. In this case the transition amplitude $U^{(id)}(x_\kappa^1,\dots,x_\kappa^n;\ x_{\kappa+1}^1,\dots,x_{\kappa+1}^n;\ \Delta\tau)$ has too many ($\sim n!$) terms corresponding to all permutations of final or initial particle coordinates, and direct account for all of them is hopeless. Fortunately, for small $\Delta\tau$ some additional small parameter arises, and the number of relevant terms reduces substantially. Indeed, let us rewrite two particle amplitude (6) in the form

$$U^{(id)} = U^{(d)} \cdot \left(1 + \eta \frac{\times}{=}\right) =$$

$$= U^{(d)} \cdot \exp\{-\delta S_{eff}\} \qquad (17)$$

$$\delta S_{eff} = -\ln\left(1 + \eta \exp\left\{-\frac{(x_\kappa - y_\kappa)(x_{\kappa+1} - y_{\kappa+1})}{\Delta\tau} + \dots\right\}\right)$$

It is close to the amplitude $U^{(d)}$ for two distinguishable particles, unless initial and/or final separations of particles are small

$$|x_\kappa - y_\kappa| \sim |x_{\kappa+1} - y_{\kappa+1}| \sim \Delta\tau^{1/2} \qquad (18)$$

In other words, the momentum of particle localized in time interval $\Delta\tau$ is $p \sim 1/(\Delta\tau)^{1/2}$, and Pauli "forces" act while the separation of particles $\Delta x \lesssim 1/p \sim (\Delta\tau)^{1/2}$. Obviously, the probability w_j to have j particles being close enough to feel their identity has a smallness

$$w_j \sim \left(\frac{(\Delta\tau)^{1/2}}{L}\right)^{j-2} w_2 \qquad (19)$$

where L is the typical scale parameter of the problem. Taking $\Delta\tau$ small enough we can make the contribution of three and higher order particle correlation be negligible. In this approximation corresponding Langevin equations take a form

$$\frac{dx_\kappa^\ell}{d\lambda} = -\frac{\partial S^{(d)}}{\partial x_\kappa^\ell} - \sum_{\ell' \neq \ell} \frac{\partial \delta S_{eff}^{(\ell,\ell')}}{\partial x_\kappa^\ell} + \xi_{\kappa,\ell}(\lambda) \qquad (20)$$

$$\ell, \ell' = 1,\dots n$$

$$\kappa = 1,\dots,N$$

and the number of arithmetical operations is proportional to n only, as if we consider just two particle interaction.

To understand the accuracy of this approximation we simulate a few fermions of mass m= 1 moving in common oscillator potential $V(x) = x^2/2$. Results are shown in fig.2, where energy of fermion system is plotted as a function of particle number n. The interval of eucleadian time is here τ =4, and periodical boundary conditions $x_N^\ell = x_1^\ell$, ℓ =1,...,n are

used. It is seen, that the larger is the number of particles n, the smaller $\Delta\tau$ is needed in order to reproduce the true result. The reason is obvious: for n-th level of the oscillator a size parameter of the problem (the period of wave function oscillation) decrease as $n^{-1/2}$ and (see eq.(19)) the role of omitted multiparticle Pauli interactions becomes more important. Nevertheless the algorithm is fast enough: to calculate a system of 10 fermions takes only 10 CPU minutes of processor with speed 2 MF lops per second!

A SIMPLE MODEL OF ALPHA CLUSTERING IN NUCLEI. Another interesting application is the alpha clustering of nucleons in nuclei [7]. We study here some oversimplified model of the phenomenon. Let us consider two pairs of identical fermions, a pair of "protons" and a pair of "neutrons", mutually interacting with a potential

$$V(x_i, x_j) = \frac{(x_i - x_j)^2}{2} \qquad (21)$$

independent of kinds of particles. However, identical particles in contrast to nonidentical ones suffer additional repulsion because of Pauli principle. As a result, they are gathered into two pairs, an analog of alpha clusters. Our results are shown in fig.3, where we present correlation of interparticle distances, defined in the following way. Taking one of the particles, we find the distance to the nearest partner of the opposite kind:

$$R_1 = \min_j | Re\, x_1 - Re\, x_j | \qquad (22)$$

Then we measure the distance R_2 between two remaining particles and the distance R_3 between first particle and another particle of the same kind. It is clearly seen, that we indeed observe two clusters of the size order of $R_{1,2} \simeq 0.7$ separated by the distance order $R_3 \simeq 1.5$.

CONCLUSIONS. We have found the method to be very convenient and not time consuming. Simplest applications presented here assumes only an illustrative goal. Extention to the three dimensional case and spin degrees of freedom is straigforward and we hope to give it in further publication.

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FIGURE CAPTURES

Fig.1. Two fermion energy versus temperature T. Points are the result of our simulations, the curve shows the exact analytical result, given by eq.(16).

Fig.2. n-fermion energy versus n. Points are obtained by numerical simulation and curve shows the exact analytical solution.

Fig.3. Probability distribution of interparticle distances (see text): a) correlation of intracluster distances, b) correlation of intra- and intercluster distances.

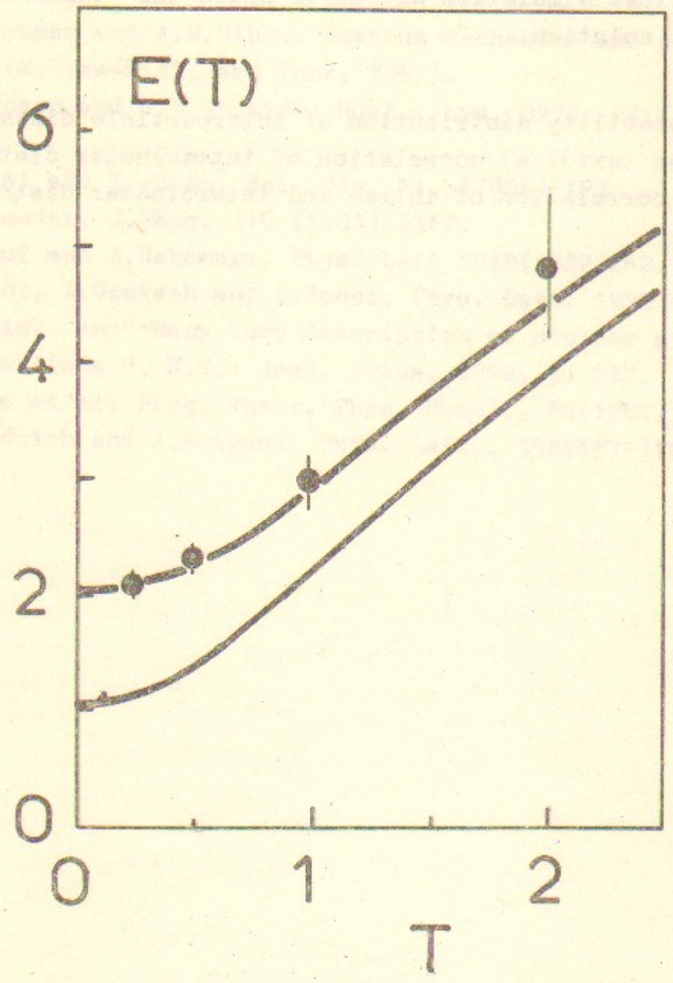

fig.1

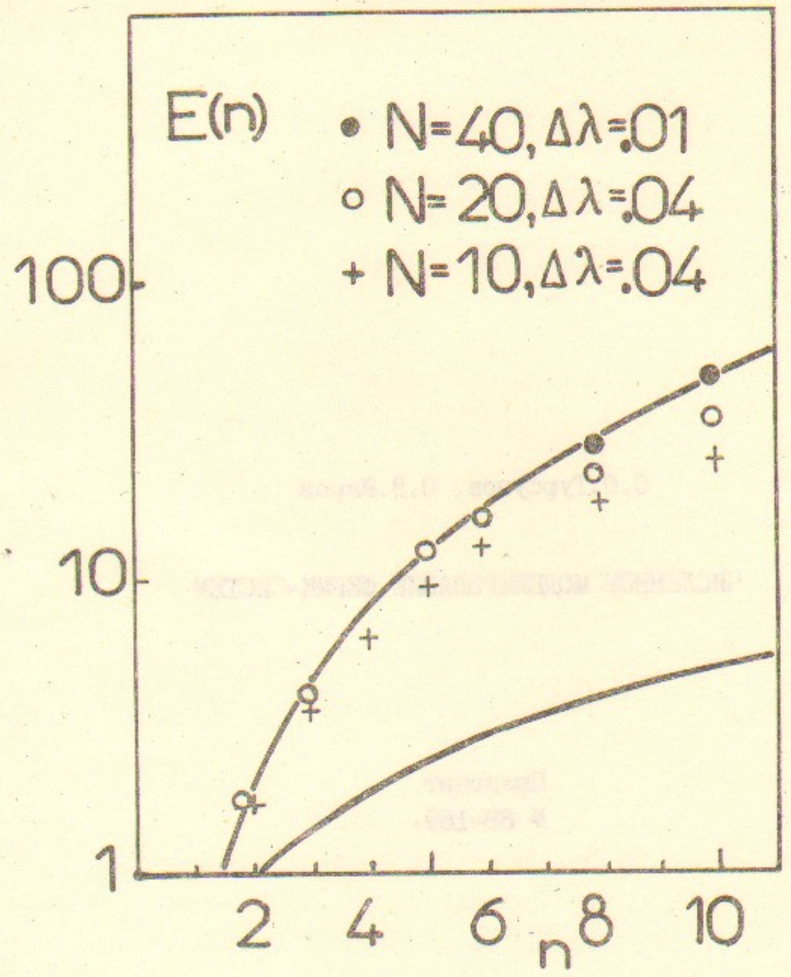

fig.2

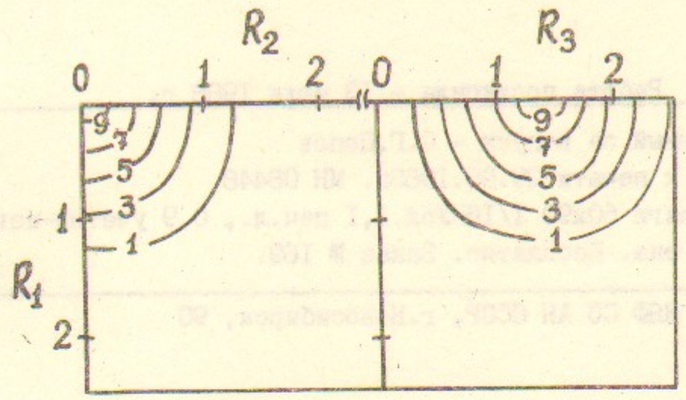

fig.3

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