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PROBABILISTIC SIMULATION OF FERMION PATHS

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Abstract

Permutation symmetry of fermion path integral allows (while spin degrees of freedom are ignored) to use in its simulation any probabilistic algorithm, like Metropolis one, heat bath, etc.

1. INTRODUCTION. In our recent Letter [1] we have proposed a way to simulate many-fermion systems. The main problem known here is that the integrand of any fermionic path integral is not positively defined, and widespread opinion claims (see, e.g. [2]) that probabilistic Monte Carlo algorithms fail in this case. We try the complex Langevin method [3], which has no explicite restriction of this kind and get a good success.

However, later on in view of works [4,5], we have realized that the Langevin method fails in simulation of any integral $\int_a^b dx f(x)$, if its integrand has a node: $f(x_o) = 0$, $x_o \in a,b$. This is a consequence [5] of the "segregation theorem" [6] proved for real x, x_0; but a direct numerical experiment shows, that simulation fails as well, even if one shifts the node point into the complex plane: $x_o \to x_o + i\varepsilon$. Therefore a puzzle occurs: why our simulation of fermions works well, although the integrand in our path integral has a lot of nodes ?

In this letter we show that our success is a consequence of the permutation symmetry of our path integral. Moreover, while spin degrees of freedom are ignored, one can reduce the whole domain of integration to some subdomain, where the integrand remains positive and therefore any probabilistic Monte Carlo algorithm (Metropolis one, heat bath, etc.) can be used.

2. Let us start with the L-fermion path integral in its time-discretized form:

$$\int Dx\, e^{-S[x]} = \int \prod_{n=1}^{N} \prod_{\ell=1}^{L} dx_n^{\ell} \prod_{n=1}^{N} U(x_n^1 \ldots x_n^L, x_{n+1}^1 \ldots x_{n+1}^L; \Delta\tau) \qquad (1)$$

where N is the number of steps $\Delta\tau$ in eucleadian time $\tau_o = \Delta\tau \cdot N$, x_n^{ℓ} is a coordinate of ℓ-th particle at time $\tau_n = \Delta\tau \cdot n$ (spatial subscripts are suppressed) and the link function $U(x_n, x_{n+1}; \Delta\tau)$ is the amplitude of L-fermion transition from the point x_n to the point x_{n+1} during a (small) time interval $\Delta\tau$. Periodical boundary conditions are imposed $x_{N+1}^{\ell} = x_1^{\ell}$. It is convenient to introduce an effective action defined as

$$\exp(-S_{eff}(x_n, x_{n+1}; \Delta\tau)) = U(x_n, x_{n+1}; \Delta\tau) \qquad (2)$$

which in the limit $\Delta\tau \to 0$ can be estimate as [1]:

$$S_{eff}(x_n, x_{n+1}; \Delta\tau) = \sum_{\ell=1}^{L} \left\{ \frac{m(x_{n+1}^{\ell} - x_n^{\ell})^2}{2\Delta\tau} + \frac{\Delta\tau}{2} \left[V(x_n^{\ell}) + V(x_{n+1}^{\ell}) \right] + \right.$$

$$\left. + \frac{1}{2} \sum_{\ell' \neq \ell}^{L} \ln \left[1 - \exp\left(- \frac{(x_{n+1}^{\ell} - x_{n+1}^{\ell'})(x_n^{\ell} - x_n^{\ell'})}{\Delta\tau} \right) \right] \right\} \qquad (3)$$

While the first two terms are a conventional form of the action for distinguishable particles, the third term arises for identical particles only, providing a needed symmetry of the link function $U(x_n, x_{n+1}; \Delta\tau)$ with respect to permutations of the initial or final particle coordinates. Since the link function $U(x_n, x_{n+1}; \Delta\tau)$ is not positively defined, the integrand in eq.(1) cannot be considered as a probability weight. However, one may simulate a path ensemble, taking instead as a weight function the absolute value of the integrand:

$$\left| \exp(-S) \right| = \left| \prod_{n=1}^{N} U(x_n, x_{n+1}; \Delta\tau) \right| \qquad (4)$$

Then any average can be calculated directly by the formula

$$\langle O \rangle = \left(\sum_{\{x\}_+} O(x) - \sum_{\{x\}_-} O(x) \right) / \left(\sum_{\{x\}_+} 1 - \sum_{\{x\}_-} 1 \right) \qquad (5)$$

where $\{x\}_+$ and $\{x\}_-$ are subsets of the whole path ensemble, whether the integrand in eq.(1) has positive or negative sign. This receipt works well while τ_o is not large: $\tau_o \cdot \Delta E \lesssim 1$, where ΔE is order of the energy splitting between the ground state and excited one: $\Delta E \sim E_1 - E_0$. In the limit of large $\tau_o \gg 1/\Delta E$ the receipt fails because of strong cancellations in eq.(5), but instead one may calculate

$$\langle O \rangle_{\pm} = \sum_{\{x\}_{\pm}} O(x) \Big/ \sum_{\{x\}_{\pm}} 1 \qquad (6)$$

We claim, that in the limit $\tau_o \gg 1/\Delta E$

$$\langle O \rangle = \langle O \rangle_+ = \langle O \rangle_- \qquad (7)$$

The motivation comes from a well-known behaviour of the correlation function

$$\langle x(\tau)\, x(\tau') \rangle \backsim \exp(- \Delta E \cdot |\tau - \tau'|) \qquad (8)$$

The same is obviously valid for a sign-sign correlation of link functions, while the links are separated by $|\tau-\tau'|\gg 1/\Delta E$. Therefore the coordinate distribution at any particular τ and the total sign of the integrand in eq.(1) do not correlate, if a path "length" in τ is large enough: $\tau_0 \gg 1/\Delta E$.

To illustrate this observation we simulate a system of L fermions with a mass $m = 1$ moving in d-dimensional oscillator potential

$$V(x) = x^2/2 \qquad (9)$$

using both the Langevin method and Metropolis one. The results given in Table 1 support well the validity of eq.(7).

3. Now we present a more exciting observation, based on a bit more subtle but convincing enough to be considered seriously arguments. Let us treat the quantity

$$S = \sum_{n=1}^{N} S_{eff}(x_n, x_{n+1}; \Delta\tau) \qquad (10)$$

as a <u>true</u> action of our fermion system. Then the integration of the Langevin equations

$$\frac{dx_n^\ell}{d\lambda} = -\frac{\partial S}{\partial x_n^\ell} + \eta(\lambda) \qquad (11)$$

is nothing but a procedure of stochastic quantization of our fermion system. If x_n are started from the real initial values, the domain of their evolution is restricted by the condition $\exp(-S[x]) > 0$ [5] due to the "segregation theorem" [6], therefore <u>any</u> link can never pass through its node and change its sign. This observation allows us to impose a restriction in eq.(1)

$$U(x_n, x_{n+1}; \Delta\tau) > 0 \qquad \text{for } \underline{\text{any}} \ n \qquad (12)$$

before the simulation. Since the integrand is ever positive in this case, any probabilistic Monte Carlo algorithm can be easily applied. In Table 2 we present some results of numerical simulation under this restriction for the system just mentioned above (Langevin method is used here). The data well support the idea.

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TABLE 1. Mean potential energy $\langle V\rangle$ of L fermions in d-dimesional oscillator potential.

d	L	$\langle V\rangle$	$\langle V\rangle_+$	$\langle V\rangle_-$	exact value	τ_0	N	algorithm used
2	2	1.662	1.561	1.508	1.5	8.	40	Langevin
2	2	1.569	1.441	1.595	1.5	8.	40	Metropolis
2	4	4.455	4.200	4.177	4.0	4.	10	Langevin
3	2	2.076	1.997	1.994	2.0	4.	10	Langevin

TABLE 2. Mean potential energy $\langle V\rangle$ of L fermions in d-dimensional oscillator potential (link positivity condition (12) is imposed).

d	L	$\langle V\rangle$	exact value	N	τ_0
2	2	1.574	1.5	10	4.
2	3	2.640	2.5	10	4.
2	4	4.016	4.0	10	4.

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