Journal of Statistical Physics, Vol. 43, Nos. 5/6, 1986

Stochastic Simulation of Fermions

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KEY WORDS: Fermions; Langevin equation; stochastic simulation; quantum Monte Carlo.

The Schrödinger equation for bosons or for distinguishable particles can be formally transformed into a Fokker–Planck equation. The stationary time-dependent correlation functions of the corresponding stochastic process (Langevin equation) coincide with the imaginary time quantum correlation functions. This relation can be used, e.g., to obtain information on the lower-lying spectrum by numerical simulation.[1] In this note we discuss the extension of these ideas for the treatment of fermions in one dimension, and some of the problems that appear in higher dimensions.

We consider the following Langevin equation, with Gaussian white noise ξ

$$\dot{\vec{x}}_i = -\nabla_i W(\vec{x}_1,...,\vec{x}_N) + \vec{\xi}_i, \qquad \langle \xi_i^{(\mu)}(t)\, \xi_j^{(\nu)}(t') \rangle = \sigma \delta_{ij}\, \delta_{\mu\nu}\, \delta(t-t') \quad (1)$$

The corresponding Fokker–Planck equation for the probability density $P(\vec{x}_1,..., \vec{x}_N, t)$ is

$$\frac{\partial P}{\partial t} = \sum_{i=1}^{N} \nabla_i \cdot (\nabla_i W P) + \frac{\sigma}{2} \sum_{i=1}^{N} \Delta_i P \quad (2)$$

Using the stationary density P_5, we express P as $P = P_5^{1/2}\psi$. Then ψ satisfies

$$\frac{\partial \psi}{\partial t} = \frac{\sigma}{2} \sum_i \Delta_i \psi - V\psi \equiv H\psi$$

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0022-4715/86/0600-0865$05.00/0

with

$$V=\sum_i\left[\frac{1}{2\sigma}(\nabla_i W)^2-\frac{1}{2}\Delta_i W\right] \tag{3}$$

P can be expanded in terms of $\{\psi_n\}$, the eigenfunctions of H. The stationary time-dependent correlation function of an observable $A(\vec{x}_1,\ldots,\vec{x}_N)$ becomes

$$S_{AA}(r)=\langle A(o)\,A(t)\rangle=\sum_n|\langle\psi_0|\,A\,|\psi_n\rangle|^2e^{-\lambda_n t} \tag{4}$$

λ_n are the eigenvalues. If one sets $\sigma=\hbar/m$, this expression coincides with the Euclidean groundstate correlation function of the quantum system defined by the Hamiltonian H. Equation (3) is the corresponding Schrödinger equation. P_5 and W can be expressed in terms of the groundstate

$$P_5=\psi_0^2, \qquad W=-\sigma\ln\psi_0 \tag{5}$$

Some of the lower eigenvalues can be obtained by numerical simulation of (1) from the long-time behavior of the correlations (5) for appropriately chosen functions A. This relation between the correlation functions of a quantum and a classical stochastic model is also useful for theoretical reasons, e.g., it allows one to relate dynamical critical properties to static ones in $d+1$ dimension.[1,2]

Equation (5) gives the main condition required to associate a Langevin equation to a quantum system: the groundstate ψ_0 must be real and positive. For bosons and distinguishable particles in any dimension this is guaranteed by the Perron–Frobenius theorem. For fermions in general ψ_0 has positive and negative regions due to the antisymmetry condition. However, in one dimension it is possible to get a relation like (4) by restricting the stochastic process to a region where ψ_0 is positive: The antisymmetrization applies to the total wave function, i.e., including the spin. If one considers spin-independent Hamiltonians, the spatial and spin parts factorize. All the calculations can be done with the spatial part alone; the spin manifests only through the restriction on the symmetry of ψ_n. For example, the He-atom has two independent series of states. The spatial part of the groundstate (singlet) is symmetric and the standard method can be applied. For more than two electrons the groundstate is always antisymmetric with respect to some permutations (since the Hilbert space of spin is two-dimensional it can only compensate the symmetry for 2 df). The states can be classified according to certain irreducible representations of the symmetric group. Since there are no transitions between different series, the

lowest state of each of them can be treated as a groundstate. We consider the case of completely antisymmetric groundstates; analogous arguments can be made for the other symmetries.

Consider first the case of two particles. We are interested in correlation funcions of the form

$$S_{AA} = \sum_n |\langle \psi_0 | A | \psi_n \rangle|^2 e^{-\lambda_n t} \tag{6}$$

where the observable A is symmetric: $A(x_1, x_2) = A(x_2, x_1)$. The expression $\langle \psi_0 | A | \psi_n \rangle$ is different from zero only if ψ_n has the same symmetry as ψ_0, in which case

$$\langle \psi_0 | A | \psi_n \rangle = \int_{\mathbb{R}^2} dx_1\, dx_2\, \psi_0 A \psi_n \equiv \int_{\mathbb{R}^2} dx_1\, dx_2\, f_n \tag{7}$$

f_n is symmetric with respect to the nodal line $x_1 = x_2$, which separates the plane into two regions, D_1 and D_2. Thus

$$\int_{\mathbb{R}^2} dx_1\, dx_2\, f_n = 2 \int_{D_1} dx_1\, dx_2\, f_n = 2 \int_{D_2} dx_1\, dx_2\, f_n \tag{8}$$

S_{AA} can be expressed in terms of integrals over one region, e.g., D_1, where ψ_0 is positive

$$S_{AA} = 2^2 S_{AA}^{D_1} \equiv 2^2 \sum_n \left| \int_{D_1} dx_1\, dx_2\, f_n \right|^2 e^{-\lambda_n t} \tag{9}$$

Since *all* the contributing eigenfunctions are zero at the boundary of D_1, $S_{AA}^{D_1}$ is identical to the correlation function of a stochastic process restricted to the region D_1. Since the potential $W = -\delta \ln \psi_0$ becomes infinite at the boundaries of D_1, the process starting in D_1 stays automatically there.

For N fermions in one dimension we have the same picture: The nodal surfaces $x_i = x_j$ separate $\mathbb{R}^N$ into $N!$ equivalent regions D_i; ψ_0 is positive, e.g., in D_1. Then

$$S_{AA} = (N!)^2 S_{AA}^{D_1} \tag{10}$$

$S_{AA}^{D_1}$ is the correlation function of the stochastic process in D_1. Thus S_{AA} can be obtained by simulating a Langevin equation in a restricted region D_1.

In higher dimensions the situation is different. The nodal surfaces determined by the antisymmetry cannot split the configuration space into disconnected regions. The zeros of the groundstate ψ_0 do give such a

splitting $E_1,..., E_M$, and the integrals in the expression for the correlation function can be restricted to a domain E_1 where ψ_0 is positive

$$S_{AA} = M^2 S_{AA}^{E_1} \equiv M^2 \sum_n \left| \int_{E_1} d\vec{x}_1,..., d\vec{x}_N \, \psi_0 A \psi_n \right|^2 e^{-\lambda_n t} \tag{11}$$

But since the other eigenfunctions ψ_n are not zero at the whole boundary of E_1 (i.e., ψ_n is not necessarily zero everywhere where ψ_0 is), $S_{AA}^{E_1}$ cannot be interpreted as the correlation function of a stochastic process restricted to the domain E_1. The eigenfunctions ψ_n do not satisfy the correct boundary conditions. This method, therefore, cannot be extended to higher dimensions. However, the lower eigenvalues for fermion systems in any dimension, in principle, can be obtained by a Langevin simulation as follows[3]: One simulates with the potential $W = -\sigma \ln(\varphi_0^B)$, where φ_0^B is the completely symmetric (i.e., bosonic) groundstate. If one chooses an $A(x_1,..., x_N)$ having the desired type of antisymmetry, the long-time behavior of S_{AA} gives the eigenvalue of the lowest state having that type of antisymmetry.

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