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LETTER TO THE EDITOR

A Langevin approach to fermion and quantum spin correlation functions

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Abstract. By using spin-coherent states, we show that correlation functions for fermions or quantum spins follow from solutions to Langevin equations associated with a functional integral representation of the partition function. Our method is applicable to any number of dimensions, may also be combined with boson variables, and is suitable for computer simulations.

A functional integral representation for the imaginary-time dynamics or partition function for quantum fermions or spin systems does not readily lend itself to conventional Monte Carlo methods (e.g. a Metropolis algorithm) since the integrand is generally non-positive. To deal with this problem various approximate or indirect techniques have been used, such as the evaluation of fermion determinants by boson functional integrals, inversion of the Dirac operator in the presence of an external field, expansion in hopping parameters, etc. (see e.g. Fucito *et al* 1981, Scalapino and Sugar 1981, Weingarten and Fetcher 1981, Blankenbecler *et al* 1981, Duncan and Furman 1981, Kuti 1981). Making use of occupation number eigenstates, Hirsch *et al* (1981, 1983) reduced a fermion problem to a (quasi-) local multiple sum which can be treated by Monte Carlo methods generally only for one space dimension. In this letter we address these problems by using spin-coherent states and obtain correlation functions of interest by studying a Langevin equation associated with the spin-coherent-state functional integral. If bosons are also present they may be treated by Langevin equations as well (see e.g. Klauder and Ezawa 1983). These methods are applicable to any number of dimensions. For the sake of illustration we confine ourselves to pure fermion or spin-$\frac{1}{2}$ problems.

For a single degree of freedom the spin-coherent states defined for all points on the unit sphere may be taken as ($S_3|0\rangle = \frac{1}{2}|0\rangle$)

$$|\Omega\rangle \equiv |\theta, \phi\rangle \equiv \exp(-\mathrm{i}\phi S_3)\exp(-\mathrm{i}\theta S_2)|0\rangle. \tag{1}$$

These states admit a resolution of unity in the form

$$\int |\Omega\rangle\langle\Omega|\, \mathrm{d}\Omega = 1, \tag{2}$$

where $\mathrm{d}\Omega \equiv (2\pi)^{-1}\sin\theta\, \mathrm{d}\theta\, \mathrm{d}\phi$, when integrated over the unit sphere (see e.g. Klauder 1963, 1982). Tensor products of such states cover multiple degrees of freedom, and fermions are represented by spin operators in the standard manner of Jordan and Wigner (1928). Hereafter, unless stated otherwise, we let $|\Omega\rangle$ and $\mathrm{d}\Omega$ denote the spin-coherent states and associated measures for as many degrees of freedom as are present.

For a Hamiltonian $\mathscr{H}$ and ε small, it follows that

$$e^{-\varepsilon\mathscr{H}} = \int |\Omega\rangle\langle\Omega| \, e^{-\varepsilon h(\Omega)} \, d\Omega, \tag{3}$$

correct to order ε, where $h(\Omega)$ is determined from $\mathscr{H}$ by

$$\mathscr{H} \equiv \int h(\Omega)|\Omega\rangle\langle\Omega| \, d\Omega. \tag{4}$$

For a single spin-$\frac{1}{2}$ degree of freedom $\mathscr{H} = a + \boldsymbol{b} \cdot \boldsymbol{S}$ for some a and $\boldsymbol{b}$; in that case $h(\Omega) = a + 3\langle\Omega|\boldsymbol{b} \cdot \boldsymbol{S}|\Omega\rangle$.† Consequently it follows that

$$Z = \mathrm{Tr}(e^{-T\mathscr{H}}) = \lim_{\varepsilon \to 0} \int \cdots \int \prod_{l=1}^{N} \langle\Omega_{l+1}|\Omega_l\rangle \exp[-\varepsilon h(\Omega_l)] \prod_{l=1}^{N} d\Omega_l \tag{5}$$

where $N \equiv T/\varepsilon$ and $|\Omega_{N+1}\rangle \equiv |\Omega_1\rangle$ (Ciafaloni and Onofri 1979, Onofri 1980).

For ε small and fixed the expression

$$\int \cdots \int e^S \prod_{l=1}^{N} d\Omega, \qquad S \equiv \sum_{l=1}^{N} [\ln \langle\Omega_{l+1}|\Omega_l\rangle - \varepsilon h(\Omega_l)], \tag{6}$$

approximately represents the partition function with $\exp(S)$ as (complex) distribution. If we introduce an auxiliary time τ, in the manner of Parisi and Wu (1981), we can characterise the evolution of any (complex) (non-) equilibrium distribution by a Fokker–Planck-like equation having $\exp(S)$ as equilibrium distribution. For a single degree of freedom this equation is given by

$$\begin{aligned} \partial G(\theta, \phi, \tau)/\partial\tau = \frac{1}{2} \sum_{l=1}^{N} \bigg[& \frac{1}{\sin\theta_l} \frac{\partial}{\partial\theta_l} \left(-\sin\theta_l \frac{\partial S}{\partial\theta_l} + \sin\theta_l \frac{\partial}{\partial\theta_l} \right) \\ & + \frac{1}{\sin^2\theta_l} \frac{\partial}{\partial\phi_l} \left(-\frac{\partial S}{\partial\phi_l} + \frac{\partial}{\partial\phi_l} \right) \bigg] G(\theta, \phi, \tau), \end{aligned} \tag{7}$$

where $\theta, \phi = \{\theta_l, \phi_l\}$. In turn, such a Fokker–Planck equation can be replaced by equivalent (complex) Langevin equations, which again for a single degree of freedom read $(1 \leqslant l \leqslant N)$

$$\begin{aligned} d\theta_l(\tau)/d\tau &= \tfrac{1}{2} \cot[\theta_l(\tau)] + \tfrac{1}{2} \, \partial S/\partial\theta_l(\tau) + \xi_l(\tau), \\ d\phi_l(\tau)/d\tau &= \tfrac{1}{2}\{\sin^2[\theta_l(\tau)]\}^{-1} \, \partial S/\partial\theta_l(\tau) + \{\sin[\theta_l(\tau)]\}^{-1} \eta_l(\tau), \end{aligned} \tag{8}$$

where ξ_l and η_l are independent standard Gaussian white noise sources, i.e. $\langle\xi_l(\tau)\rangle = 0$, $\langle\xi_l(\tau)\xi_l'(\tau')\rangle = \delta_{ll}'\delta(\tau - \tau')$, etc. For almost all solutions of the Langevin equations and for any choice of initial conditions $\theta(0), \phi(0) \equiv \{\theta_l(0), \phi_l(0)\}$, an analogue of the ergodic theorem asserts that

$$\lim_{\Lambda \to \infty} \Lambda^{-1} \int_0^{\Lambda} F\{\theta(\tau), \phi(\tau)\} \, dt = \frac{\int \cdots \int F\{\theta, \phi\} \, e^S \prod_{l=1}^{N} d\Omega_l}{\int \cdots \int e^S \prod_{l=1}^{N} d\Omega_l}. \tag{9}$$

† For a general spin s, $h(\Omega)$ is given simply by reweighting of l $(\leqslant 2s)$ components in an expansion of $\langle\Omega|H|\Omega\rangle$ into spherical harmonics $Y_{l,m}(\Omega)$; see e.g. Gilmore (1976).

Thus we are led to an approximate evaluation of the correlation function $F\{\theta, \phi\}$ in the distribution $\exp(S)$ by means of a long-time average in the auxiliary time τ of $F\{\theta(\tau), \phi(\tau)\}$, where $\theta(\tau)$, $\phi(\tau)$ is a solution of the associated Langevin equation. Note in this approach that the distributions G or $\exp(S)$ and their integrals are not explicitly needed!

The procedure sketched above lends itself to computer simulation where τ plays a role quite analogous to Monte Carlo time†. In this regard we observe that although h is typically non-local for fermions, this non-locality is strictly algebraic and thus easily treated. As defined h may entail large numbers, but they may be eliminated by using another rule to associate $\mathscr{H}$ to a c-number function. For quantum spins no such complications arise. Numerical examples will be presented elsewhere.

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† Since positivity or reality of the distribution is not required by the Langevin method it can be used to evaluate correlation functions for distributions involving general spin-coherent matrix elements (rather than a trace) and/or real time, quantum mechanical systems.