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LETTER TO THE EDITOR

Partition function from the Green function

Y Avishai and J Richert

Centre de Recherches Nucléaires et Université Louis Pasteur de Strasbourg, Groupe de Physique Nucléaire Théorique, BP 20 67037 Strasbourg-Cedex, France

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Abstract. The partition function in quantum statistical mechanics can be expressed as an energy integral of $\exp(-\beta E)$ times the discontinuity of the Green function. A Monte Carlo approach for its evaluation which is not based on path integral representation is suggested. The fermion problem is avoided in the sense that all integrands are positive. Some weak points are underlined. We also discuss the evaluation of statistical averages using the pertinent procedure.

In his study of multiparticle scattering problems, Weinberg discussed the physical content of the many-particle Green function $G(W)$ for energies W outside the spectrum of the Hamiltonian H (Weinberg 1964). Among others, he suggested an obvious expression which relates $G(E \pm i\varepsilon)$ to the partition function in quantum statistical mechanics

$$Z(\beta) \equiv \text{Tr}[\exp(-\beta H)] = \frac{i}{2\pi} \int_0^\infty \exp(-\beta E) \text{Tr}[\Delta G(E)] dE, \quad (1)$$

where

$$\Delta G(E) = G(E + i\varepsilon) - G(E - i\varepsilon). \quad (2)$$

Since an exact solution of the many-body problem is impossible, one should regard (1) as an effective approximation for finite ε .

A great deal of effort has been devoted in recent years to the generation of methods and algorithms for calculating the partition function. Most of them are based on path integrals resulting from a division of the (imaginary) time axis and the use of the generalised Trotter formula (Suzuki *et al* 1977). For the many-fermion problem, it is not always possible to perform the ensuing Monte Carlo simulations since some configurations give negative contributions to the partition function. Thus, a much more sophisticated scheme is required (Hirsch *et al* 1982) which presently is formulated only for one-dimensional models with hopping and nearest-neighbour interactions. Another kind of approach is to use Langevin equations for the time evaluation of the configurations in which the complex 'probability' appears as a force term (G Parisi 1983, Klauder 1983). Numerical tests of this method have not yet been given.

The purpose of the present letter is to examine the possibility of evaluating $Z(\beta)$ by a Monte Carlo procedure starting from (1). The arguments presented below are quite elementary but we are unaware of a similar approach. It should be stressed once

more that, in this equation, ε is fixed but finite so that (1) is only an approximation. In addition, we show how one can evaluate statistical averages using the above procedure.

The algorithm suggested below could be useful mainly for systems which can be described by matrix Hamiltonians. As an example we may consider a system of N fermions occupying $M > N$ single particle levels interacting through the Hamiltonian

$$H = \sum_{\alpha, \beta} t_{\alpha\beta} a_{\alpha}^{\dagger} a_{\beta} + \sum_{\alpha, \beta, \gamma, \delta} v_{\alpha\beta\gamma\delta} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\gamma} a_{\delta},$$

where the indices run over single-particle states, and the fermion operators anticommute, namely $\{a_{\alpha}^{\dagger}, a_{\beta}\} = \delta_{\alpha\beta}$. The basic states are the $\binom{M}{N}$ Slater determinants

$$|\Phi_i\rangle = (N!)^{-1/2} \prod_{k=1}^N a_{\alpha_k}^{\dagger} |0\rangle$$

where $|0\rangle$ is the vacuum and $i = 1, 2, \dots, \binom{M}{N}$ runs over all the N -tuples $\alpha_1 \dots \alpha_N$ of different integers between 1 and M . The evaluation of the matrix elements $H_{ij} = \langle \Phi_i | H | \Phi_j \rangle$ is tedious but standard.

Another system we have in mind is a quantum spin system consisting of N spins, interacting through the Hamiltonian

$$H = \sum_{\langle ij \rangle} H_{ij} \equiv \sum_{\langle ij \rangle} (K_x \sigma_i^x \sigma_j^x + K_y \sigma_i^y \sigma_j^y + K_z \sigma_i^z \sigma_j^z),$$

where the sum runs over nearest neighbours. The Hilbert space is spanned by 2^N states of k spins up and $N - k$ spins down, which we can order by a single index $n = 1, 2, \dots, 2^N$. The evaluation of the matrix elements $H_{mn} = \langle m | H | n \rangle$ is then reduced to $\langle m | H_{ij} | n \rangle$ which is easily evaluated (Suzuki *et al* 1977, equation (2.18)).

It is evident that, as the number of particles becomes large, the matrices H cannot be stored. This is of course a general feature which appears elsewhere. Actually, it is possible in our case to avoid the storage problem by generating the matrix elements each time they are needed. This procedure will consume much more time of course. We can now explain briefly our Monte Carlo approach.

First, let us notice that some modification is needed with regard to the integration range. To be specific, we assume H to be an $N \times N$ matrix so that there is a symmetric interval $[-M, M]$ which includes all the eigenvalues E_n of H . Then, in the energy representation $\text{Tr}(\Delta G) = -2\pi i \varepsilon \sum_n [\varepsilon^2 + (E - E_n)^2]^{-1}$, and (1) should then read

$$Z(\beta) = \varepsilon \int_{-M}^M \exp(-\beta E) \sum_n [\varepsilon^2 + (E - E_n)^2]^{-1} dE. \quad (3)$$

In the limit $\varepsilon \rightarrow 0$ using $\varepsilon/(\varepsilon^2 + x^2) \rightarrow \delta(x)$, equation (3) gives indeed $Z(\beta) = \sum_n \exp(-\beta E_n)$. Actually, some change of variable is needed since we need the δ -function on finite interval so let us assume that this has already been done.

Now, the first point to be noticed is that the term

$$I(E) \equiv \sum_n [\varepsilon^2 + (E - E_n)^2]^{-1} \quad (4)$$

is almost 'naturally' suitable for Metropolis-type Monte Carlo calculation. To see this,

define the operator

$$O(E) \equiv \varepsilon^2 + (E - H)^2 \quad (5)$$

so that $I(E) = \text{Tr}(O^{-1})$. Evidently, $O(E)$ is positive definite, and therefore the integral (summation convention implied)

$$z(E) \equiv \int_{-\infty}^{\infty} \prod_{k=1}^N dx_k \exp(-O_{ij}x_i x_j) \quad (6)$$

exists and is equal to $\pi^{N/2}[\det(O)]^{-1/2}$. Then clearly

$$I(E) = z(E)^{-1} \int_{-\infty}^{\infty} \prod_{k=1}^N dx_k 2 \left(\sum_{m=1}^N x_m^2 \right) \exp(-O_{ij}x_i x_j), \quad (7)$$

which can be regarded as the statistical average of the random variable $y = 2\sum_i x_i^2$ with normalised probability density $P = z^{-1} \exp(-O_{ij}x_i x_j)$. It is now tempting to rush and evaluate $I(E)$ on an energy mesh after which the partition function $Z(\beta)$ can be calculated by one quadrature. However, before elaborating on the positive points, there are two disadvantages of this procedure which should be underlined. The first one is that when the energy E is equal to one of the eigenvalues E_n , then the variance $\sigma = (y^2 - \bar{y}^2)^{1/2}$ is proportional to $1/\varepsilon$ so that many Metropolis iterations may be required just at the most important points. The second disadvantage is that the probability used is not related to the underlying temperature. The equilibrium configuration from which we sample is determined from the distribution of eigenvalues and not from the thermalisation of the system. The attractiveness of (7) is due firstly to the relatively small number of integration variables (namely N) compared with the large number appearing in the time-slicing procedure. Secondly, the probability density is Gaussian, which is always welcome from a practical point of view. Finally, even if the RHS of (7) is evaluated with fewer Metropolis iterations (so that $I(E)$ is poorly approximated) it is expected to exhibit maxima at the eigenvalues $E = E_n$, so that a plot of the approximated $I(E)$ can give a great deal of information about the spectrum of H .

At this point one may notice that in Monte Carlo calculations one computes statistical averages but not the partition function itself. However, from the works of Yang and Lee (1952) it appears that the partition function contains valuable information even without being used in calculation of averages. They have shown that for N Ising spins in an external magnetic field \mathcal{H} the zeros of the partition function $Z(\mathcal{H}, \beta)$ in the complex fugacity ($u \equiv \exp(-2\beta\mathcal{H})$) plane, lie on lines (in the thermodynamic limit) and that in this limit the lines might approach the real axis. A zero of $Z(\mathcal{H}, \beta)$ for real u marks the occurrence of a phase transition. The question of whether zeros of Z (for zero field) in the complex temperature plane fall on lines has recently been discussed (Saarloos and Kurtze 1984). We are unaware of an analogous consideration of quantum spin systems but it is obvious that the zeros of Z have equal significance also in the quantum case.

Thus, the partition function has a merit of its own, but in order to analyse its analytic behaviour its numerical evaluation must be reliable. It is our belief that a Monte Carlo calculation for $I(E)$ equation (7) (on an energy mesh) is feasible, from which $Z(\beta)$ is evaluated according to (3).

Now we can use our formalism also to calculate statistical averages proper and not the partition function itself. Replacing $z(E)^{-1}$ in (7) with $[\det(O)]^{1/2}$ and using

(3) we get (up to an unimportant constant)

$$Z(\beta) = \int dE \prod_{k=1}^N dx_k \exp\{-\beta E + \frac{1}{2} \log[\det O(E)] + \log y - O_{ij} x_i x_j\}$$

$$\equiv \int dE d\mathbf{x} \exp[-S(E, \mathbf{x})] \quad (8)$$

where $y = 2 \sum_i x_i^2$ and the 'action' $S(E, \mathbf{x})$ is real since O is positive definite. Consider for example the statistical average of the energy. It is given by

$$\langle E \rangle = -\partial \log Z / \partial \beta = \int dE d\mathbf{x} E \exp[-S(E, \mathbf{x})] / Z(\beta) \quad (9)$$

which is suitable for Metropolis-type Monte Carlo evaluation, using the normalised probability density $P \equiv \exp(-S) / Z(\beta)$. The price is that $\det(O)$ must be calculated at each iteration, but evaluation of determinants (unlike eigenvalue problems) is a direct procedure. The number of elementary arithmetic operations required to evaluate a determinant grows as $(\frac{2}{3})N^3$ (Knuth 1968).

Another possibility is to use (3) and (4) together with the definition of $\langle E \rangle = -\partial \log Z / \partial \beta$. We then obtain the relation

$$\langle E \rangle = \int \exp(-\beta E) I(E) E dE / \int \exp(-\beta E) I(E) dE, \quad (10)$$

and can evaluate this integral by sampling the energy with probability density

$$P(E) = \exp(-\beta E) I(E) / \int \exp(-\beta E) I(E) dE. \quad (11)$$

The Metropolis test requires the evaluation of the ratio $P(E')/P(E)$ in which the value of I can be calculated in a Monte Carlo algorithm as in (7). The advantage of this method is that the temperature enters explicitly into the probability density so that the sampled energy need not be close to the eigenvalues E_n . Hence the variance in the evaluation of $I(E)$ is reduced. (See the discussion after (7).)

We will now test this last method numerically. Consider a system of two fermions in a truncated space of four single particle levels. This system is described by the second quantised Hamiltonian introduced previously, in which $\alpha, \beta, \gamma, \delta$ run from 1 to 4 on the single particle levels.

Although this is a toy problem, the fermionic degrees of freedom (implied by the anti-commutation relations $\{a_\alpha, a_\beta\} = \delta_{\alpha\beta}$) show up and affect other attempts to apply Monte Carlo simulations (Avishai and Richert 1983).

For the kinetic energy terms $t_{\alpha\beta}$ we took $t_{11} = 0.2, t_{22} = 0.5, t_{33} = 1.0, t_{44} = 2.5, t_{13} = t_{31} = 0.6$, while the potential energy terms assumed the value $v_{\alpha\beta\gamma\delta} (\beta > \alpha, \delta > \gamma) = 1.0$. Our calculations have been performed with $\beta = (kT)^{-1} = 0.5$. At this value of β , the exact value of the averaged energy is $\langle E \rangle_{\text{exact}} = 1.448$. Applying the Metropolis algorithm on (10) we iterated it 450 times and sampled the value of the energy at intervals of ten iterations apart (thus maintaining statistical independence). The arithmetic mean of these 45 samplings was $\langle E \rangle_{\text{MC}} = 1.4626$. This result cannot of course lead to a conclusive statement about the feasibility of the present schemes but it is quite encouraging.

Finally, we want to stress that in this formalism there is no fermion problem. The system under consideration can be bosonic, fermionic, or both. It is sufficient to know the matrix elements of the Hamiltonian H in some (conveniently chosen) complete basis. The operator $O(E)$ defined in (5) is always positive definite.

In summary, we have started from expression (1) (Weinberg 1964) and discussed a Monte Carlo algorithm for calculating the partition function itself as well as statistical averages. This algorithm is not based on a path integral, and is applicable also to fermion systems. We hope to present numerical results in the near future.

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