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Published in:
Physical Review Letters

DOI:
10.1103/PhysRevLett.46.77

Publication date:
1981

PHYSICAL REVIEW
LETTERS

VOLUME 46 | 12 JANUARY 1981 | NUMBER 2

Monte Carlo Calculation of the Thermodynamic Properties of a Quantum Model: A One-Dimensional Fermion Lattice Model

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(Received 29 September 1980)

Starting from a genuine discrete version of the Feynman path-integral representation for the partition function, calculations have been made of the energy, specific heat, and the static density-density correlation functions for a one-dimensional lattice model at nonzero temperatures. A Monte Carlo technique has been used to calculate the temperature-dependent properties. The results are compared with exact calculations for short chains, the Hartree-Fock approximation, and a classical model.

PACS numbers: 05.30.Fk, 05.30.Ch

Starting from the generalized Trotter formula, Suzuki[1] proved that the partition function of a d-dimensional quantum spin model is equivalent to a partition function of a $(d+1)$-dimensional Ising model. A similar correspondence has been established for other quantum models.[2] Because of this equivalence between a d-dimensional quantum model and a $(d+1)$-dimensional classical model, the quantum system can be studied by performing Monte Carlo calculations on the classical model.[3]

In this paper we present results of such a calculation for the one-dimensional (1D) spinless fermion lattice model described by the Hamiltonian

$$H = H_0 + H_1; \tag{1a}$$

$$H_0 = -t\sum_{l=1}^{M} c_l^{\dagger} c_{l+1} + c_{l+1}^{\dagger} c_l, \qquad c_l = c_{l+M}, \quad t > 0; \tag{1b}$$

$$H_1 = v\sum_{l=1}^{M} c_l^{\dagger} c_l c_{l+1}^{\dagger} c_{l+1} = v\sum_{l=1}^{M} n_l n_{l+1}. \tag{1c}$$

The operator $c_l^{\dagger}$ creates a fermion at a site l, n_l is the number operator, t is the energy associated with the motion of the particles, and v is the strength of the interaction. The total number of particles is denoted by N. It is well known that (1) is equivalent to the spin-$\frac{1}{2}$ Ising-Heisenberg chain if $M \to \infty$.[4] For a half-filled band $M = 2N$, the ground state of (1) is the same as the ground state of the antiferromagnet for which quantum effects are known to be very important. As pointed out by Hubbard,[5] the model (1) might be used to describe some of the properties of the tetracyanoquinodimethane salts if more distant interactions are taken into account. These effects are easily included in the scheme presented below.

We now present the essential steps of our calculation. We also start from the Trotter formula[6] but our approach differs substantially from that of Suzuki, Miyashita, and Kuroda.[3] Because H_0 and H_1 are bounded, we have

$$Z \equiv \mathrm{Tr} e^{-\beta H} = \lim_{m\to\infty} Z_m, \tag{2a}$$

$$Z_m = \mathrm{Tr}[\exp(-\beta H_0/m)\exp(-\beta H_1/m)]^m. \tag{2b}$$

The basic idea is to calculate the approximant Z_m and the corresponding thermodynamic quantities and to study the convergence of the results as a function of m. Note that[7] $Z_{2p} \geq Z_{2p+1} \geq Z$ and $Z_m = Z$ for $t = 0$, $v \neq 0$ or for $t \neq 0$, $v = 0$.

By using the fact that H_0 can be diagonalized by

Fourier transformation and introducing complete sets of states, a straightforward calculation yields

$$Z_m = e^{2t\beta N} \sum_{\{P^{(j)}\}} \sum_{\{X_l^{(j)}\}} \rho(\{X_l^{(j)}\}, \{P^{(j)}\}) \operatorname{sgn}(P^{(1)} \cdots P^{(m)}), \tag{3a}$$

$$\rho(\{X_l^{(j)}\}, \{P^{(j)}\}) = \prod_{j=1}^{m} \prod_{l=1}^{N} J(2t\beta/m,\ X_l^{(j)} - X_{P_l^{(j+1)}}^{(j+1)}) \exp[(-\beta v/m)\delta_{(X_l^{(j)} - X_{l+1}^{(j)}) \pmod M, 1}], \tag{3b}$$

$$J(y, X) = M^{-1} \sum_{k=1}^{M} \cos(2\pi k X/M) \exp[-2y \sin^2(k\pi/M)]. \tag{3c}$$

The position of the (l, j)th particle in the 2D model is given by $X_l^{(j)} = X_l^{(j+m)} = X_{l+M}^{(j)}$, $P_l^{(j)}$ is a permutation operator acting on the particle label l, and the superscript (j) labels the distance along the new "Trotter" direction. By a change of variables, (3) can be written as a genuine discrete version of Feynman's path-integral representation[8] for the partition function. In Eq. (3), permutation operators appear in a more symmetric form which is more convenient for numerical calculations. The result (3) is easily extended to the case of more-distant interactions because we have written (3) in the representation that diagonalizes H_1.

For short chains ($M \leq 8$), the summation in Eq. (3) can be done exactly and we have also calculated Z_m, using the formulation of Suzuki, Miyashita, and Kuroda.[3] Comparing these results with those obtained from diagonalizing the Hamiltonian, we concluded that Eq. (3) is a much better approximant than the one used in Ref. 3. For long chains, we calculate the thermodynamic properties by means of importance sampling.

Obviously, a Monte Carlo calculation for a given permutation is feasible[9] but the standard Monte Carlo method for the calculation of Z_m breaks down because it requires all contributions to the partition function to be positive in order to define a transition probability. This problem is solved by defining the following average of a quantity A by $\langle\langle A \rangle\rangle = \mathrm{Tr}(\rho A)/\mathrm{Tr}\rho$ where Tr denotes the sum over all possible configurations and permutations.

Using $E_m = -Z_m^{-1} \partial Z_m / \partial\beta$, we find that the mth approximant for the energy is given by

$$E_m = -\langle\langle \operatorname{sgn}(P) \sum_{j=1}^{m} \sum_{l=1}^{N} \{(t/m)[J(2t\beta/m, Y_l^{(j)} - 1) + J(2t\beta/m, Y_l^{(j)} + 1)] \times [J(2t\beta/m, Y_l^{(j)})]^{-1} - (v/m)\delta_{(X_l^{(j)} - X_{l+1}^{(j)}) \pmod M, 1}\} \rangle\rangle / \langle\langle \operatorname{sgn}(P) \rangle\rangle, \tag{4}$$

where $P = P^{(1)} \cdots P^{(m)}$ and

$$Y_l^{(j)} = X_l^{(j)} - X_{P_l^{(j+1)}}^{(j+1)}.$$

A similar expression is easily obtained for the specific heat. The density-density correlation function is given by

$$\langle n_i n_{i+k} \rangle = \langle\langle \operatorname{sgn}(P) m^{-1} \sum_{j=1}^{m} M^{-1} \sum_{l=1}^{M} \sum_{l'=1}^{M} \delta_{X_l^{(j)} - X_{l'}^{(j)}, k \pmod M} \rangle\rangle \langle\langle \operatorname{sgn}(P) \rangle\rangle. \tag{5}$$

This simple but essential trick allows us to calculate the relevant thermodynamic properties because $\rho/\mathrm{Tr}\rho$ is positive and Monte Carlo techniques can be used to estimate the quantities between double brackets.

It is interesting to note that there is an exact relation between this fermion model and a boson model with a hard-core interaction. In second-order perturbation theory, this boson model is equivalent to the large-U limit of the extended Hubbard model.[10]

The results presented here have been obtained by averaging data of more than four statistically independent runs of at least 10^5 Monte Carlo steps per particle each. In each run more than the first 10^4 Monte Carlo steps per particle were discarded for the sampling procedure. In practice, the maximum value of m is limited, not because of memory requirements, but because the acceptance rate decreases with decreasing β/m. Note also that the statistical errors are proportional to $m^{-1/2}$.

We now discuss the numerical results for $t = 1$, $v = 2$, $N = M/2$, and $M = 32$. For this particular choice of parameters, quantum effects are very

TABLE I. The energy and specific heat for the fermion (boson) model for $\beta = 2$ as a function of m. For comparison, the results obtained by the Hartree-Fock (HF) approximation, the classical limit (CL) $t = 0$, and the exact $N = 4$, $M = 8$ diagonalization are also given.

m	E	C
8	-0.38 ± 0.04 (-0.485 ± 0.002)	0.6 ± 0.1 (0.44 ± 0.02)
16	-0.37 ± 0.03 (-0.421 ± 0.003)	0.1 ± 0.6 (0.36 ± 0.06)
20	-0.36 ± 0.03 (-0.411 ± 0.002)	0.6 ± 0.5 (0.32 ± 0.08)
24	-0.35 ± 0.01 (-0.393 ± 0.006)	0.4 ± 0.4 (0.31 ± 0.08)
HF	-0.293	0.399
CL	0.269	0.420
EX ($M = 8$)	-0.3595	0.0892

important. Obviously, a diagonalization of the Hamiltonian is impossible because this requires the solution of the eigenvalue problem for a $2^M \times 2^M$ matrix.

In Table I, we present results for the energy and specific heat per site for different values of m and $\beta = 2$ which corresponds to a very low temperature. As explained previously, the properties of the fermion model are calculated by simulating a boson model and therefore the results for the latter are also included. In general, the statistical errors on the boson data are considerably smaller than the statistical errors on the fermion data.

Because of the weak m dependence for large values of m, we estimate the energy at $\beta = 2$ to be $E \simeq -0.35$ and comparing this result with the exact ground-state energy[11] $E_0 = -0.345$, we may conclude that we are in the low-temperature regime where quantum effects dominate.

The statistical errors on the specific heat for the fermion model are rather large. This is due to the fact that the fluctuations in the energy are small and therefore difficult to sample, and many more samples would be needed to obtain reasonable statistics. For comparison, the exact results (EX) for eight sites, the results of the Hartree-Fock (HF) approximation, and of the classical limit (CL) $t = 0$ are also given. Because HF approximation is equivalent to a variational principle, it should yield reasonable values for the energy and this is indeed the case.

In Figs. 1 and 2 we have plotted the Fourier-transformed density-density correlation functions

$$S(q) = \langle n_l n_l \rangle + 2 \sum_{k=1}^{M} \cos(2\pi kq/M) \langle n_l n_{l+k} \rangle - \delta_{q,0}(N/M)^2 \tag{6}$$

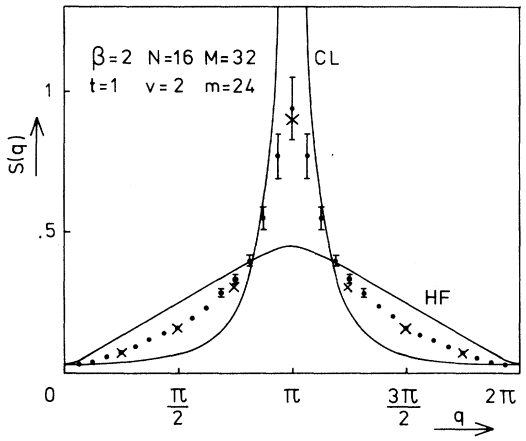

FIG. 1. Comparison between the density-density correlation functions obtained by the Monte Carlo calculation (solid circles), the Hartree Fock (HF) approximation, the classical limit (CL) $t = 0$, and the exact $N = 4$, $M = 8$ diagonalization (crosses). Note that $\beta = 2$ corresponds to a very low temperature.

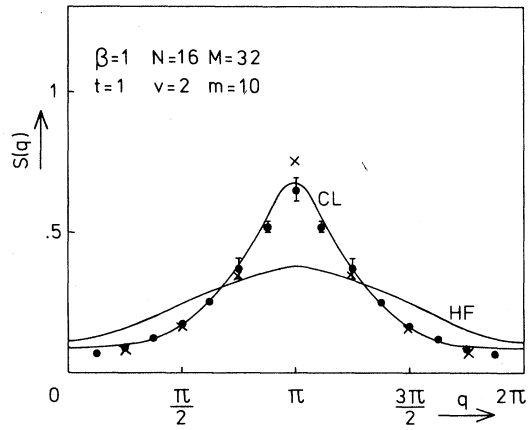

FIG. 2. Comparison between the density-density correlation functions obtained by the Monte Carlo calculation (solid circles), the Hartree Fock (HF) approximation, the classical limit (CL) $t = 0$, and the exact $N = 4$, $M = 8$ diagonalization (crosses).

for different temperatures.

At low temperatures $\beta = 2$, both the HF and the CL approximation are qualitatively wrong. In the CL model, which is equivalent to the 1D Ising model in a field, the correlation function $S(q=\pi)$ diverges as $T \to 0$. For modest temperatures $\beta = 1$, the CL limit and the Monte Carlo results for $S(q)$ are in very good agreement but the energy and specific heat are not. Both figures clearly demonstrate that HF approximation should not be used to calculate correlation functions for this strongly interacting system. Comparing the Monte Carlo data with the exact $N=4$, $M=8$ results, we conclude that it is not necessary to increase the number of sites.

We have shown that it is possible to calculate the temperature-dependent properties of a quantum model with sufficient accuracy. Although we only studied a very simple model, we have chosen a model for which quantum effects are very large. Our approach can be extended to other models such as the spin-$\frac{1}{2}$ Heisenberg model and the extended Hubbard model. An extension to 2D or 3D models is straightforward but it is an open question whether the actual simulations can be done with a reasonable amount of computer time.

The authors thank J. Fivez and B. De Raedt for interesting discussions. This work is supported by the projects "Neutronenverstrooiing" and "Een-dimensionale magnetische systemen" of the Interuniversitair Instituut voor Kernwetenschappen, Belgium.

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Astrophysical Constraints on the Radiative Lifetime of Neutrinos with Mass between 10 and 100 eV/c^2

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Upper limits to astronomical photon backgrounds are used to derive constraints on the radiative lifetime of neutrinos. With the assumption that the radiative decay dominates the decay routes available, comparisons with predicted fluxes exclude radiative lifetimes between 10^{13} and 10^{22}–10^{23} sec for neutrinos which decay to lighter neutrinos and 5–50-eV photons. For $m_{\nu_L} \ll m_{\nu_H}$, this photon-energy range corresponds to a parent-neutrino–mass range of 10–100 eV/c^2.

PACS numbers: 14.60.Gh, 95.85.Mt, 98.70.Vc

Constraints on the radiative lifetime of massive neutrinos have been widely discussed.[1-10] Here we concentrate on the observational constraints on neutrinos in the 10–100-eV/c^2 range, since recent experimental evidence suggests that the mass of the electron antineutrino is within the range 14–46 eV/c^2.[11] Within this mass range, neutrinos would dominate the mass density of the universe without violating the current observational limits on that density.[12-14]

Arguments[4-8] based on distortions to the microwave background, effects on big-bang nucleosynthesis, and the results of laboratory experiments rule out lifetimes less than the decoupling time (10^{12}–10^{14} sec); hence we concentrate on longer lifetimes. We assume throughout that the radiative decay dominates the total decay routes and that the secondary neutrino is very light compared to the parent neutrino. The 10–100-eV/c^2 parent neutrinos then correspond to 5–50-eV decay photons. Note that the lifetime limits as a function of decay photon energy will be independent of this latter assumption.

The most direct limits come from considera-

