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MONTE CARLO METHODS FOR QUANTUM LATTICE MODELS

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Abstract

We discuss a Monte Carlo technique to calculate the thermodynamic properties of quantum lattice models. We use Suzuki's generalized Trotter formula to reformulate the problem in terms of path integrals. Applications treated in detail include the influence of quantum fluctuations on the generalized 1-dimensional classical Wigner lattices introduced by Hubbard and super-localization in Holstein's 1-,2- and 3-dimensional molecular crystal model.

1. Introduction

Although Monte Carlo methods have been widely used in classical statistical mechanics, it is difficult to apply them directly to quantum statistical problems mainly because such theories are formulated in terms of non-commuting variables. Recently Suzuki (1) suggested that this fundamental problem might be solved by using a generalization of the Trotter formula (1). Given the Hamiltonian $H = \Sigma_{\ell=1}^{p} H_\ell$ where each H_ℓ is bounded we have (2)

$$\|\hat{\rho}-\hat{\rho}_m\| \leqslant \frac{2\beta^2}{m} \left(\sum_{q=1}^{p} \|H_q\|\right)^2 \exp\left[\frac{\beta(m+2)}{m} \sum_{q=1}^{p} \|H_q\|\right] , \tag{1.1a}$$

where

$$\hat{\rho}_m \equiv [\exp(\frac{-\beta H_1}{m}) \ldots \exp(\frac{-\beta H_p}{m})]^m \quad , \tag{1.1b}$$

is the m-th approximation to the non-normalized density matrix

$$\hat{\rho} \equiv e^{-\beta H} = \lim_{m\to\infty} \hat{\rho}_m \quad . \tag{1.1c}$$

This formula is used to approximate the partition function

$$Z \equiv \mathrm{Tr}\, e^{-\beta H} = \lim_{m\to\infty} Z_m \quad , \tag{1.2a}$$

by

$$Z_m = \mathrm{Tr}\, \hat{\rho}_m \quad . \tag{1.2b}$$

In practical applications we have to choose H_ℓ such that it is easy to diagonalize each H_ℓ separately. We then insert complete sets of states between all exponential operators, work out all matrix elements analytically and obtain an expression which looks very much like a partition function of a (d + 1)-dimensional classical model (3,4). Formally this approach is closely related to the path integral formulation of quantum statistical mechanics (5,6), the distance in the extra "Trotter" direction playing the same role as the imaginary-time variable appearing in the path integral. In general the (d + 1)-dimensional system is complicated and a rigorous treatment is extremely difficult.

We know from classical statistical mechanics that the Metropolis Monte Carlo method (7) is an efficient importance sampling technique for estimating physical properties within certain statistical errors. The relationship between the quantum problem and the (d + 1)-dimensional lattice model then suggests that one should try to use this computational method to calculate the properties of quantum models. However from (1.1) it is clear that the equivalence between a d-dimensional quantum lattice model and a (d + 1)-dimensional lattice model becomes exact if and only if the size of the lattice in the Trotter direction goes to infinity whereas in most applications and especially in the case where the (d + 1)-dimensional model is simulated by means of a Monte Carlo method it is impossible to calculate the properties of the infinitely large system. Furthermore the quantum nature of the problem causes a number of additional difficulties, which are not present in a Monte Carlo simulations of a genuine classical model. Due to conservation laws (such as conservation of the number of particles, magnetization etc.) there are a large number of configurations with zero weight and

as it is very inefficient to generate these states during the simulation; a substantial amount of extra, complicated, code is required to solve this problem (8,9). In the case of fermion statistics a fundamental problem arises because in most representations some matrix elements of $\hat{\rho}_m$ are negative (5,6).

The basic idea of our approach is to regard (1.1 - 2) as a means of generating systematic approximations to the partition function of the quantum model. Since the Trotter formula (1.1) does not specify how one has to compose the Hamiltonian it is clear that there is the possibility of finding several useful (d + 1)-dimensional representations. Therefore it is necessary to be able to compare the properties of the various approximations on a quantitative basis and more important , it is absolutely necessary to study the convergence of the physical quantities as a function of m. An advantage of working with lattice models is that it is possible to carry out exact (numerical) calculations as long as the system is not too large. Indeed, for small systems one often can diagonalize the full Hamiltonian directly and therefore we can investigate the properties of the approximations as a function of the Trotter dimension. Note that the upper bound Eq. (1.1a) implies that the convergence of the results will be very slow if the temperature goes to zero ($\beta \to \infty$). It is only because detailed model calculations for small systems (10-12) have shown that it is possible to obtain accurate estimates of the thermodynamic properties of the quantum model at low temperatures for a relatively small value of m, that this approach can be expected to work well. In addition we can and should use these exact (numerical) results to check the Monte Carlo algorithm.

2. One-dimensional fermion model

In this section we consider a ring of M sites described by the Hamiltonian

$$H = -t \sum_{i=1}^{M} (c_i^+ c_{i+1} + c_{i+1}^+ c_i) + \frac{1}{2} \sum_{i=1}^{M} \sum_{j=1}^{M} V_{|i-j|} n_i n_j \quad . \tag{2.1}$$

The hopping energy t will usually be taken to be 1 and V_ℓ denotes the ℓ-th neighbor interaction. The fermion operator $c_i^+ (c_i)$ creates (removes) a particle at (from) site i, the operator $n_i \equiv c_i^+ c_i$ counts the number of fermions at sits i, the total number of particles being N.

Model (2.1) is relevant to the description of electron motion in quasi one-dimensional organic conductors (13-15). To a good approximation the electron motion in some of these charge transfer salts is determined by

the spinless fermion Hamiltonian (2.1): $4k_F^e$ in the electron system corresponds to wave vector $2k_F$ in the spinless fermion model (2.1). In the classical limit (t = 0) the model is equivalent to an Ising model with competing interaction which is already a non-trivial many-body system. Pokrovski and Uimim (16) and also Hubbard (14) have given an algorithm to determine the ground-state of this classical (Ising-like) model. It has been shown that this classical model has a rich variety of Wigner lattice ground state configurations (14) and exhibits a complete devil's staircase (17). The classical Wigner lattice picture has been put forward by Hubbard (14) and Torrance (18) as a possible mechanism to explain the presence of $4k_F^e$ scattering in X-ray and neutron diffraction experiments on TTF-TCNQ salts (19). If there is only nearest-neigbor interaction the Jordan-Wigner transformation maps the Hamiltonian (2.1) onto the anisotropic spin-1/2 Heisenberg chain

$$H = -\frac{t}{2}\sum_{i=1}^{M}\left(\sigma_i^x\sigma_{i+1}^x + \sigma_i^y\sigma_{i+1}^y + \frac{v_1}{2t}\,\sigma_i^z\sigma_{i+1}^z\right) , \qquad (2.2)$$

where σ_i^x, σ_i^y and σ_i^z stand for the Pauli matrices. The properties of this spin model have been studied very extensively and one can show that if the fermion density $\rho \equiv N/M = 1/2$, the fermion system (with $v_2 = 0$) undergoes a ground-state metal-insulator phase transition at $v_1 = 2t$. For $\rho \neq 1/2$ the system is always metallic (20).

For the sake of simplicity we will confine the discussion of the approximations to the case with nearest-neighbor interaction only. For model (2.1) we can either split up the Hamiltonian in kinetic and potential energy or we can write the Hamiltonian as a sum of local two-site Hamiltonians. The first choice yields an expression for $\hat{\rho}_m$ (10,11) which is formally identical to the path integral of a continuum fermion system (5,6). In the local split-up approach there is the additional freedom of chosing a particular ordering of the site-dependent Hamiltonians and therefore the expression for the approximate partition function will depend on the particular ordering of the site-dependent blocks. (3,4,8)

To study the convergence of the approximations as a function of the Trotter dimension m we first calculate the energy, specific heat and static correlation functions for short chains and we compare these data with the results obtained by diagonalizing the full Hamiltonian (2.1) numerically.

From our exact numerical calculations we conclude that results obtained by means of the path integral representation converge faster than

those obtained by using the local decomposition. We have also carried out a similar calculation for the spin model (2.2) and came to the conclusion that in the case of the isotropic ($v_1 = 2t$) Heisenberg chain the two-site approach is superior (12). We have chosen the path integral approach as the basis for our Monte Carlo work because it is more general and converges faster. To simulate the fermion system we only need to make a slight modification to the standard Monte Carlo algorithm in order to remove the problem of negative transition probabilities (10, 11). To test the Monte Carlo procedure we first reproduce the exact (numerical) results for small systems for a set of model parameters and several values of m. We have found good agreement between exact and simulation data for all systems for which the exact (numerical) results can be obtained with modest computational efforts. This apparently is not the case for an algorithm (22) that implements the Barma and Shastry break-up (4). This shortcoming can be due to the fact that their algorithm is unable to select all possible states: it does not generate an ergodic Markov chain.

We now discuss some of our simulation results. Detailed information about the arrangement of the particles can be extracted from the static structure factor S(q). We have previously demonstrated (10,11,23) that our simulation data are in agreement with the behavior expected in all special cases of the model (2.1). An interesting problem that is not yet amenable to conventional treatment but can be studied by means of our method is the influence of a non-zero transfer energy t on classical 1 - d Wigner lattices. For $\rho = 13/32$ (which is approximately equal to the charge transfer in TTF-TCNQ) the classical ($t = 0$) ground state configuration is given by $|1010010100101001010010100101010 0>$ (23). For this configuration S(q) peaks at $q = 13\pi/32$, $19\pi/32$. The arrows in Fig. 1 indicate the position of the wave vectors $2k_F$ ($= 13\pi/16$) and $2(\pi - k_F)$. In Fig. 1 we show simulation data for the set of parameters that should correspond to the case of TTF-TCNQ (14). The plots demonstrate the effect of turning on the more-distant interactions. Our simulation data indicate that the nearest neighbor interaction is not sufficient to have a pronounced maximum at $2k_F$. The hopping term redistributes the spectral weight in such a way that a large number of configurations gives a large contribution to the structure factor and wipes out most of the details of the classical Wigner lattice. As soon as the next-nearest neighbor interaction is turned on S(q) peaks in the neighborhood of the expected

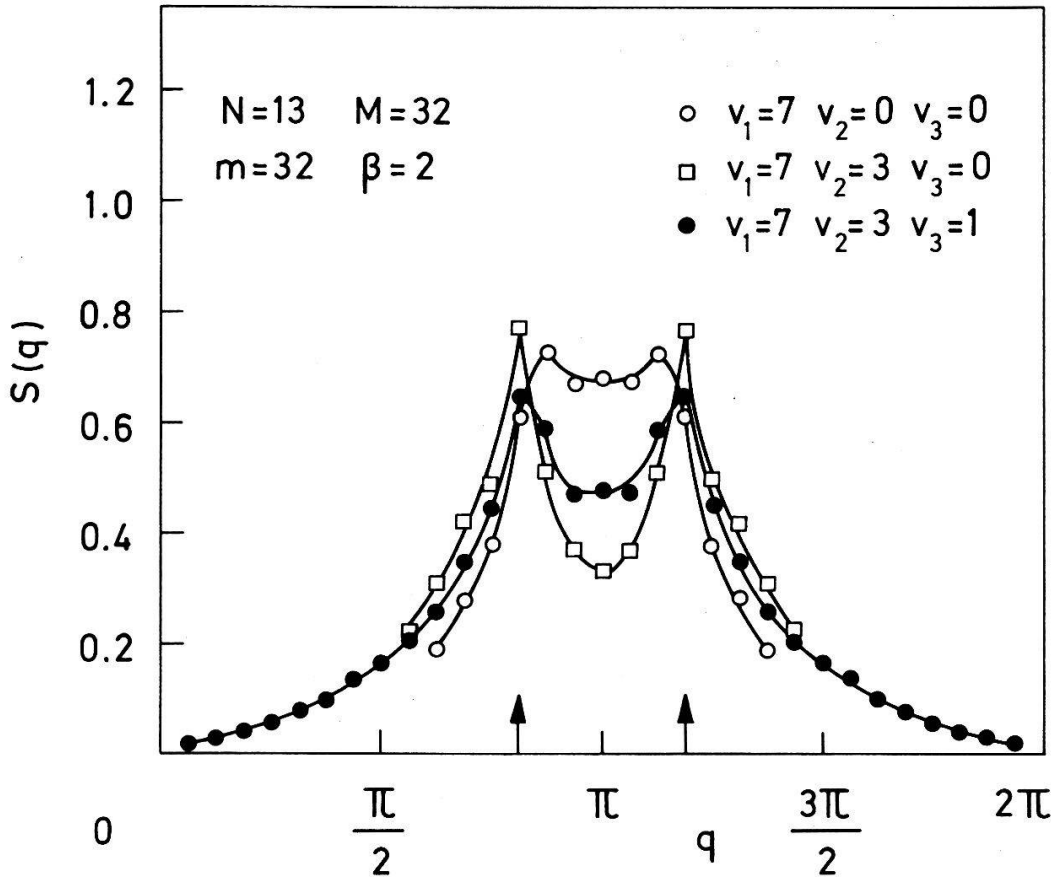

Fig. 1. The wave vector dependent static structure factor S(q) of a one-dimensional system of interacting spinless fermions for several values of the near-neighbor couplings V_ℓ. Solid lines are guides to the eye only.

q-values. Apparently a non-zero next-next-nearest neighbor interaction reduces the difference between the weights of the $2k_F$ satellites and the $q = \pi$ configuration, a behavior which is difficult to understand on the basis of simple intuitive arguments. From our simulation data (23) we conclude that the behavior of a system with a half-filled band ($\rho = 1/2$) is different from that of a system where the band is not half-filled ($\rho \neq 1/2$).

3. Electron-phonon model

In this section we study a lattice model in which one electron is coupled linearly to the lattice displacement of the site where it resides. Our goal is to calculate the thermodynamic properties of Holstein's molecular crystal model (24-27), a model that is frequently used to describe small

polarons. We assume that the electron moves in a d-dimensional hypercube of linear size M and that there is only one lattice degree of freedom per site. For simplicity of notation we will formulate the theory in one space-dimension. The formulas for 2- and 3-d systems can be derived in exactly the same way. The model Hamiltonian reads

$$H = H_1 + H_2 + H_3 \,, \tag{3.1a}$$

$$H_1 = \frac{1}{2} \sum_{i=1}^{M} p_i^2 \,, \tag{3.1b}$$

$$H_2 = \frac{\omega_0^2}{2} \sum_{i=1}^{M} x_i^2 + \frac{\omega_1^2}{2} \sum_{i=1}^{M} x_i x_{i+1} + \lambda \sum_{i=1}^{M} x_i c_i^+ c_i \,, \tag{3.1c}$$

$$H_3 = -t \sum_{i=1}^{M} (c_i^+ c_{i+1} + c_{i+1}^+ c_i) \,. \tag{3.1d}$$

The mass of the oscillators is taken to be 1, $\Omega(q) \equiv (\omega_0^2 + \omega_1^2 \cos q)^{1/2}$ is the frequency of a vibration with wavevector q, λ is the electron-lattice coupling strength and t is the kinetic energy associated with the nearest-neighbor hopping motion of the electron or hole. Momentum and displacement of the lattice distortion at site i are denoted by p_i and x_i.

To derive a path integral representation of the partition function we decompose the Hamiltonian according to (3.1a) and use the Trotter formula (1.1). We can evaluate the integrals over all phonon coordinates and electron momenta analytically and find that $Z_m = cZ_m^B Z_m^F$, where c is an unimportant numerical factor . Formally our result (28-30) is identical to the Feynman path integral for the large polaron model (5). Z_m^B is the approximation to the partition function of the free-phonon system,

Z_m^F describes an effective electron system with nearest-neighbor coupling and retarded long-range interactions caused by the electron-phonon coupling. The calculation of the electron contribution Z_m^F is not trivial and we are forced to use the Monte Carlo method to calculate estimators of the expectation values.

The thermodynamic functions of interest are the approximations to the polaron energy and derivatives of the polaron free energy $F_m^F = -\frac{1}{\beta} \ln Z_m^F$ with respect to the coupling λ. The first derivative of the free energy is related to the expectation value of the electron-phonon interaction energy $\Sigma_i x_i c_i^+ c_i$. The fluctuation on this quantity is given by

$$\Delta F_m^F = \frac{\partial^2 F_m^F}{\partial \lambda^2} + \frac{1}{\lambda}\frac{\partial F_m^F}{\partial \lambda} \tag{3.2}$$

A discontinuity in $\partial F_m^F/\partial\lambda$ or ΔF_m^F as a function of λ means that the free energy is not an analytic function of the coupling λ and in analogy with the theory of phase transitions this indicates that the system undergoes a (ground state) transition.

We now summarize some of our simulation results. From a comparison of simulation data, weak-coupling and strong-coupling results for the energy (28,29) we conclude that the simulation data are in good agreement with either weak-coupling theory as long as λ is smaller than a critical value λ_c or strong coupling theory if $\lambda > \lambda_c$. This is illustrated in Fig. 2 where we compare E_m^F and the results of weak- and strong coupling theory for the ground state energy in the case of 2- and 3-dimensional electron motion. This plot also shows that $\beta = 5$ corresponds to a very low temperature for these systems. The kinetic energy decreases rapidly as the coupling λ increases. In the

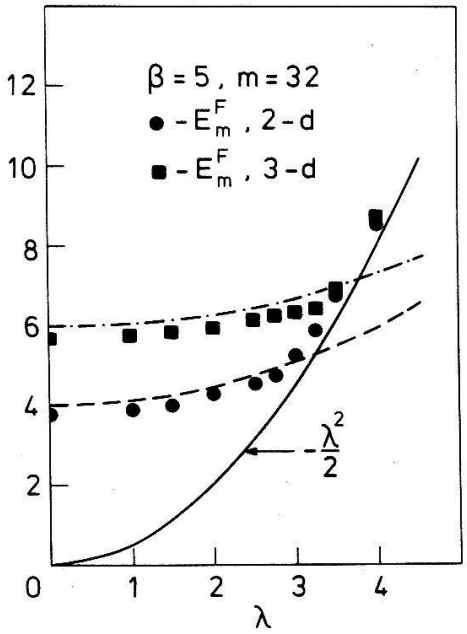

Fig. 2. Comparison between the ground state energy (dashed line: 2-d model, dashed-dot line: 3-d model) obtained from second order perturbation theory, the energy in the strong-coupling regime (solid line) and simulation data for E_m^F (solid dots: 2-d model, solid squares: 3-d model). This plot shows that in our units ($t = 1$, $\Omega = 1$) the inverse temperature $\beta = 5$ corresponds to a very low temperature.

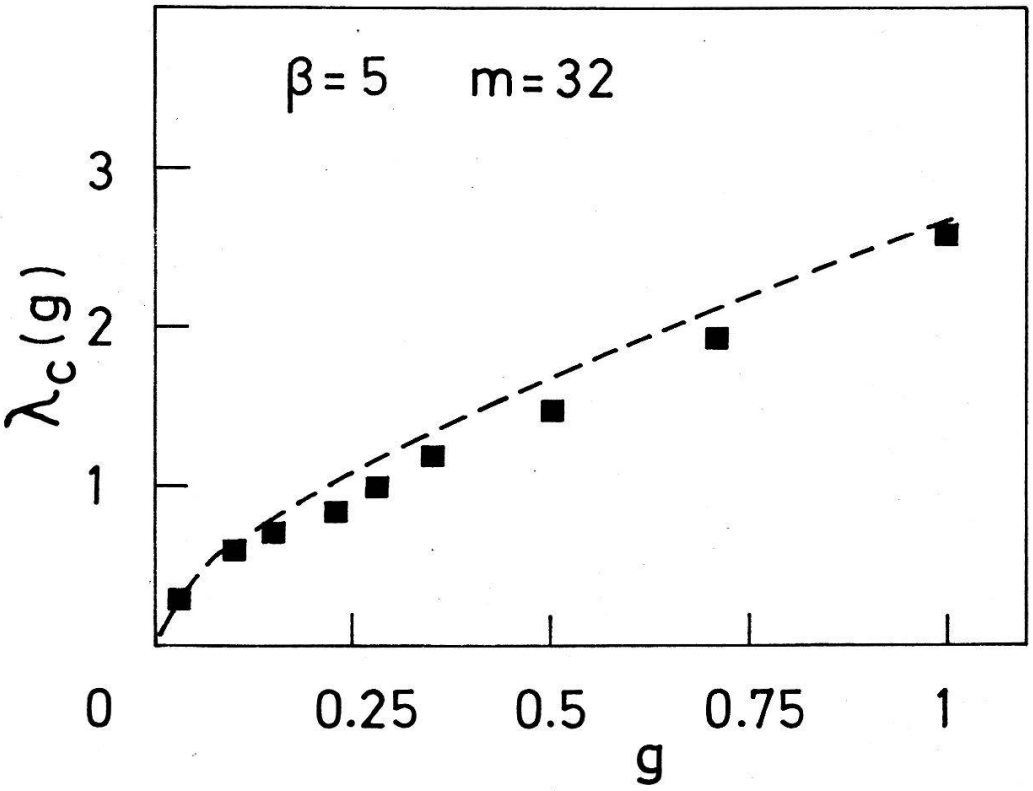

Fig. 3. The critical value λ_c of the electron-phonon coupling as a function of the phonon gap g at the Brillouin zone boundary. The dashed line is a theoretical result obtained from comparison of weak and strong coupling expansions.

neighborhood of λ_c, ΔF_m^F has a pronounced maximum. To a good approximation, the peak position λ_c can be found by equating the weak- and strong-coupling expansion of the ground state energy. Simulation data for 1-, 2- and 3-dimensional systems show essentially the same features. The larger the spatial dimensionality, the larger are the fluctuations ΔF_m^F. The fluctuations decrease with increasing temperature. In the critical region the kinetic energy of the 2- and 3-model drops more rapidly than in the 1-d case. This is consistent with the observation that the transition in two and three dimensions is more abrupt than in one dimension.

In Fig. 3 we depict the dependence of the critical coupling λ_c on the gap g of the phonon dispersion at the Brillouin-zone boundary $q = \pi$. Here we have chosen the parameters ω_0 and ω_1 such that $\omega_0 = (1 + g^2)/2$ and $\omega_1 = (1 - g^2)/2$. We conclude that within the limitations of the Monte Carlo method (7) there is strong evidence that the critical value of λ below which

self-trapping does not occur, goes to zero if the optical phonons become soft (30).

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