Numerical study of a Projected Hubbard Model

K. Michielsen and H. De Raedt
University of Groningen
NL 9700 AV Groningen, The Netherlands

Abstract. The extension of a generalized Hubbard model, recently introduced by A. Montorsi and M. Rasetti, is studied by means of numerical diagonalization, Quantum Monte Carlo and variational methods. Exact results for lattices up to 4×4 are presented. Quantum Monte Carlo simulations reproduce our exact numerical results. We use these data to assess the accuracy of variational (including generalized BCS like) methods.

Introduction

Recently A. Montorsi and M. Rasetti (MR) [1] showed that a generalization of the Kivelson, Schrieffer, Su, and Heeger (KSSH) model [2] is exactly solvable in any dimension by expressing the free energy in terms of a simple quadrature [1]. As the MR model describes (strongly) interacting fermions on a lattice, it is of considerable interest to explore its phase diagram and other physical properties. To this end it is necessary to develop numerical techniques to calculate quantities other than the free energy (or derivatives of it). In this paper we present the first results of exact numerical diagonalizations, Quantum Monte Carlo simulations and variational calculations and compare our results to those of MR where possible.

The MR model is defined by the Hamiltonian $H = H_0 + H_1$ where $H_0 = -\mu \sum_{i,\sigma} n_{i,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow}$ where μ is the chemical potential, U is the on-site electron interaction and $n_{i,\sigma}$, $\sigma = \uparrow, \downarrow$ denotes the number operator at site i. The kinetic energy $H_1 = (1/2) \sum_{<i,j>} \sum_{\sigma,\sigma'} t^{\sigma,\sigma'} (a^+_{i,\sigma} a_{j,\sigma'} + h.c.) - (1/2) \sum_{<i,j>} \sum_{\sigma,\sigma'} \tilde{t}^{\sigma,\sigma'} (a^+_{i,\sigma} a_{j,\sigma'} + h.c.)(n_{i,-\sigma} + n_{j,-\sigma'})$ differs from the usual Hubbard model kinetic energy in many respects. Firstly, the kinetic energy does not conserve the spin. Physically this may be due to the presence of spin-orbit interactions in the more general Hamiltonian of which the MR model is only the tight-binding approximation. Secondly the last term in H_1 represents the bond charge repulsion, characteristic of the KSSH model. The kinetic energy H_1 assigns different hopping amplitudes depending on the relative site-occupation. Of particular importance is the case where $t^{\sigma,\sigma'} = \tilde{t}^{\sigma,\sigma'} = t$. Then hopping processes between two singly-occupied sites and a doubly and an empty site are inhibited and H_0 and H_1 commute, i.e. the total number of doubly occupied sites and empty sites are conserved quantities. Note that this is also the case for the original KSSH model so that this feature is not a consequence of incorporating spin-flip hopping processes. As it stands H_1 assigns equal amplitudes for hopping from singly-occupied to empty sites and as for hopping from doubly to singly occupied sites. This constraint can be removed by modifying the bond charge term such that $H_1 = (1/2) \sum_{<i,j>} \sum_{\sigma,\sigma'} t^{\sigma,\sigma'} (a^+_{i,\sigma} a_{j,\sigma'} + h.c.) - (1/2) \sum_{<i,j>} \sum_{\sigma,\sigma'} \tilde{t}^{\sigma,\sigma'} (a^+_{i,\sigma} a_{j,\sigma'} + h.c.)(n_{i,-\sigma} + n_{j,-\sigma'} - \gamma n_{i,-\sigma} n_{j,-\sigma'})$.

The key feature of the MR model is that by introducing a new set of local operators $A_i = (a^+_{i,\uparrow} + a^+_{i,\downarrow})/\sqrt{2}$, $N_i = A^+_i A_i$, and $D_i = (a_{i,\downarrow} a^+_{i,\uparrow} + a_{i,\uparrow} a^+_{i,\downarrow} + n_{i,\uparrow} + n_{i,\downarrow})/2$, Hamiltonian H can be rewritten as $H = -\mu \sum_{i,\sigma} (N_i + D_i) + U \sum_i N_i D_i + t \sum_{<i,j>} \kappa_{i,j} (A^+_i A_j + h.c.)$ where $\kappa_{i,j} = 1 - D_i - D_j + \gamma D_i D_j$. As all D_i commute with all A_i and all A^+_i it follows immediately that the grand canonical partition function can be written [1] as $Z = Tr e^{-\beta H} = Tr e^{-\beta H_0} e^{-\beta H_1} = \sum_{s_i=0,1} tr e^{-\beta H}$ where tr denotes the trace over all spinless fermions (A^+_i, A_i) and the s_i denote the eigenvalues of the idempotent operators D_i. As H is a quadratic form of the spinless fermion operators the trace tr can be performed analytically [3] yielding $Z = \sum_{s_i=0,1} \prod_i e^{\beta \mu s_i} det[1 + \exp(-\beta M(\{s_i\}))]$, where $M_{i,i} = -\mu + U s_i$, $M_{i,j} = t(1 - s_i - s_j + \gamma s_i s_j)$ if i and j are nearest neighbors and $M_{i,j} = 0$

otherwise. We use this exact expression for the partition function as the starting point for our numerical work. In contrast to the expression for Z one obtains for the Hubbard model [3], the determinant entering our expression is always positive. This assures that we will not encounter minus-sign problems in the simulations [3], a very nice and important feature.

Exact, Quantum Monte Carlo and Variational Calculations

The most straightforward way to analyse the model is to perform the sum over all possible configurations of the s_i. This requires 2^N (N is the number of sites) evaluations of the determinant of an $N \times N$ matrix. As we have to calculate the exponent of the matrix M in any case, it is expedient to diagonalize M first, then take the exponent and calculate the determinant as a product of all eigenvalues. With modest computational effort we can in this way calculate any relevant quantities for lattices containing up to $N = 16$ sites. For larger lattices we employ the Metropolis Monte Carlo method to sample the space of s_i configurations. We have carefully checked that our Quantum Monte Carlo simulation code reproduces the exact results for lattices up to $N = 16$ sites [4]. Our results [4] do not agree with those obtained from the numerical evaluation of Eq.(19) of [1].

To asses the usefulness of approximation schemes frequently used to explore the properties of models for strongly correlated electrons, we have compared our exact and simulation data with the results of variational calculations [4]. To this end we invoke the variational principle $F \leq F_T + < H - H_T >_T$, where H_T is a suitable trial Hamiltonian and $< X >_T$ is the thermal expectation value of the observable X with respect to the ensemble defined by H_T. Alternatively, we have used the expression for Z and employed the inequality $< e^x > \geq e^{<x>}$ to obtain an upper bound for the free energy F. Our calculations [4] show that taking a Hartree-Fock like trial Hamiltonian or using the inequality mentioned above yield the same expression for the upper bound namely $\beta F/N \leq -\ln(1+e^{\beta\mu}) - \sum_k \ln(1+e^{-\beta E_k})$ where $E_k = -\mu + Us + 2t(1-2s+\gamma s^2)\epsilon_k$, $\epsilon_k = \sum_{i=1,d} \cos k_i$, $s = 1/(1+e^{-\beta\mu})$ and d is the dimensionality of the lattice.

To account for the presence of the spin-flip hopping processes, we take as a generalized BCS trial Hamiltonian $H_{GBCS} = \sum_k \sum_{\sigma,\sigma'} E_k(a^+_{k,\sigma}a_{k,\sigma'} + h.c.) + \sum_k \sum_\sigma a^+_{k,\sigma}a_{k,\sigma} + \sum_k \sum_{\sigma,\sigma'} \Delta_k(a^+_{k,\sigma}a_{k,\sigma'} + h.c.)$. As a first step we specialize to the case $\gamma = 0$. Taking $E_k = -\mu + Us + 2t(1-2s)\epsilon_k$, the corresponding upper bound to the free energy reads $F/N \leq -(1/\beta)\ln(1+e^{\beta\mu}) + \sum_k (E_k/2 - e_k) - (1/\beta)\sum_k \ln(1+e^{-2\beta e_k}) + (U/4-2t)(\sum_k \Delta_k f_k)^2 - 4\sum_k \Delta_k^2 f_k$. Minimizing the upper bound with respect to Δ_k we obtain the gap equation $\Delta_q = -(U/8)\sum_k \Delta_k f_k + (t/2)\sum_k \epsilon_k \Delta_k f_k + (t/2)\epsilon_q \sum_k \Delta_k f_k$ with $f_k = \tanh(\beta e_k)/e_k$ and $e_k = \sqrt{E_k^2/4 + 4\Delta_k^2}$. This gap equation has the same structure as the one studied in the context of layered superconductors [5]. Solving this gap equation numerically, we can compute the upper bound to the free energy [4].

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References

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