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Correlation functions of the Hubbard model at low density in a crossing-symmetric approximation: comparisons with Monte Carlo simulations.

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The accuracy of a simple crossing-symmetric approximation for the fully reducible vertex is tested by comparisons of the spin, charge, and pairing correlations with those obtained by Monte Carlo simulations of the two-dimensional Hubbard model. The approximation under study consists in assuming that for parallel spins the fully reducible vertex vanishes, while for anti-parallel spins it is equal to the *T*- matrix. Up to quarter-filling, accuracies better than 10% are obtained.

1. INTRODUCTION

There are two broad classes of self-consistent approximations used in calculating correlation functions of many-body systems: conserving[1,2] and crossing- symmetric.[3,4] There is no known general scheme which garantees that a crossing-symmetric approximation will also be conserving. What is known however, is that for the one-band Hubbard model, crossing-symmetric approximations built on parquet equations give better agreement with Monte Carlo calculations than conserving approximations[5].

Given the complexity of the above calculations, it is still useful to have some simpler approximation schemes which a) are easier to generalize to more complex models than the nearest-neighbor Hubbard model and b) give more insight into the Physics. For example, it has been shown[6] that even in the intermediate-coupling regime, magnetic correlation functions can quite accurately be computed using the standard generalized random phase approximation (GRPA) scheme, as long as a renormalized value of the interaction U is used. The renormalization comes from short-range T-matrix effects, and hence may be estimated. This approach however fails for the density-density correlation functions, in the sense that there is no known way of estimating the renormalized U.

We propose a simple approximation scheme which is remarkably accurate in the low-density limit. Accuracy here means that up to about quarter-filling, all the usual correlation functions obtained by Monte Carlo in both the particle-hole and particle-particle channels are reproduced to better than 10%.

2. CROSSING SYMMETRIC APPROXIMATION FOR THE FULLY REDUCIBLE VERTEX

It is known[7,8] that for short-range potentials, the two-body potential should be replaced by the T-matrix in computing low-energy properties. We go one step further for the Hubbard model by approximating the fully-reducible vertex by the T-matrix. This vertex is defined diagrammatically in Fig 1. In this approximation, incoming particles scatter only if they have opposite spins. The particle-hole channel is obtained by crossing the legs of the above vertex. Self-energy effects are neglected in the Green's function.

Fig. 1: Definition of the fully reducible vertex Γ and its approximation in terms of the T-matrix.

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3. COMPARISONS WITH MONTE CARLO SIMULATIONS

3.1 Particle-hole channel

Simulations are done with the determinental Monte Carlo approach for the two-dimensional nearest-neighbor Hubbard model. A comparison of the spin-spin correlation function appears in Fig. 2. The maximum for the interacting system is displaced from that in the non-interacting one, a qualitative change that our approximation is able to reproduce. The agreement is of the same order for charge-charge correlations.

3.2 Particle-particle channel

The more widely studied particle-particle correlation functions in the context of high-temperature superconductivity are the equal-time autocorrelation functions for the *d*-wave and extended *S*-wave order parameters. Within our approximation, the *d*-wave correlation function is independent of interactions. Fig. 3a shows that this is very well verified up to fillings of order *0.7* where the *d*-wave correlations are enhanced compared with the non-interacting case. The extended *S*-wave case shown in Fig. 3b is non-trivially influenced by interactions. Below quarter-filling $(\langle n \rangle = 0.5)$, interactions reduce the correlations compared with the $U = 0$ case, while above quarter filling they enhance them. This is also reproduced in a quite satisfactory way by our approximation.

4. CONCLUSION

Equal-time correlation functions compare very well with Monte Carlo simulations in the low density limit $(\langle n \rangle < 0.5)$ when the fully-reducible vertex is approximated by the *T*-matrix in a crossing-symmetric manner. Preliminary results indicate that frequency-dependent correlations may be more difficult to reproduce.

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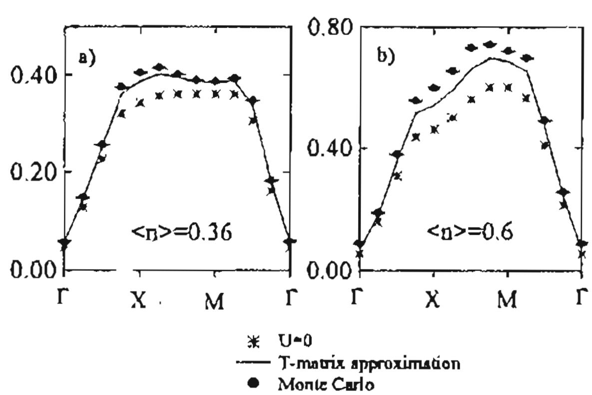

Fig. 2: spin-spin correlation functions as q moves in the Brillouin zone, for U=4t, βt=5 and an 8*8 lattice.

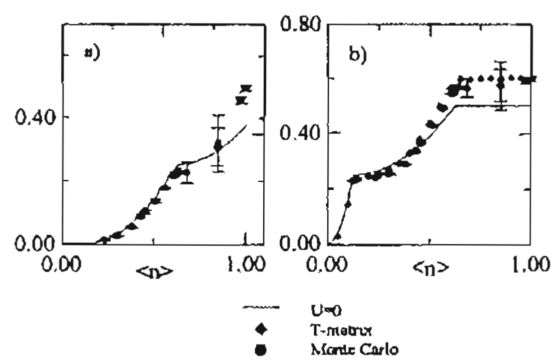

Fig3: $\langle \Delta_D^+ \Delta_D \rangle$ and $\langle \Delta_S^+ \Delta_S \rangle$ as a function of filling for U=4t, βt=6 and an 4*4 lattice.