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Finite-Size Effects in the Negative U Hubbard Model

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Abstract. Using the BCS approach and Quantum Monte Carlo (QMC) simulations, we investigate the size dependence of the pairing correlations in the weak and intermediate coupling regimes. Pronounced finite size effects appear as long as the average spacing of the single-particle levels is larger than or comparable to the characteristic energy scale (superconducting gap). The irregularity of the size dependencies are traced back to variations in the occupation of the highest non-empty energy levels with the system size. We propose means to reduce the size dependence and its irregularity.

Introduction

The occurrence of superconductivity in models for strongly correlated fermions is a topical issue. Numerical methods have been developed to study these models without further approximations in small systems. Studying finite-size effects, we concentrate on the negative U Hubbard model,

$$H = -t \sum_{\langle i,j\rangle\alpha} (c^\dagger_{i\alpha} c_{j\alpha} + \text{h.c.}) - U \sum_i n_{i\uparrow} n_{i\downarrow} \tag{1}$$

as a generic system exhibiting supeconductivity. Because the physical properties of a fermion system strongly depend on the density of states (DOS) at the Fermi level, the shell structure in the DOS on the finite lattice has drastic consequences [1,2]. These effects are significant as long as the average level spacing exceeds the energy scale of the superconducting gap.

Comparison between BCS and QMC

We performed Projector QMC simulations [3] on a two-dimensional lattice to obtain ground state properties and compared the (exact) results with a BCS treatment of (1) at fixed particle number (FBCS [4]). The corresponding component of the variational BCS wave function is projected out, before performing the variation of the parameters in the wave function. The variational equations are then solved numerically.

In Fig.(1), the results of the two methods for the Cooper pair vertex correlation functions

$$\chi_\nu = \frac{1}{N^2} \sum_{kl} f^\nu_k f^{\nu *}_l (\langle c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} c_{-l\downarrow} c_{l\uparrow}\rangle - \langle c^\dagger_{k\uparrow} c_{l\uparrow}\rangle\langle c^\dagger_{-k\downarrow} c_{-l\downarrow}\rangle). \tag{2}$$

are compared in the weak-coupling regime. The perfect agreement with the PQMC data shows that the FBCS wave function serves as a good variational wave function for the ground state on the finite lattice. The FBCS method improves the BCS results. Discrepancies at half-filling can be traced back to enhanced charge-density wave correlations. In the intermediate coupling regime, the FBCS scheme overestimates the superconducting correlations, which are reduced due to quantum fluctuations [5].

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Finite-size effects

Fig.(1) shows the pronounced effects of the DOS shell structure on χ_0. Open shell configuration exhibit strongly enhanced superconducting correlations, which can be understood as a DOS effect. Moreover, we find that the symmetry of the Fermi surface is reflected in the symmetry of the Cooper pair. The fluctuations between open and closed shell configuration get reduced with increasing coupling strength and band filling. However, they complicate any extrapolation to the thermodynamic limit, especially for weak coupling. Finite-size effects are prominent as long as the average level spacing exceeds the energy scale of the superconducting gap. In the weak-coupling regime, this criterion yields as a lower bound on the lattice sizes, where these shell effects disappear,

$$N > \frac{gW}{U}\exp(\frac{W}{U}), \qquad (3)$$

where $W = 4Dt$ denotes the band width on a D-dimensional lattice and g the average level degeneracy. However, the feasability of an extrapolation is improved, if only closed shell configurations are used, as shown in fig.(2). The number of these configurations is enlarged by considering tilted clusters on the square lattice.

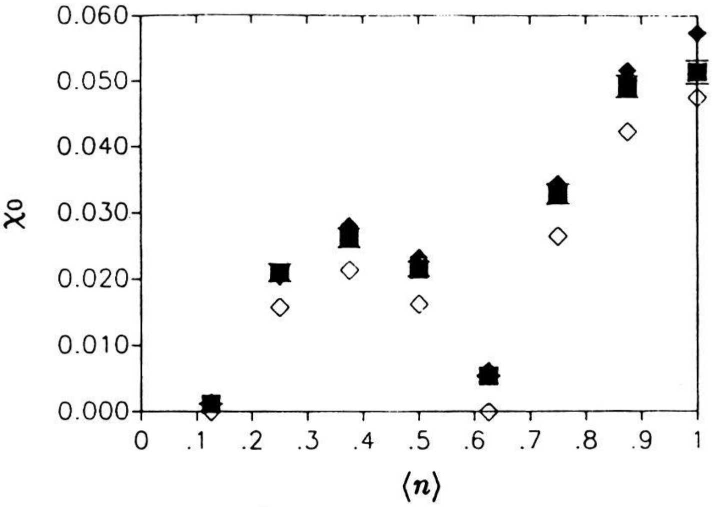

Figure 1. χ_0 ($f_k^0 = 1$) as a function of the band filling $\langle n \rangle$. $4 \star 4$ lattice, $U/t = 1$. Comparison of BCS (◇), FBCS (◆) and PQMC (■) data.

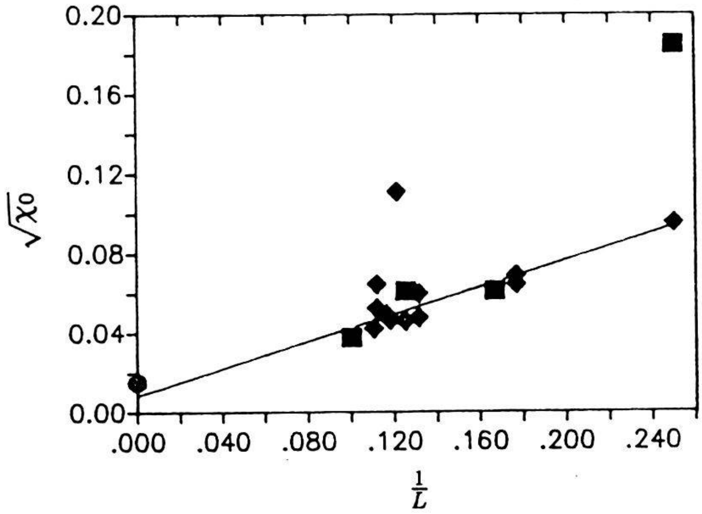

Figure 2. $\sqrt{\chi_0}$ ($f_k^0 = 1$) as a function of the inverese linear lattice size $1/L$. $U/t = 1, \langle n \rangle = 0.75$. FBCS data. The infinite lattice BCS result is indicated.

References

[1] D.Bormann, T.Schneider and M.Frick, *Europhys.Lett.* 14, 101 (1991)

[2] D.Bormann, T.Schneider and M.Frick, submitted to *Z.Phys.B* (1991)

[3] S.E.Koonin, G.Sugiyama and H.Friederich in *Proc.Intl.Symp., Bad Honnef*, Springer, Heidelberg (1982)

[4] P.Ring and P.Schuck, *The Nuclear Many-Body Problem*, Springer, Heidelberg (1980)

[5] R.T.Scalettar, E.Y.Loh, J.E.Gubernatis, A.Moreo, S.R.White, D.J.Scalapino, R.L.Sugar and E.Dagotto, *Phys.Rev.Lett.* 62, 1407 (1989)