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Superconducting ground state of the two-dimensional Hubbard model: a variational study

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Abstract

A trial wave function is proposed for studying the instability of the two-dimensional Hubbard model with respect to d-wave superconductivity. Double occupancy is reduced in a similar way as in previous variational studies, but in addition our wave function both enhances the delocalization of holes and induces a kinetic exchange between the electron spins. These refinements lead to a large energy gain, while the pairing appears to be weakly affected by the additional term in the variational wave function.

1. Introduction

The insulating antiferromagnetic phase of layered cuprates is well described by the two-dimensional Hubbard model at half filling. It is less clear whether this model is also able to describe the superconducting phase observed for hole concentrations $0.05 < p < 0.25$. It has been shown a long time ago that fermions with purely repulsive interactions can become superconducting, but the initial estimates for the critical temperature of continum models were deceptively low [1]. In the mean-time, both analytical and numerical studies have indicated that for electrons on a lattice the situation may not be hopeless. Unfortunately, reliable estimates for the superconducting gap Δ, the condensation energy $W_n - W_s$ or other important quantities for the two-dimensional repulsive Hubbard model and variants thereof are still missing.

Here we report on the current status of our variational studies of the two-dimensional Hubbard model for intermediate values of U and a hole doping $p \approx 0.19$. Our preliminary results for the gap and the condensation energy are consistent with typical experimental values.

2. Variational approach

There are two competing terms in the Hubbard Hamiltonian $\hat{H} = -t\hat{T} + U\hat{D}$, the hopping term between nearest-neighbour sites

$$\hat{T} = \sum_{\langle i,j\rangle,\sigma} (c^{\dagger}_{i\sigma}c_{j\sigma} + c^{\dagger}_{j\sigma}c_{i\sigma}) \,, \tag{1}$$

where $c^{\dagger}_{i\sigma}$ creates an electron at site i with spin σ, and the on-site interaction (the number of doubly occupied sites)

$$\hat{D} = \sum_i n_{i\uparrow}n_{i\downarrow} \,, \quad n_{i\sigma} = c^{\dagger}_{i\sigma}c_{i\sigma} \,. \tag{2}$$

Several variational studies have been performed for the limiting case $U \to \infty$, where double occupancy is completely suppressed [2,3]. This limit is not appropriate for intermediate values of U. We have thus chosen the variational ansatz

$$|\Phi\rangle = e^{-h\hat{T}}e^{-g\hat{D}}|d\text{BCS}\rangle \,, \tag{3}$$

where double occupancy is only partially suppressed (variational parameter g). At the same time both the delocalization of holes and kinetic exchange between spins are enhanced (parameter h). The parent state

$|d\mathrm{BCS}\rangle$ is a BCS state with parameters describing d-wave pairing, *i.e.,*

$$u_{\mathbf{k}}^2 = \frac{1}{2}(1 + \frac{\epsilon_{\mathbf{k}} - \mu}{E_{\mathbf{k}}}), \qquad u_{\mathbf{k}} v_{\mathbf{k}} = \frac{\Delta_{\mathbf{k}}}{2E_{\mathbf{k}}}$$

with

$$E_{\mathbf{k}} = \sqrt{(\epsilon_{\mathbf{k}} - \mu)^2 + \Delta_{\mathbf{k}}^2}, \ \Delta_{\mathbf{k}} = \Delta \cdot (\cos k_x - \cos k_y).$$

We notice that our wave function contains two additional variational parameters, the gap Δ and the "chemical potential" μ (μ is a variational parameter and not the true chemical potential).

The expectation value of the Hamiltonian with respect to our trial state is computed using a Monte Carlo simulation. This is straightforward for $h = 0$, where the BCS state can be projected onto a subspace with a fixed number of particles and written as a superposition of real space configurations. For $h > 0$ the projection onto a state with a fixed number of particles is found to lead to minus sign problems, which worsen as the gap parameter increases. The problem can be solved by using a fixed "chemical potential" (instead of a fixed number of particles) together with a momentum space representation. A Hubbard-Stratonovich transformation is used to decouple the on-site interaction in the Gutzwiller projector. Unfortunately, this approach results in a very slow convergence.

3. Results and conclusions

We have first considered the particular case $h = 0$, which has been studied previously [4]. Fig. 1 shows the energy per site as a function of the gap Δ for several values of U. For $U = 2t$ the numerical precision does not allow to draw any conclusion about pairing, but for $U = 4t$ and $U = 8t$ there are clear minima at $\Delta \approx 0.04t$ and $\Delta \approx 0.05t$, respectively.

Allowing h to vary improves significantly both the energy and the wave function [5,6]. For $U = 8t$, the energy gain due to the refinement of the variational ansatz is two orders of magnitude larger than the condensation energy of Fig. 1. Nevertheless, our first results for $h > 0$ confirm the trend towards d-wave superconductivity, with a gap of about the same size as in Fig. 1.

We briefly comment on the comparison between our results (for $U = 8t$, $t = 300$ meV and $n = 1 - p \approx 0.81$) and experimental data for the layered cuprates. Typical data for the gap parameter found in photoemission experiments are $\Delta \approx 10 - 15$ meV

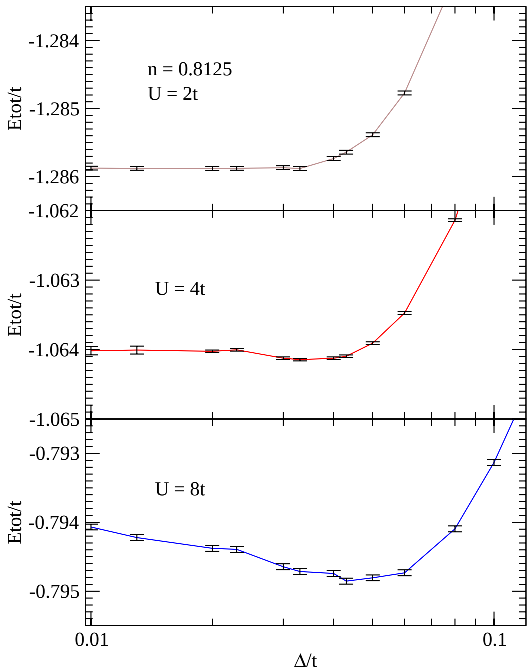

Fig. 1. Total energy per site of a 8x8 square lattice for a density corresponding to the slightly overdoped region of the phase diagram of cuprates.

[7], while the condensation energy obtained from specific heat data is of the order of 0.1 meV [8]. Both experimental values agree surprisingly well with our variational results.

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References

[1] W. Kohn and J. M. Luttinger, Phys. Rev. Lett. **15**, 524 (1965).

[2] C. Gros, Phys. Rev. B **38**, 931 (1988).

[3] A. Paramekanti, M. Randeria and N. Trivedi, Phys. Rev. B **70**, 054504 (2004).

[4] T. Giamarchi and C. Lhuillier, Phys. Rev. B **43**, 12943 (1991).

[5] H. Otsuka, J. Phys. Soc. Jpn. **61**, 1645 (1991).

[6] M. Dzierzawa, D. Baeriswyl and M. Di Stasio, Phys. Rev. B **51**, 1993 (1995).

[7] A. Damascelli, Z. Hussain and Z.-X. Shen, Rev. Mod. Phys. **75**, 473 (2003).

[8] J. W. Loram et al, Physica C **341**, 831 (2000).