ELSEVIER

Physica B 284–288 (2000) 415–416

PHYSICA B

www.elsevier.com/locate/physb

Bulk limit of superconducting condensation energy in 2D Hubbard model

K. Yamaji*, T. Yanagisawa, S. Koike

Electrotechnical Laboratory, 1-1-4 Umezono, Tsukuba Ibaraki 305-8568, Japan

Abstract

We have studied the possibility of superconductivity (SC) in the titled model by computing the SC condensation energy per site as the energy gain in the d-pairing SC state using the variational Monte Carlo method. Its bulk limit was obtained by finite-size scaling with approximately fixed electron density ρ. This value survived finite for $\rho \geqslant 0.84$ when next n.n. transfer energy t' satisfied $-0.25t \leqslant t' \leqslant -0.10t$ with on-site Coulomb energy $U = 8t$; here t is the n.n. transfer energy. The obtained values are of the order of the experimental one for YBCO. © 2000 Elsevier Science B.V. All rights reserved.

PACS: 74.20.Mn; 74.25.Bt; 75.25.Dw; 74.72. − h

Keywords: Hubbard model; Superconducting condensation energy; Variational Monte Carlo method

The possibility of occurrence of superconductivity [1] in the two-dimensional (2D) Hubbard model was denied by several groups [2–6] but supported by some [7,8]. In preceding works [9,10] we performed variational Monte Carlo (MC) calculations with various values of on-site Coulomb energy U, next nearest-neighbor (n.n.n.) transfer energy t', and the lattice sizes. The results indicated that the d-wave superconducting (SC) state has a definite energy gain with reference to the normal state, when t' takes a suitable negative value. In order to judge if the SC energy gain remains finite in the bulk limit, we have extended such calculations to larger lattices with number of sites N_s up to 22×22 with approximately fixed electron density ρ in the range from 0.80 to 0.86 with $t' = 0 \sim -0.30$; energy unit is n.n. transfer t. $U = 8$ is fixed since the energy gain in the SC state is largest around this value [9,10]. Competition with SDW will be studied elsewhere.

Our model is the 2D Hubbard model defined by $H = -t\sum_{\langle jl\rangle\sigma}(c^\dagger_{j\sigma}c_{l\sigma} + \text{h.c.}) - t'\sum_{\langle\langle jl\rangle\rangle\sigma}(c^\dagger_{j\sigma}c_{l\sigma} + \text{h.c.}) + U\sum_j c^\dagger_{j\uparrow}c_{j\uparrow}c^\dagger_{j\downarrow}c_{j\downarrow}$, with the standard notation. $\langle jl\rangle$ and $\langle\langle jl\rangle\rangle$ denote summation over n.n. and n.n.n. pairs, respectively. We evaluate the total energy in the SC state for this Hamiltonian using the variational MC method. Our trial wavefunction is a Gutzwiller-projected BCS-type wavefunction $\Psi_s = P_{N_e}P_G\prod_k(1 + w_k c^\dagger_{k\uparrow}c^\dagger_{-k\downarrow})|0\rangle$, where P_G is the Gutzwiller projection operator with variational parameter g. Projector P_{N_e} assures a fixed total electron number N_e. Coefficient w_k is given by $\Delta_k/(\xi_k + \sqrt{\xi_k^2 + \Delta_k^2})$, where $\xi_k = -2t(\cos k_x + \cos k_y) - 4t'\cos k_x \cos k_y - \mu$ and $\boldsymbol{k}$-dependent gap function $\Delta_k = \Delta(\cos k_x - \cos k_y)$ for d-pairing. $c_{k\sigma}$ is the Fourier transform of $c_{j\sigma}$. The boundary conditions along the x- and y-axis are periodic and anti-periodic, respectively. The ground state energy $E_g = \langle\Psi_s|H|\Psi_s\rangle/\langle\Psi_s|\Psi_s\rangle$ was calculated using an MC procedure. For fixed values of ρ and t' we optimized variational parameters g, Δ and μ by means of the correlated measurements method and then computed E_g with 4×10^8 MC steps. We computed E_g also for a fixed small value of Δ with g and μ optimized again. Assuming the parabola dependence of E_g on Δ we estimated from the two sets of data the energy gain ΔE_g in the SC state with reference to the normal state.

Our main results are shown in Fig. 1. $\Delta E_g/N_s$, which is nothing but the *SC condensation energy*, is plotted as

* Corresponding author. Tel. + 81-298-54-5368; fax: + 81-298-54-5099.

E-mail address: yamaji@etl.go.jp (K. Yamaji)

PII: S0921-4526(99)01983-3

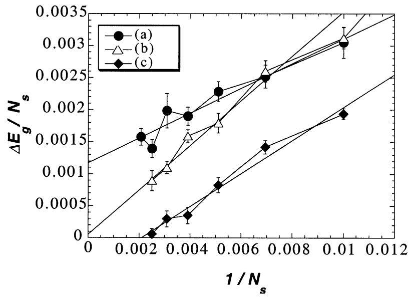

Fig. 1. Energy gain per site $\Delta E_g/N_s$ in the SC state with reference to the normal state is plotted as a function of $1/N_s$ in cases (a), (b) and (c) mentioned in the text.

a function of $1/N_s$. The displayed three series of plots are for the cases of (a) $\rho \simeq 0.86$ and $t' = -0.20$, (b) $\rho \simeq 0.84$ and $t' = -0.15$, and (c) $\rho \simeq 0.80$ and $t' = -0.10$. The treated are square lattices with edge length $L = 10$–22. In case (a) the linear fitting line indicates very clearly that the limit to $N_s \to \infty$, i.e., *bulk limit*, remains finite, giving 0.00117 ± 0.00013. We get the bulk limit of $\Delta = 0.049 \pm 0.005$ similarly. On the other hand, in case (c) the bulk limit vanishes. Case (b) shows a transient situation in-between. The gain per site sharply increased with increasing ρ. When $\rho = 0.84$, it also increased with increase of $|t'|$ in the range $-0.25 \leqslant t' \leqslant 0$ and it started to decrease at $t' = -0.30$. At $t' = 0$ the bulk-limit value vanished in the whole range $0.80 \leqslant \rho \leqslant 0.86$. Thus, the present result indicates that the bulk SC state survives with finite appropriate values of negative t' although at relatively large values of ρ, e.g., $\rho \geqslant 0.84$ when $U = 8$, corresponding to low hole doping. This result strongly supports the assertion that the 2D Hubbard model has SC when t' is finite [7]. It is also not inconsistent with the statement that it has no SC in its simplest form [2–6]. In order to delineate the SC parameter region correctly the present work clearly shows the necessity to take the bulk limit. This work is the first to succeed in obtaining this limit for the SC condensation energy.

The above-mentioned bulk-limit value of SC condensation energy is equal to 0.59 meV/site, if we take $t = 0.5$ eV following [11]. This is in a reasonable range around experimental values ~ 0.26 meV/site estimated from the critical magnetic field [12] and the specific heat [13]. This indicates the relevance of the 2D Hubbard model for the high-T_c cuprates. It should be noted that the t–J model gives a huge condensation energy on the contrary [14].

Acknowledgements

The main part of computation was carried out on the massively parallel computer, Center for Computational Physics, University of Tsukuba.

References

[1] J.E. Hirsch, Phys. Rev. Lett. 54 (1985) 1317.
[2] S.R. White et al., Phys. Rev. B 40 (1989) 506.
[3] N. Furukawa et al., J. Phys. Soc. Japan 61 (1992) 3331.
[4] F.F. Assaad et al., Phys. Rev. B 50 (1994) 12835.
[5] E. Dagotto, Rev. Mod. Phys. 66 (1994) 763.
[6] S. Zhang et al., Phys. Rev. Lett. 78 (1997) 4486.
[7] T. Husslein et al., Phys. Rev. B 54 (1996) 16179.
[8] K. Kuroki et al., Phys. Rev. B 56 (1997) R14287.
[9] K. Yamaji et al., Physica C 304 (1998) 225.
[10] K. Yamaji et al., in: N. Koshizuka, et al., (Eds.), Advances in Superconductivity XI, Springer, Tokyo, 1999, p. 343.
[11] L.F. Feiner et al., Phys. Rev. B 53 (1996) 8751.
[12] Z. Hao et al., Phys. Rev. B 43 (1991) 2844.
[13] J.W. Loram et al., Phys. Rev. Lett. 71 (1993) 1740.
[14] H. Yokoyama et al., J. Phys. Soc. Japan 65 (1996) 3615.