Parameter dependence of the superconducting condensation energy of the two-dimensional Hubbard model

Kunihiko Yamaji [a,1], Mitake Miyazaki [a], Takashi Yanagisawa [a]
[a] *Nanoelectronics Research Institute, AIST Tsukuba Central 2, Tsukuba 305-8568, Japan*

Abstract

Using the variational Monte Carlo method we have computed the t'-dependence of the superconducting condensation energy for the titled model of the size up to 20×20 with electron densities $\cong 0.86$ and 0.84. The energy starts to sharply rise when t' decreases from zero to -0.10, reaching the maximum around $-0.05 \sim -0.10$ and turns to slow decrease, vanishing around -0.35 (in energy unit t). The rising part is in a qualitative agreement with observations.

Key words: superconducting condensation energy; Hubbard model; t'; Monte Carlo; high-T_c

1. Introduction

The possibility of occurrence of superconductivity in the two-dimensional (2D) Hubbard model has a long history of controversy. In preceding works [1,2] we performed variational Monte Carlo (M.C.) calculations with various values of on-site Coulomb energy U, next nearest neighbor (n.n.n.) transfer energy t', and the lattice sizes. These results gave strong positive indications. In particular, the energy gain per site in the the d-wave superconducting (SC) state in reference to the normal state was shown to remain finite in the bulk limit in an appropriate parameter range [2], giving the SC condensation energy E_{cond} comparable to the values obtained from experiments. Recently the superconducting state was rigorously shown to be the most stable state of this model in the weak coupling limit [3]. For these reasons the two-dimensional Hubbard model is believed to contain essential electronic ingredients which give rise to the high-T_c superconductivity. The strongest material dependence giving rise to a wide range of T_c is considered to be extracted into t'. Therefore, its evaluation and how and to what extent it enhances superconductivity are very important issues. In this report by using the variational Monte Carlo method we have computed the t'-dependence of E_{cond} for this model of the size up to 20×20 lattice sites with doped hole densities ~ 0.14 and 0.16 around the optimal hole doping. E_{cond} starts to sharply rise when t' decreases from zero to around $t' \sim -(0.05 \sim -0.10)$ and turns to slow decrease, vanishing around $t' = -0.35$ (energy unit is t). The rising part is in a qualitative agreement with observations.

2. Model and method

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 M. C. method. Our trial wavefunction is a Gutzwiller-projected BCS-type wavefunction $\Psi_{\rm S} = P_{N_e} P_{\rm G} \prod_k (1 + w_k c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}) |0\rangle$, where $P_{\rm G}$ is the Gutzwiller projection operator with variational parameter g. Projector P_{N_e} picks up the component having a fixed total electron number N_e. Coeffi-

[1] Corresponding author. E-mail: yamaji-kuni@aist.go.jp

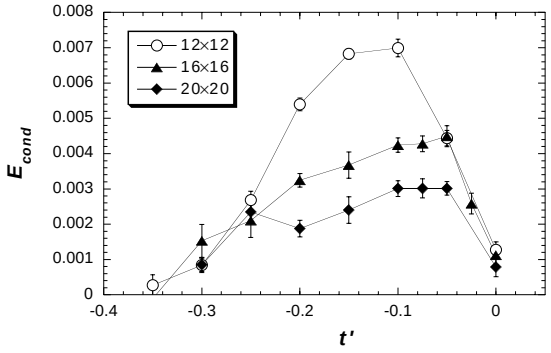

Fig. 1. Computed SC condensation energy E_{cond} plotted against n.n.n. transfer energy t' for $\rho \simeq 0.86$ and $U = 8$ for 12 × 12, 16 × 16 and 20 × 20 lattices.

cient 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 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-axes 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 computed by using a M.C. procedure. For fixed values of electron density ρ and t' we optimized variational parameters g, Δ and μ by means of the correlated measurements method, obtaining E_g. We also computed E_g for the normal state with g optimized. The difference between the two total energies divided by site number N_s is our calculated condensation energy E_{cond}. This way of determining E_{cond} is more faithful to the definition than the way employed previously [1,2].

3. SC condensation energy

Since experimental values of E_{cond} take the maximum when electron density per Cu site $\rho \sim 0.86$ in each family of cuprates, we first compute E_{cond} for $\rho \cong 0.86$ with $U = 8$ (energy unit is t). In Fig. 1 our main results for E_{cond} are shown againt t' for three lattices with 12×12, 16×16 and 20×20 sites. Although E_{cond} values decrease with increasing system size, similar tendencies of the t'-dependence are shared by three curves. The three curves clearly show the tendency that E_{cond} sharply increases as t' starts from zero to the negative side until $t' \sim -(0.05 \sim 0.10)$. The latter values are smaller in the absolute magnitude than the special value of $t' \simeq -0.167$ for which the Fermi level coinsides with the level of the van Hove singularity in the case of $\rho = 0.86$. Then, E_{cond} turns to slow decrease until $t' \sim -0.30$ where it almost vanishes. This overall feature is confirmed to be shared by the case with $\rho \cong 0.84$. These results indicate that E_{cond} is maximized when the Fermi energy for the normal one-electron states lies slightly below the energy level of the van Hove singularity. In such an optimized situation one can confirm that the k-points in the close neighborhood of the van Hove singularity are empty but those slightly far from and below the singularity are occupied. This is understandable from the viewpoint that the present d-wave superconductivity is mainly driven by the electron pair transfer due to the Coulomb scattering between the two sets of the van Hove singularity regions around $(\pm\pi, 0)$ and $(0, \pm\pi)$, respectively, from where the electronic state density is largely contributed.

The shell structure of the electronic filling to the k-points does not seem to give an important influence to the result. In the cases of the 12×12 and 16×16 lattices, all the data points in Fig. 1 are from closed shell except for $t' = -.15$; in the case of 20×20, data points for $t' = -0$, $-.025$, $-.15$ and $-.20$ are from closed shell.

If one represents each family of cuprates by the family member having the maximum T_c in each family, the family with the higher T_c should have the larger value of E_{cond} in the optimally doped state. In the region $-0.1 \leq t' \leq 0$, Fig. 1 is in accord with the result in Fig. 9 of Raimondi et al.[4] plotting the maximum T_c of the family against the calculated value of t'. Another similar result in Fig. 5 of Pavarini et al.[5] shows a similar tendency of T_c against t' while $\mid t' \mid$ is small but its range of this tendency is expanded to $t' \sim -0.40$. This range looks too far in the negative side of t' in view of the present result.

With decreasing doped-hole density E_{cond} was shown to increase [1]. However, this trend was shown to stop around the optimal hole density due to the appearance of the SC state coexisting with the SDW having a stripe structure [6]. These results qualitatively explain the experimental hole-doping dependence of T_c.

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

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