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Spin fluctuations and holon dynamics in the large-U Hubbard model

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Abstract. The spin–holon effective Hamiltonian proposed by Zou and Anderson is used to calculate the chemical potential and the self-energy correction of spinons. Our results show that the effect of spin–exchange interaction is to enlarge the spinon bandwidth. For low temperatures and fixed doping fraction δ, the renormalized bandwidth and the chemical potential are nearly independent of temperature, but both change rapidly with the doping fraction. In the superfluid phase, the effect of increasing the doping fraction or increasing the on-site Coulomb repulsion U is to increase the relative kinetic energy of spinons, leading to a decrease in the superfluid transition temperature $T_s(\delta)$, which is sensitive to various choices of U and the band parameter t; the increase in U tends to shift the boundary of $T_s(\delta)$ towards a lower doping fraction. The correction due to spin fluctuations is extremely important for small doping fractions, leading to modification of the results of Baskaran, Zou and Anderson, and Ruckstein, Hirschfeld and Appel. Moreover, in the region of $\delta \lesssim 8t/\pi^2 U$, the effect of paramagnon fluctuations renders the mean-field theory invalid. We also discuss the effects of holon fluctuations on the mean-field results.

1. Introduction

Recent neutron and Raman scattering experiments have shown clearly that the low-temperature phase of high-temperature superconductors (HTSCs) is antiferromagnetic (AFM) for small doping fractions [1, 2]. The strong two-dimensional AFM correlations extend to the HTSC phase. In the material La_2CuO_4, the correlation length for AFM order in the copper oxide layer decreases from 200 Å in the AFM phase to 10–20 Å in the superconducting phase, as the doping fraction increases [3]. This shows that the spin correlations between the copper atoms are very important on the copper–oxygen plane. Until recently, not much theoretical work has been devoted to the AFM phase transition of HTSC materials.

Recently, the two-dimensional Hubbard model has been extensively used for analysing the physical properties of HTSC materials. The research can be roughly divided into two categories. The most notable is based on the resonating valence bond (RVB) mean-field analysis [4], and the other on the investigation of what the role is played by spin fluctuations [5] in the HTSC mechanism. Research reveals that probably the principal mechanism of HTSCs is similar to that of heavy-fermion superconductivity, i.e. AFM spin *fluctuations lead to anisotropic superconductivity* [6].

In this paper, we discuss the effect of spin fluctuations on the HTSC mechanism [7]. Starting with the effective Hamiltonian of the large-U Hubbard model proposed by Zou and Anderson [8], we investigate the effect of paramagnon fluctuations on the spinon chemical potential and the self-energy correction. The results indicate that, when the doping fraction δ is small, the effect of paramagnon fluctuations on the spinon chemical potential and the self-energy correction cannot be neglected, leading to the modification of the results of Baskaran, Zou and Anderson (BZA) and Ruckenstein, Hirschfeld and Appel (RHA) [4]. In the region $\delta \leqslant 8t/\pi^2U$, the effect of paramagnon fluctuations renders the mean-field theory invalid. The format of the paper is as follows. In the following section, we derive the Zou–Anderson effective Hamiltonian. Then in section 2, within the random-phase approximation (RPA), we calculate the spinon self-energy correction and chemical potential. Recent RPA calculations on the Hubbard model have been attempted [9]; however, it is not the same approximation as used in our present work because our starting point is the Zou–Anderson effective Hamiltonian. In section 3, we discuss the spinon superfluid phase and derive the spinon system Gorkov equations. From that, we solve for the s-wave superfluid phase transition temperature and its relation with the temperature and the doping fraction. The results are compared with the simple BZA and RHA calculations. We finally discuss the effect of holon fluctuations on our mean-field results.

2. Effective Hamiltonian

We start with the Zou–Anderson large-U effective Hamiltonian [8]. In the case of large on-site Coulomb repulsion U, after taking averages of the holons, the effective Hamiltonian can be written as

$$H_{\rm eff} = -t\delta \sum_{\langle ij\rangle\sigma} S^\dagger_{i\sigma} S_{j\sigma} - J \sum_{\langle ij\rangle} (S^\dagger_{i+} S^\dagger_{j-} S_{j-} S_{i+} + S^\dagger_{i+} S_{j+} S^\dagger_{j-} S_{i-}) \tag{1}$$

with

$$\sum_{i,\sigma} S^\dagger_{i\sigma} S_{i\sigma} = N(1-\delta)$$

where $J = 4t^2/U$, and $S_{i\sigma}$ is the neutral fermion field operator; the summations over i and j are confined to pairs of nearest-neighbour sites, and N is the total number of lattice sites on the X–Y plane. The first term describes the kinetic energy of spinons and the second the exchange interaction. This model has three independent parameters: t, J and the doping fraction δ. After taking the Fourier transformation, the Zou–Anderson effective Hamiltonian can be written as

$$H_{\rm eff} = H_t + H_J. \tag{2}$$

In equation (2), the corresponding terms are

$$H_t = \sum_{k,\sigma} \varepsilon_{k,\sigma} S^\dagger_{k,\sigma} S_{k,\sigma}$$
$$H_J = -\frac{ZJ}{2N} \sum_{k,k',q,\sigma} \gamma_q [S^\dagger_{k+q,\sigma} S^\dagger_{k',-q,\bar\sigma} (S_{k',\bar\sigma} S_{k,\sigma} - S_{k',\sigma} S_{k,\bar\sigma})] \tag{3}$$

where $\varepsilon_{k,\sigma} = -Z\delta t\gamma_k$, $\gamma_k = (1/Z)\Sigma_z \exp(\mathrm{i}k \cdot \hat z)$, Z being the number of nearest neighbours denoted by $\hat z$ ($Z = 4$ for square lattice).

3. Spinon self-energy correction and chemical potential

The lowest-order correction (in J) for the spinon self-energy can be obtained from the RPA calculation [10]; one gets

$$\tilde\varepsilon_k = \varepsilon_k - \frac{ZJ}{N} \sum_{k'} \gamma_{k-k'} f_{k'} \tag{4}$$

where f_k is the Fermi–Dirac distribution at a temperature T, $\beta = 1/k_{\mathrm{B}}T$ is the reciprocal temperature and

$$f_k = \{1 + \exp[\beta(\varepsilon_k - \mu)]\}^{-1}. \tag{5}$$

We emphasize here that f_k depends on the chemical potential μ, which is related to the spinon density $N_s/N = 1 - \delta$ being determined only at the end of the calculations.

The paramagnon fluctuations lead to the renormalization of the bare energy of spinons. In order to obtain the lowest-order self-energy correction, we use the bare density of states (DOS) which involves the bare energy ε_k and the bare bandwidth. The approximate DOS in two dimensions can be written as

$$\rho(\varepsilon) = (2/\pi^2 D) \ln|4D/\varepsilon| \tag{6}$$

where $D = 4t\delta$ is the bare half-width. By a lengthy but straightforward calculation, one obtains

$$\tilde\varepsilon_k = -\tilde D \gamma_k. \tag{7}$$

In the notation of BZA and RHA [4], we can write the renormalized half-width as $\tilde D = 4\delta t + 2PJ$ and

$$P = \frac{1}{\pi^2}\Bigg(\left\{1 + 4\ln 2 - \left|\frac{\mu}{D}\right|^2 \left[1 + \ln\left(\left|\frac{4D}{\mu}\right|^2\right)\right]\right\}$$
$$+ \frac{2}{D'^2} \sum_{k=1}^{\infty} \frac{(-1)^k}{k} \left[\!\left[\ln\left(\frac{4D'}{|\mu'|}\right)\left[\left(|\mu'| + \frac{1}{2k}\right)\right.\right.\right.$$
$$\left. - \exp[-2k(D' - |\mu'|)]\left(D' + \frac{1}{2k}\right)\right] - \frac{1}{2k}\Bigg\{1 - \exp(2k|\mu'|)\,\mathrm{Ei}(-2k|\mu'|)$$
$$- \ln(4D')\left[\exp[-2k(D' - \mu')]\left(D' + \frac{1}{2k}\right) - \left(\mu' + \frac{1}{2k}\right)\right]\Bigg\}$$
$$- \exp(2k\mu')\left[\frac{1 - C - \ln(2k)}{2k} - \ln|\mu'|\left[\exp(2k|\mu'|)\left(|\mu'| - \frac{1}{2k}\right) + \frac{1}{2k}\right]\right.$$

$$- |\mu'| \sum_{l=1}^{\infty} \frac{1}{l} \left(\sum_{j=1}^{l} \frac{l(l-1)\dots(l-j+1)}{(2k|\mu'|)^j} \right.$$

$$\left. - \sum_{j=1}^{l+1} \frac{(l+1)l(l-1)\dots(l-j+1)}{(2k|\mu'|)^{j+1}} \right) \Bigg] \Bigg] \Bigg). \tag{8}$$

Here $\mu' = \frac{1}{2}\beta\mu$, $D' = \frac{1}{2}\beta D$ and $C = 0.577215$ is Euler's constant. The function Ei is defined by

$$-\nu^{-1}\,\mathrm{Ei}(-\nu) = \int_1^{\infty} \exp(-\nu x) \ln x \, \mathrm{d}x.$$

In the original BZA and RHA analysis, the term P in equation (8) was set to zero. We find that it is not a true solution to the simultaneous integral equations.

The expression for $\tilde{D}$ is fairly complicated; however, at low temperatures ($\beta \to \infty$) a simple limit can be obtained. The band half-width is increased by an amount $\Delta D = (2J/\pi^2)(1 + 4\ln 2)$. Since the spinon bare energy is given by $\varepsilon_k = -4\delta t \gamma_k$, it can be understood that the effect of the spin correlation on the spinon self-energy correction is to enlarge the bare energy band of spinons. The leading terms of equation (8) can be verified directly from equation (1). The direct term gives the renormalized chemical potential μ, and the exchange term renormalizes the spinon bandwidth, that is

$$- t\delta \sum_{\langle ij\rangle\sigma} S^{\dagger}_{i\sigma} S_{j\sigma} \to -(t\delta + J\langle S^{\dagger}_i S_j\rangle) \sum_{\langle ij\rangle\sigma} S^{\dagger}_{i\sigma} S_{j\sigma}.$$

Let us define

$$\frac{P}{2} = \langle S^{\dagger}_i S_j \rangle = \frac{1}{ZN} \left\langle \sum_i \sum_{\delta} S^{\dagger}_{i+\delta} S_i \right\rangle.$$

Taking the Fourier transform with respect to the spinons,

$$P = \frac{2}{N} \sum_k \gamma_k \langle S^{\dagger}_k S_k \rangle = \frac{1}{N} \sum_k \gamma_k \tanh\left(\frac{\beta}{2}\right)(\varepsilon_k - \mu). \tag{8'}$$

Taking $\beta \to \infty$ and using equation (6) for the DOS, we obtain

$$\lim_{\beta\to\infty} P(\mu, \beta) = \frac{4}{\pi^2 D^2} \int_0^D \ln\left|\frac{4D}{\varepsilon}\right| \varepsilon \, \mathrm{d}\varepsilon = \frac{1}{\pi^2} \left\{ 1 + 4\ln 2 - \left|\frac{\mu}{D}\right|^2 \left[1 + \ln\left(\left|\frac{4D}{\mu}\right|^2 \right) \right] \right\}$$

in exact agreement with equation (8) in the same limit [11].

In view of equation (7), the renormalized bandwidth $\tilde{D}$ is obtained as a function of the chemical potential μ and the temperature T through the Fermi–Dirac distribution. A simple numerical analysis shows that $\tilde{D}$ is not sensitive to the change in temperature. However, as discussed in the following, the chemical potential changes rapidly with the doping fraction δ, and we thus need the study of the chemical potential as a function of the doping fraction and the temperature.

The calculation of the spinon chemical potential is as follows. For large U, the relation between the spinon number and the doping fraction can be approximated by

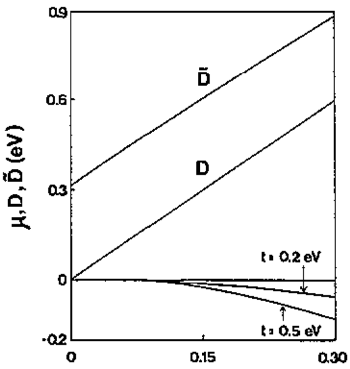

Figure 1. The chemical potential μ and the renormalized bandwidth $\tilde{D}$ versus the doping fraction δ at $t = 0.5$ eV and $U = 2.5$ eV.

$N_s = N(1 - \delta) = \Sigma_{k\sigma} f_k$; hence we get the relation between the chemical potential μ and the doping fraction δ:

$$\delta = \sum_k \tanh\left(\frac{\beta}{2}(\tilde{\varepsilon}_k - \mu)\right). \tag{9}$$

Here, for consistency, we use the renormalized spinon energy $\tilde{\varepsilon}_k$ after considering the corrections of the spinon self-energy by the spin correlation. We expect the computation using the renormalized bandwidth and DOS to be a better approximation. Hence equation (8) can be approximated by the following integral:

$$\delta = \frac{2}{\pi^2 \tilde{D}} \int_{-\tilde{D}-\mu}^{\tilde{D}-\mu} \ln\left|\frac{4\tilde{D}}{x+\mu}\right| \tanh\left(\frac{\beta x}{2}\right) \mathrm{d}x. \tag{10}$$

We obtain the following expression:

$$\delta = \frac{4}{\pi^2 \beta \tilde{D}} \left\{ \ln(2\beta\tilde{D}) \ln\left(\frac{\cosh(\beta/2)(\tilde{D}-\mu)}{\cosh(\beta/2)(\tilde{D}+\mu)}\right) + \beta\mu\left[\ln\left(\frac{\beta|\mu|}{2}\right) - 1\right] \right.$$
$$+ \sum_{k=1}^{\infty} \frac{(-1)^k \exp(-\beta k|\mu|)}{k} \{[\ln(2\beta k|\mu|) + \exp C]$$
$$\left. - \exp(2\beta k|\mu|)\,\mathrm{Ei}(-2\beta k|\mu|)\} \right\}. \tag{11}$$

In equation (11), we obtain the doping fraction δ as a function of μ, $\tilde{D}$ and T. The desired results $\mu(\delta, T)$ and $\tilde{D}(\delta, T)$ can, in principle, be obtained by solving equations (7) and (11). However, owing to the complexities of the equations, we are only able to solve them numerically.

The numerical results show that for low temperatures and fixed δ, with the band parameter $t = 0.2$–0.5 eV and the potential $U = 2$–5 eV, the chemical potential μ and the renormalized spinon half-bandwidth $\tilde{D}$ are nearly independent of temperature, but both change rapidly with the doping fraction δ. From figure 1 we can see that, the larger t becomes, the faster μ decreases with increasing δ, but μ remains nearly zero in the region $\delta < 0.05$, with $\mu = 0$ when $\delta = 0$, which satisfies the half-filled condition. Moreover, the correction of spin fluctuations is extremely important for small δ. For $t =$

0.5 eV and $U = 2.5$ eV, the correction doubles the bare half-width when $\delta \simeq 0.15$, thus rendering the RPA invalid.

In the original BZA and RHA analysis [4], the term P in equation (8′) was completely ignored. We find that in the region $\delta \leqslant t/U$, the spinon fluctuations cannot be neglected. If ε_k is taken as $\bar{\varepsilon}_k$ in equation (8′), a self-consistent integral equation for P is obtained. We also solved this integral equation with equation (9) self-consistently and obtained $\mu(\delta)$ and $P(\delta)$. When the self-consistent solutions were compared with the RPA results, we find excellent agreement, the discrepancy being less than 7% in the whole $\delta \leqslant t/U$ region.

4. Spinon superfluid phase

In the following we discuss the effect of spin fluctuations on the spinon superfluid phase. We introduce the Matsubara Green functions

$$\begin{aligned} G(p, \tau - \tau') &= -\langle T_\tau S_{p,\sigma}(\tau) S^\dagger_{p,\sigma}(\tau')\rangle \\ F_{-+}(-p, \tau - \tau') &= -\langle T_\tau S^\dagger_{-p,-}(\tau) S^\dagger_{p,+}(\tau')\rangle \end{aligned} \tag{12}$$

where T_τ is the time-ordered operator. Using the method of equation of motion, we obtain the following Gor'kov equations [10]:

$$\begin{aligned} -(\partial_\tau - \xi_p) F^\dagger_{-+}(-p, \tau - \tau') + \Delta(p)\, G(p, \tau - \tau') &= 0 \\ -(\partial_\tau + \xi_p) G(p, \tau - \tau') + \Delta(p)\, F^\dagger_{-+}(-p, \tau - \tau') &= \delta(\tau - \tau') \end{aligned} \tag{13}$$

where $\partial_\tau = \partial/\partial\tau$ and

$$\begin{aligned} \xi_p &= \bar{\varepsilon}_p - \mu \\ \Delta(p) &- \frac{J}{N}\sum_q \gamma_q \langle S_{q-p,+} S_{p-q,-} - S_{q-p,-} S_{p-q,+}\rangle. \end{aligned} \tag{14}$$

In equation (14), $\Delta(p)$ is the singlet pair order parameter of the spinon superfluid phase and the gap equation is

$$\begin{aligned} \Delta_p &= \frac{ZJ}{N}\sum_q \gamma_q \frac{\Delta_{p-q}\tanh(\beta E_{p-q})}{E_{p-q}} \\ E_p &= \sqrt{\xi_p^2 + \Delta_p^2}. \end{aligned} \tag{15}$$

By taking Δ_p as $\cos p_x + \cos p_y$ and by using the renormalized bandwidth and DOS, we obtain the following integral equation which determines the s-wave superfluid transition temperature T_s:

$$\frac{\pi^2 \tilde{D}}{8J} = \int_0^1 x^2 \ln\left(\frac{4}{x}\right)\left(\frac{\tanh[\beta_c \tilde{D}(x+y)]}{x+y} + \frac{\tanh[\beta_c \tilde{D}(x-y)]}{x-y}\right) \mathrm{d}x \tag{16}$$

where $y = \mu/\tilde{D}$ and $\beta_c = 1/k_B T_s$. Taking $t = 0.5$ eV and $t/U = 0.2$, and by numerical calculations, we obtain the relation between the s-wave transition temperature T_s and

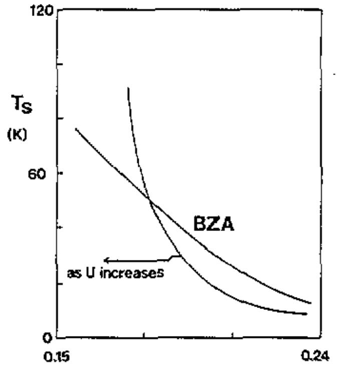

Figure 2. The s-wave superfluid transition temperature T_s versus the doping fraction δ at $t = 0.5$ eV and $U = 2.5$ eV. The results of BZA are also plotted for comparison. As U increases, our curve tends to shift to the left.

the doping fraction δ. As shown in figure 2, the effect of increasing the doping fraction or increasing U is to increase the relative kinetic energy of spinons, leading to a decrease in the superfluid transition temperature $T_s(\delta)$, which is sensitive to different choices of the parameters t and U. The increase in U tends to shift the boundary of $T_s(\delta)$ to the left.

In figure 2, the BZA results are also plotted for comparison. While our results agree qualitatively with those of BZA at large doping fractions, the discrepancy becomes significant for small doping fractions, indicating that the correction due to spin fluctuations cannot be ignored for small δ. The present analysis using the method of spinon self-energy correction is more convenient for studying the magnetic properties of the two-dimensional large-U Hubbard model [12].

5. Discussion

In the above treatment, we consider the collection of holons as a nearly free-boson system which undergoes the Bose–Einstein condensation in the spinon superfluid phase. The mean-field approximation corresponds to taking the Bose condensation of holons and will be valid if a sufficient number of holons exist. We expect the transition temperature of holon Bose–Einstein condensation to be given by $T_b \simeq t(\delta - \delta_c)$, where δ_c denotes the doping fraction at which the superfluid phase starts to emerge.

Here we would like to comment on the above mean-field treatments. In the above calculations we adopt the effective Hamiltonian approach in which the holon operators are replaced by their averages. In this respect the spin fluctuations have explicitly been taken into account and we obtained the spinon self-energy correction. However, in the small-δ region, we expect the holon fluctuations to be equally important.

BZA and RHA [4] explicitly pointed out the inadequacy of the mean-field approximation, which can be overcome by doing a systematic expansion in holon fluctuations. It turns out that by doing this the holon fluctuations couple to the spin fluctuations and the mean-field results are modified. We shall see that the holon fluctuations introduce a ferromagnetic (FM) coupling into the problem. Before taking the average, the kinetic part of the effective Hamiltonian is written as

$$H_t = -t \sum_{\langle ij \rangle} e_i e_j^\dagger S_{i\sigma}^\dagger S_{j\sigma}$$

where e_i is the holon operator. Let us take $e_i = \langle e_i \rangle + B_i = \sqrt{\delta} + B_i$, where B_i represents the fluctuation about the mean-field value $\langle e_i \rangle$. Then H_t is written as

$$H_t = -t\delta \sum_{\langle ij \rangle \sigma} S_{i\sigma}^\dagger S_{j\sigma} + H_{\mathrm{fl}}$$

where H_{fl} is the fluctuation part and

$$H_{\mathrm{fl}} = -t\sqrt{\delta} \sum_{\langle ij \rangle \sigma} S_{i\sigma}^\dagger S_{j\sigma}(B_i + B_j^\dagger) - t \sum_{\langle ij \rangle \sigma} B_i B_j^\dagger S_{i\sigma}^\dagger S_{j\sigma}.$$

Let us assume B_i to be small and ignore the second-order fluctuations. Using the second-order perturbation, we obtain a contribution to the Hamiltonian from the holon fluctuations:

$$H' = \sum_n \frac{H_{\mathrm{fl}}^1 |n\rangle\langle n| H_{\mathrm{fl}}^{1\dagger}}{E_i - E_n}$$

where H_{fl}^1 denotes the first term of H_{fl} and the symbol † denotes Hermitean conjugate. The intermediate state $|n\rangle$ has one extra holon compared with the initial state and thus $E_i - E_n = -E_{\mathrm{h}}$, with $E_{\mathrm{h}} < 0$ being the energy of a holon. Taking the mean holon energy as $\langle E_{\mathrm{h}} \rangle$, we obtain

$$H' = \frac{2t^2\delta}{\langle E_{\mathrm{h}} \rangle} \sum_{\langle ij \rangle \sigma} n_{i\sigma} n_{j\sigma} + \text{self-energy correction term} + \text{chemical potential term}.$$

We can see that H' has exactly the same form as the second term of the effective Hamiltonian (equation (1)) but with opposite sign (since $E_{\mathrm{h}} < 0$). This term introduces a FM coupling which will give a FM phase under appropriate conditions. In order to obtain the FM phase, we calculate the zero-temperature ($\beta \to \infty$) state magnetic susceptibility in the RPA [12]. We obtain the following condition for the FM phase:

$$1 + 4J_{\mathrm{eff}} N(\mu) < 0$$

where $J_{\mathrm{eff}} = J + 2t^2\delta/\langle E_{\mathrm{h}} \rangle$. For a rough estimate, we let $\langle E_{\mathrm{h}} \rangle = -2t < 0$, $N(\mu) = (2/\pi^2 D) \ln|4D/\mu|$ and $\mu(\delta) = 0.5\delta - 1.5\delta^2$, then

$$1 - (4/\pi^2)(1 - \theta/\delta) \ln(16/|3\delta - 0.1|) \leqslant 0$$

where $\theta = 2t/U$. Here we have chosen $t = 0.5$ eV. We obtain a result consistent with the Monte Carlo simulation of Yokouyama and Shiba [13].

In conclusion, we have employed the spin–holon effective Hamiltonian to calculate the chemical potential and the self-energy correction of spinons. Our results show that the effect of spin–exchange interaction is to enlarge the bandwidth. For low temperatures and fixed doping fraction, the renormalized bandwidth and the chemical potential are nearly independent of temperature, but both change rapidly with the doping fraction. In the superfluid phase, the effect of increasing the doping fraction or increasing the on-site Coulomb repulsion is to increase the relative kinetic energy of spinons, leading to a decrease in the superfluid transition temperature, which is sensitive to various choices of U and the band parameter t. The increase in U tends to shift the boundary of $T_{\mathrm{s}}(\delta)$ towards lower doping fractions. The correction due to spin fluctuations is extremely important for small doping fractions, leading to the modification of the results of

BZA and RHA [4]. Moreover, in the region of $\delta \leqslant 8t/\pi^2 U$, the effect of paramagnon fluctuations renders the RPA invalid. We also discuss the inadequacy of the mean-field approximation and the effects of holon fluctuations on the mean-field results.

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