Spin-density wave and superconductivity in an extended two-dimensional Hubbard model with nearest-neighbor attraction

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We study the interplay of antiferromagnetic and superconducting orders in a two-dimensional Hubbard model with on-site repulsion and nearest-neighbor attractive interaction. This type of interaction has been widely used to model *d*-wave superconductivity. Our mean-field calculations indicate that such an attractive interaction enhances the staggered magnetization produced by the on-site repulsion. As a result, superconductivity is strongly suppressed. Stripe formation is also affected.

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I. INTRODUCTION

A salient feature of the high-temperature superconductivity in the cuprates is the association with antiferromagnetism. Besides being an interesting subject by itself, the interaction between those two orders may provide important information on the mechanism of superconductivity.

The current theoretical understanding of the antiferromagnetic order is more complete than that of the superconductivity. A simple on-site Hubbard model seems capable of explaining some features of the antiferromagnetism. In particular, the antiferromagnetic domain-wall-like structures (the stripes[1,2]), which have been receiving increasing experimental support,[3,4] emerge naturally from mean-field study of the Hubbard model.

Most of our knowledge about superconductivity comes from experiment. A completely microscopic understanding of the mechanism is not available yet. There has nonetheless been theoretical activity of modeling superconductivity by employing some effective Hamiltonian. Just like the case where one uses the on-site attractive Hubbard model to study *s*-wave pairing, one is interested in studying models which would generate *d*-wave superconductivity. Indeed, this has been done by adding a nearest-neighbor attractive interaction[5] to the on-site repulsive Hubbard model. Many phenomenological studies of *d*-wave superconductivity[6–12] have been based on this model. In those studies, however, the spin-density wave (SDW) produced by the repulsive interaction has been ignored. A more complete treatment involving both the SDW and superconductivity has been done only recently by Martin *et al.*[13] They showed that superconducting stripes are inhomogeneous solutions of the linearized (mean-field) Hamiltonian.

In deriving the mean-field Hamiltonian, Martin *et al.* have dropped a Hartree term coming from the attractive interaction. They have assumed that such a term is not going to overwhelm the charge and spin order determined by the on-site repulsion. The purpose of this paper is to assess the effect of this term. As we will see, this term does significantly affect the spin and charge orders and thereby strongly suppresses the superconductivity as well.

The extended Hubbard Hamiltonian runs as

$$H=-t\sum_{\langle ij\rangle\sigma} c_{i\sigma}^{\dagger}c_{j\sigma}+U\sum_{i} n_{i\uparrow}n_{i\downarrow}+V\sum_{\langle ij\rangle} n_{i\downarrow}n_{j\uparrow}, \tag{1}$$

the linearization of which leads to the following mean-field Hamiltonian:

$$H_{mf}=-t\sum_{\langle ij\rangle\sigma} c_{i\sigma}^{\dagger}c_{j\sigma}+U\sum_{i} (n_{i\uparrow}\langle n_{i\downarrow}\rangle+\langle n_{i\uparrow}\rangle n_{i\downarrow}) +V\sum_{\langle ij\rangle} (n_{i\downarrow}\langle n_{j\uparrow}\rangle+\langle n_{i\downarrow}\rangle n_{j\uparrow})+\sum_{\langle ij\rangle} c_{i\downarrow}c_{j\uparrow}\Delta_{ij}^{*}+\text{H.c.}, \tag{2}$$

where $\Delta_{ij}=V\langle c_{i\downarrow}c_{j\uparrow}\rangle$ is the superconducting order parameter and $n_{i\sigma}$ is the number operator (the Hamiltonian H_{mf} is the subject of the present study) and

$$V\sum_{\langle ij\rangle} (n_{i\downarrow}\langle n_{j\uparrow}\rangle+\langle n_{i\downarrow}\rangle n_{j\uparrow}) \tag{3}$$

is the Hartree term that has been ignored by Martin *et al.*

II. METHODOLOGY

To solve H_{mf} we follow the standard iterative procedure. For a given initial set of $\langle n_{i\sigma}\rangle$ and Δ_{ij}, the Bogoliubov–de Gennes equations are solved numerically and the electronic wave functions obtained are used to calculate the new $\langle n_{i\sigma}\rangle$ and Δ_{ij} for the next iteration step. The calculation is repeated until the solution converges. By varying the chemical potential, one obtains solutions corresponding to various doping concentrations. Periodic boundary conditions are adopted for both the x and y directions. We refer to earlier publications[6,13] for details of this numerical procedure.

III. RESULTS

Hereafter we take $t=1$, $U=4$ and measure energies in units of t. For $V=0$, the ground-state configuration of the half-filled case is well known to be a uniform spin-density wave. The magnitude of the staggered magnetization $|m_i|=|\langle n_{i\uparrow}\rangle-\langle n_{i\downarrow}\rangle|$ is about 0.69. A negative V enhances the magnetization. It also widens the single-particle energy gap, as shown in Fig. 1. This enhancement can be understood by noting that at half-filling, apart from a constant, the expectation value $\langle n_{j\downarrow}\rangle$ in Eq. (3) can be replaced by $-\langle n_{i\uparrow}\rangle$ assuming a uniform SDW in the ground state. The Hartree term is

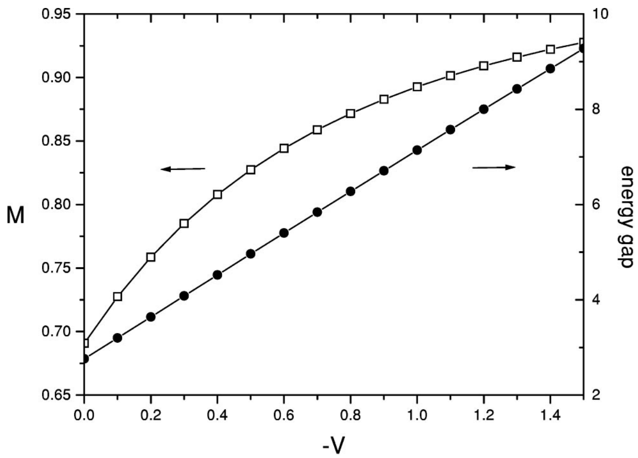

FIG. 1. Staggered magnetization (□) and single-particle energy gap (●) as a function of $-V$ for a 12×12 lattice at half-filling.

then equivalent to a linearized on-site Hubbard term with $U=-4V$.

As we have alluded to in the Introduction, the original intention of introducing a negative V is to produce d-wave superconductivity. In the absence of the Hartree term, a SDW ground state produced by U can be made superconducting by making V sufficiently negative. For example, for $U=4$ the d-wave superconducting order parameter Δ_d is essentially zero for $|V|$ less than 3.6 but it increases to 0.4 for $V=-4.4$, as seen in Fig. 2. It turns out that the order parameters are not uniform even for the half-filled case. The range of the order parameters is indicated by the error bars. The magnitude of the SDW is also displayed in Fig. 2.

As soon as the Hartree term (3) is reinstated, however, Δ_d is always negligible for half-filling and for any doping concentration. The result can be interpreted as the enhancement of antiferromagnetism by the Hartree term. In other words, a negative V will generate a SDW which is strong enough to suppress the superconductivity.

An enhanced SDW also affects the formation of stripes. To get some idea, we examine a few solutions on a 12×12

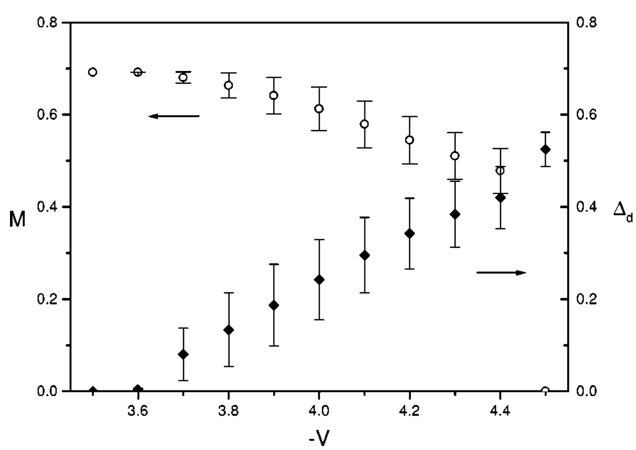

FIG. 2. Staggered magnetization (○) and d-wave superconducting order parameter (◆) as a function of $-V$ for an 8×8 lattice at half-filling calculated without the Hartree term (3).

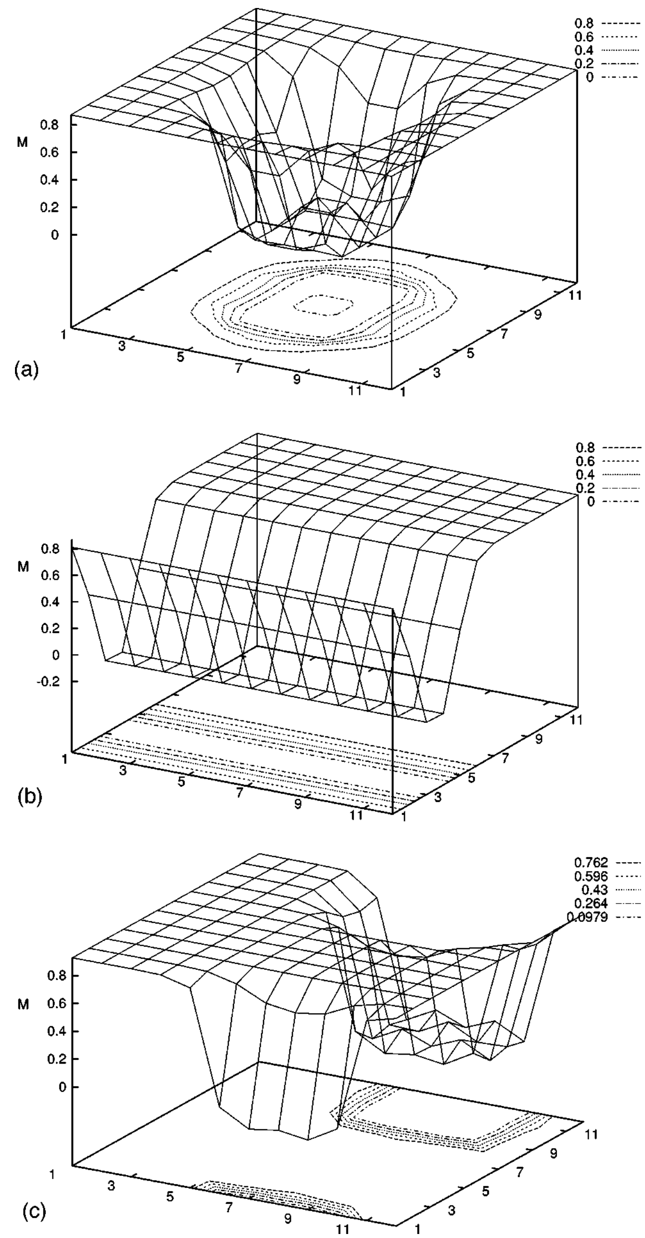

FIG. 3. Distribution of staggered magnetization on a 12×12 lattice for (a) 20 holes with $V=-0.8$, (b) 24 holes with $V=-0.8$, and (c) 24 holes with $V=-1.5$.

lattice for $U=4$. Figure 3(a) depicts the staggered magnetization profile for 20 holes with $V=-0.8$. In the $V=0$ case, the valley of the surface would reach -0.69 with a looplike domain wall (line of zero magnetization). In contrast, here the staggered magnetization stays far above -0.85. As one proceeds to a slightly higher doping (24 holes), one expects to see two straight domain walls (stripes). That indeed happens, but the separation between the two stripes narrows as V becomes more negative. At $V=-0.8$ they almost annihilate each other as shown in Fig. 3(b). For an even more negative $V=-1.5$ the depression in SDW no longer appears straight; instead it becomes square like and the bottom is shallower than before. It should be emphasized again that for all the solutions in Fig. 3, we do not detect any trace of

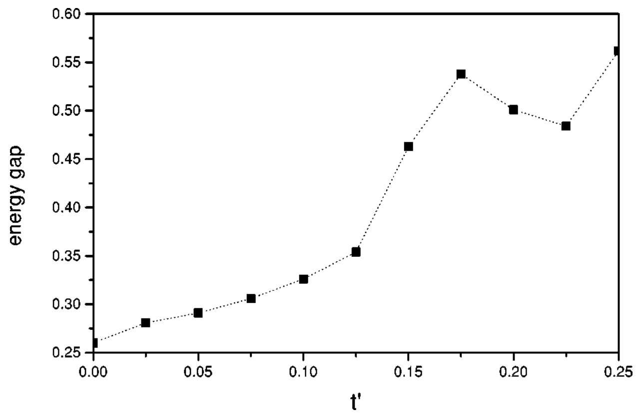

FIG. 4. Single-particle energy gap as a function of the diagonal hopping strength t'.

superconductivity.

Martin *et al.* have argued that the addition of a diagonal hopping term to the Hamiltonian (2) would reduce the single-particle gap in the SDW energy spectrum, thereby making pairing more likely. We have added such a term of magnitude $-t'$ and calculated the SDW gap for 16 holes on an 8×8 lattice. As shown in Fig. 4, the gap actually increases with t'. In any case, we fail to find any superconductivity again.

IV. DISCUSSION

From our study so far it seems that nearest-neighbor attractive interaction leads to stronger antiferromagnetism instead of *d*-wave superconductivity, in line with the observation made by Emery, Kivelson, and Zachar[14] regarding the difficulty of achieving high-temperature superconductivity through strong effective attractions. Previous employment of this interaction to generate *d*-wave superconductivity is not self-consistent at the mean-field level. Whether consideration of a more long-range or more complicated interaction might change the conclusion remains to be investigated.

We end by emphasizing that our study is a mean-field one and has its limitations. It is well known that mean-field theory tends to overestimate the stability of the SDW phase. In particular Hellberg and Manousakis[15] have investigated the *t*-*J* model and have shown that the striped phases are excited states rather than the ground-state in the periodic geometry. They have attributed[16] the ground state stripe phase found by White and Scalapino[17] in another approach to a cylindrical boundary condition. While we have used full periodic geometry in all our calculations, the possibility remains open that correlation effect may favor superconductivity over SDW.

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