RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 37, NUMBER 16 1 JUNE 1988

Spin polarons in the two-dimensional Hubbard model: A numerical study

W. P. Su

Department of Physics, and Texas Center for Superconductivity, University of Houston, Houston, Texas 77004

(Received 11 January 1988; revised manuscript received 9 March 1988)

We study the two-dimensional Hubbard model on a finite lattice. By numerically iterating the Hartree-Fock equations one obtains baglike polaron solutions for nearly half-filled-band cases. The profile of the polaron and the interaction potential between the polarons are calculated. Comparison with analytical results of Schrieffer, Wen, and Zhang is made. We also discuss a scenario in which the polarons are turned into the superconducting state by their mutual attraction.

Among the many theoretical models proposed to explain high-T_c superconductivity, the so-called "spin-bag" mechanism advanced by Schrieffer, Wen, and Zhang[1] (SWZ) is particularly attractive. Their idea is closely related to that of the polaron excitation in polyacetylene.

As is known, polyacetylene is particularly stable at half filling. The system undergoes a spontaneous distortion to form a commensurate charge-density wave, i.e., bond alternation. Any attempt to deviate the system from this stable state results in creating localized excitations so that the bulk of the condensate remains undisturbed. Thus doping proceeds by creating solitons or polarons.[2]

The two-dimensional Hubbard model is also known to possess a commensurate spin-density wave (or antiferromagnetic ordering) in the half-filled band case. Previous mean-field calculation[3] indicates that SDW persists up to a certain doping concentration. In such a calculation a uniform SDW is always assumed. Schrieffer *et al.*[1] made the analogy with polyacetylene and argued that in this case light doping should also create spin polarons. Each spin polaron is accompanied by a local depression of the SDW order parameter. Two polarons are attracted toward each other by sharing a common area of depression. Using this as the pairing potential between the Bloch states in the presence of SDW Schrieffer *et al.*[1] made an estimate of the superconducting energy gap.

In this paper we solve the Hubbard Hamiltonian by numerically iterating the Hartree-Fock (HF) equations. By working on a finite lattice with free boundary condition many quantities of interest can be straightforwardly calculated. Besides confirming some of the ideas in Ref. 1, the results presented below also yields additional insight.

The Hubbard Hamiltonian is given by

$$H=-t\sum_{\langle i,j\rangle,\sigma}(c_{i\sigma}^{\dagger}c_{j\sigma}+\text{H.c.})+U\sum_{i}n_{i\uparrow}n_{i\downarrow}\ , \tag{1}$$

where $\langle i,j\rangle$ denotes nearest neighbors and $n_{i\sigma}=c_{i\sigma}^{\dagger}c_{i\sigma}$ are the number operators. In the HF approximation the interaction term of the above Hamiltonian is linearized to

$$U\sum_{i}(\langle n_{i\uparrow}\rangle n_{i\downarrow}+\langle n_{i\downarrow}\rangle n_{i\uparrow}-\langle n_{i\uparrow}\rangle\langle n_{i\downarrow}\rangle)\ . \tag{2}$$

The linearized Hamiltonian is then solved self-consistently. In this paper this is done by numerical iteration. In the following discussion we set $t=1$ and choose $U=3$. At half filling the HF solution is an antiferromagnetic SDW with a staggered magnetization 0.6. The single-particle gap is about 1.5, which is a sizable fraction of the bandwidth $8t$.

To obtain the profile of a spin polaron we iterate the HF equations on a 10×10 lattice, with 51 spin-up electrons and 50 spin-down electrons. Starting with a small initial value, the full SDW pattern develops in about 20 iterations. The negative staggered spin density (after subtracting off the uniform background) is tabulated in Table I. A strong depression of the SDW is clearly seen at the center of the lattice. The adoption of free boundary condition makes the center of the lattice a slightly preferred site for the spin depression. This facilitates the calculations, but it is not essential, as we have been able to reproduce the same results with periodic boundary condition.

TABLE I. Staggered spin density associated with a spin polaron.

Site	1	2	3	4	5	6	7	8	9	10
1	−0.089	−0.002	0.001	0.000	0.001	0.000	0.001	0.000	−0.003	−0.074
2	−0.002	0.001	0.030	0.025	0.023	0.024	0.023	0.028	0.025	−0.003
3	0.001	0.030	0.033	0.049	0.040	0.038	0.046	0.078	0.028	0.000
4	0.000	0.025	0.049	0.047	0.086	0.067	0.146	0.046	0.023	0.001
5	0.001	0.023	0.040	0.086	0.081	0.365	0.067	0.038	0.024	0.000
6	0.000	0.024	0.038	0.067	0.365	0.081	0.086	0.040	0.023	0.001
7	0.001	0.023	0.046	0.146	0.067	0.086	0.047	0.049	0.025	0.000
8	0.000	0.028	0.078	0.046	0.038	0.040	0.049	0.033	0.030	0.001
9	−0.003	0.025	0.028	0.023	0.024	0.023	0.025	0.030	0.001	−0.002
10	−0.074	−0.003	0.000	0.001	0.000	0.001	0.000	0.001	−0.002	−0.089

TABLE II. Staggered charge density associated with a spin polaron.

Site	1	2	3	4	5	6	7	8	9	10
1	0.001	0.003	0.001	0.000	0.000	0.000	0.001	0.001	0.002	0.012
2	0.003	0.001	0.005	0.002	0.001	0.001	0.001	0.003	0.017	0.002
3	0.001	0.005	0.002	0.011	0.004	0.004	0.007	0.031	0.003	0.001
4	0.000	0.002	0.011	0.005	0.031	0.013	0.064	0.007	0.001	0.001
5	0.000	0.001	0.004	0.031	0.016	0.170	0.013	0.004	0.001	0.000
6	0.000	0.001	0.004	0.013	0.170	0.016	0.031	0.004	0.001	0.000
7	0.001	0.001	0.007	0.064	0.013	0.031	0.005	0.011	0.002	0.000
8	0.001	0.003	0.031	0.007	0.004	0.004	0.011	0.002	0.005	0.001
9	0.002	0.017	0.003	0.001	0.001	0.001	0.002	0.005	0.001	0.003
10	0.012	0.002	0.001	0.001	0.000	0.000	0.000	0.001	0.003	0.001

The spin density at the corner sites is a boundary effect. It is present also in the half-filled band case.

The spin depression has a cigar shape oriented in a diagonal direction as anticipated in Ref. 1. The corresponding charge density is shown in Table II. In the single-particle energy spectrum there is a state located in the SDW gap, at about 0.1 below the upper band. This is a localized HF state associated with the spin depression. The length of the depression extends over several lattice spacings, which is comparable to the coherence length defined as the ratio of the bandwidth to the SDW gap.

Once the existence of the spin polarons is established, the next thing is to study their interactions. It is of critical importance to determine if the interaction is attractive or repulsive. To check this we use a 6×20 lattice this time, with 61 spin-up electrons and 61 spin-down electrons. The rectangular geometry is so chosen that the two spin polarons have enough space to keep away from each other if they want.

The negative staggered spin density of the self-consistent solution is shown in Table III. The result is essentially the superposition of two slightly contracted spin depressions: one spin up, the other spin down. The two cigars are perpendicular to each other.

The fact that in the minimum energy configuration two spin depressions lie on top of each other indicates that the interaction between two depressions with opposite spins is attractive. To further determine the interaction potential, we displace one spin depression rigidly with respect to the other and calculate the change in energy. The change in energy as a function of the interpolaron separation (in units of lattice spacing) is shown in Table IV. An attractive potential well 0.03 deep and a few lattice spacings wide is clear. The interaction between two similar spin polarons can be studied in a similar fashion. The result resembles that of the spin singlet case discussed above.

At this point it is of interest to rescale the energy so that the above numbers might be relevant to high-T_c oxides.[4,5]

TABLE III. Staggered spin density of a singlet bipolaron.

Site	1	2	3	4	5	6
1	−0.090	−0.007	−0.001	−0.001	−0.007	−0.090
2	−0.007	−0.001	0.022	0.022	−0.001	−0.007
3	0.000	0.023	0.030	0.030	0.023	0.000
4	0.000	0.023	0.036	0.036	0.023	0.000
5	0.003	0.026	0.033	0.033	0.026	0.003
6	0.011	0.025	0.033	0.033	0.025	0.011
7	0.010	0.026	0.036	0.036	0.026	0.010
8	0.048	0.050	0.050	0.050	0.051	0.049
9	0.033	0.150	0.135	0.135	0.153	0.034
10	0.022	0.126	0.465	0.467	0.127	0.022
11	0.022	0.126	0.470	0.471	0.125	0.022
12	0.033	0.153	0.138	0.136	0.151	0.033
13	0.049	0.052	0.050	0.050	0.051	0.048
14	0.010	0.026	0.036	0.036	0.026	0.010
15	0.011	0.025	0.033	0.033	0.025	0.011
16	0.003	0.026	0.033	0.033	0.026	0.003
17	0.000	0.023	0.036	0.036	0.023	0.000
18	0.000	0.023	0.030	0.030	0.023	0.000
19	−0.007	−0.001	0.022	0.022	−0.001	−0.007
20	−0.090	−0.007	−0.001	−0.001	−0.007	−0.090

TABLE IV. Potential energy vs separation between two polarons with opposite spin.

Interpolaron separation (lattice spacing)	Potential energy
0	0
2	0.018
4	0.030
6	0.031
8	0.032
10	0.032

Since the bandwidth of the Cu-O d-p antibonding band is about 2 eV, our result above translates into a binding energy of bipolarons to be about 0.01 eV. The actual value of U is probably larger than $3t$, so is the corresponding binding energy. Of course the mean-field theory should be taken only with care, as emphasized by Hirsch.[3]

So far we have considered static polaron solutions only. Just like the polarons in polyacetylene the spin polarons here can move readily over the lattice. They can thus be treated like quantum-mechanical particles with an effective mass m^* over a distance scale larger than the coherence length. The attractive interaction between the polarons found before corresponds to a short-range interaction between the fermions. The Fermi gas of the spin polarons becomes superconducting because of the attractive potential. Details remain to be worked out.

The author thanks C. W. Chu, D. J. Scalapino, J. R. Schrieffer, and C. S. Ting for stimulating discussions; and G. Reiter for providing a copy of Ref. 1. This work was supported by the Texas Advanced Technology Research Program through the University of Houston and the Texas Center for Superconductivity at the University of Houston.

[1]J. R. Schrieffer, X. G. Wen, and S. C. Zhang, Phys. Rev. Lett. **60**, 944 (1988).

[2]W. P. Su, J. R. Schrieffer, and A. J. Heeger, Phys. Rev. B **22**, 2099 (1980).

[3]J. E. Hirsch, Phys. Rev. B **31**, 4403 (1985).

[4]J. G. Bednorz and A. K. Müller, Z. Phys. B **64**, 189 (1986).

[5]M. K. Wu, J. R. Ashburn, C. J. Torng, P. H. Hor, R. L. Meng, L. Gao, Z. J. Huang, W. Q. Wang, and C. W. Chu, Phys. Rev. Lett. **58**, 908 (1987).