PHYSICAL REVIEW B VOLUME 46, NUMBER 3 15 JULY 1992-I

Effect of electron interaction on the two-dimensional Peierls instability

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(Received 13 June 1991; revised manuscript received 25 February 1992)

The effect of electron interaction on the two-dimensional Peierls instability is studied by using the screened Coulomb potential to describe the electron interaction. Meanwhile, the calculation in this paper can avoid the uncertainty caused by the finite-size effect. Our results show that, in contrast to the one-dimensional case, the dimerization of the two-dimensional system is reduced by the electron interaction. Furthermore, the weaker the screening of the interaction, the larger the reduction.

I. INTRODUCTION

Low-dimensional systems possess various instabilities, which are responsible for many different orders, such as a charge-density wave (CDW), a spin-density wave (SDW), a bond-order wave (BOW), superconductivity, etc. In two-dimensional (2D) systems, competition between different orders is an important issue in condensed-matter physics. One example is the 2D electron-phonon system. Monte Carlo calculation shows that, when this system is half-filled, the Peierls instability suppresses superconductivity, but, away from half-filling, superconducting pairing appears.[1] Experiments have demonstrated that $BaBiO_3$ has a Peierls instability, but doping with K or Pb can suppress this instability and form the superconductors $Ba(Pb,Bi)O_3$ or $(BaK)BiO_3$.[2]

It has been realized that the electron interaction plays an important role in competition in 2D systems. The 2D Hubbard model shows that a long-range SDW can be established in the case of half-filling,[3] and antiferromagnetism has been found in undoped copper oxides.[4] The effects of the electron interaction on various orders are topics of great significance. This paper studies the effect of the electron interaction on 2D Peierls instability.

The same problem once arose in the one-dimensional (1D) case, and its story is instructive for us in studying the 2D system. For years there was a dispute as to whether the electron interaction enhanced or reduced 1D Peierls instability. When using the Hubbard model to describe the electron interaction, the 1D Peierls instability is surely enhanced.[5-10] This conclusion is true even for arbitrary long-range diagonal interaction.[11] But, if one takes the bond-charge repulsion into account, the 1D Peierls instability can be reduced.[12,13] This confusion is clarified by a more general description of the electron interaction.[14,15] Starting from a screened Coulomb interaction, it is found that the screening is a crucial factor in determining the behavior of the 1D Peierls instability under the influence of the electron interaction.[14] In the usual screening ($\beta \sim 1$), the dimerization is enhanced by the electron interaction. When the screening increases, the enhancement decreases. Finally, if the screening becomes strong enough ($\beta > 2$), the opposite behavior occurs, i.e., the dimerization is reduced by the electron interaction. Why does the dimerization have such qualitatively different behaviors in different screenings? The answer lies in the competition between the diagonal and off-diagonal components of the electron interaction.[16] If the screening is weak (long-range interaction) and the off-diagonal part of the electron interaction is negligible, then the site-charge repulsion (diagonal part) increases the dimerization. However, if the screening is strong (short-range interaction), the off-diagonal part becomes effective, and then the bond-charge repulsion can reduce the dimerization. It should be noted that, for the realistic screening, the off-diagonal part is much smaller than the diagonal one and the bond-charge repulsion does not reduce the bond alternation.[10]

It seems that the 2D system is a different story. By using the Hubbard model, some numerical calculations on a small 2D lattice show that the dimerization is slowly or rapidly reduced by the on-site repulsion.[17] This is different from the 1D case. This difference is understandable,[18] since the 2D Hubbard model can have long-range antiferromagnetic order, whereas the 1D model cannot. The competition between the SDW and the BOW suppresses the dimerization in the 2D system. Nevertheless, there are still some uncertainties to be clarified. First, the existing calculations are done only in small systems consisting of about ten sites. In such small systems, the pronounced finite-size effect can severely, even qualitatively, affect the conclusion. In order to get a definite answer, it is necessary to study a large system. Second, the 1D studies have shown that the off-diagonal part of the electron interaction can have a substantial effect on the dimerization. However, the existing 2D calculations are based on the Hubbard model, which contains only the first component of the diagonal part of the electron interaction and is unable to show the effect of the off-diagonal interaction on the 2D instability.

The theory presented in this paper will provide a better answer to the above problems, with two improvements. On one hand, the correlated-basis-function (CBF) method,[19] which is used in this paper and has been successfully used in the 1D case,[14] can deal with any large system. Therefore, it eliminates the uncertainty caused by the finite-size effect. On the other hand, the screened Coulomb interaction is used to describe the electron interaction. It includes both the diagonal and off-diagonal parts of the electron interaction.

Section II gives the framework of the theoretical formulation. The result and conclusion are presented in Sec. III; some discussions are also made there.

II. THEORETICAL FORMULATION

We consider a square lattice with the lattice constant a. If the hopping between the nearest-neighbor sites is dominant, the Fermi surface of a half-filled 2D system has a nesting with a wave vector (π,π). In this case the original square lattice is unstable and results in a distortion with that wave vector—it is the well-known Peierls instability. The physics of this instability is understandable: the original lattice can be imagined as a complex lattice formed by two sublattices A and B (see Fig. 1). Once a displacement d between these two sublattices appears, the primitive cell is doubled, and the border of the new Brillouin zone will coincide with the Fermi surface. Then a gap is opened at the Fermi surface, and the total energy of the system is reduced. This means that the distorted lattice has lower energy than the original one, and a lattice distortion or dimerization d results. The reduction of the energy in this dimerization is called the energy gain ΔE,

$$\Delta E = E_0 - E_d \ , \tag{1}$$

where E_0 and E_d are the energies of the system before and after dimerization. Therefore, the energy gain ΔE is a quantitative measure of the Peierls instability. The larger ΔE, the more instable the system.

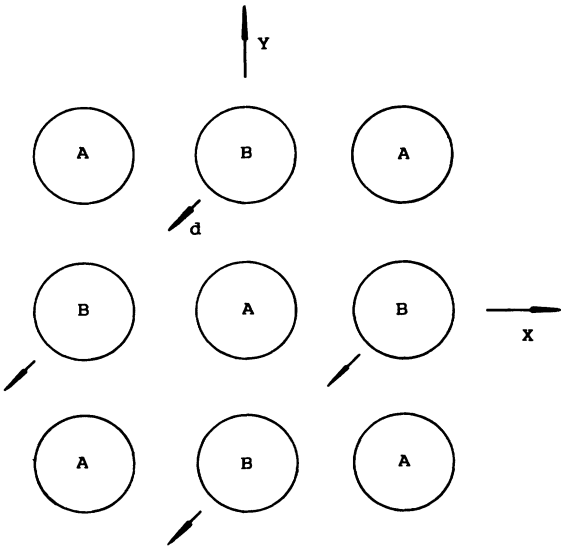

FIG. 1. The sublattices and dimerization.

When the electron interaction U is taken into account, the energy gain $\Delta E(U)$ with the same dimerization will depend on U. The U dependence of $\Delta E(U)$ reflects the effect of the electron interaction on the instability. If $\Delta E(U)$ decreases with increasing U, it means that the instability is reduced by the electron interaction; but, if $\Delta E(U)$ increases with increasing U, the instability is enhanced by electron interaction. Thus, the main task in the theoretical study is to calculate the interaction dependence of the energy gain $\Delta E(U)$. As mentioned in the Introduction, in order to include the effect of the off-diagonal part of the electron interaction, a screened Coulomb repulsion $v(r)$ should be used to describe the electron interaction,

$$v(r_{ij}) = \frac{U}{r_{ij}} \exp(-\beta r_{ij}) \ , \tag{2}$$

where U and β are the strength and screening factor, respectively, of the electron interaction. In the second quantized representation, the interaction (2) contains all the diagonal and off-diagonal matrix components. If we only take the first diagonal component, we have the Hubbard model. The first off-diagonal component, the exchange term, is the bond-charge repulsion.[12] Based on this general description (2), the result for the effect of the electron interaction will be more comprehensive than that from the Hubbard model. Hence, in our theory, the energy gain $\Delta E(U,\beta)$ will depend on both the strength U and the screening β of the electron interaction.

With the electron interaction (2), the Hamiltonian of the system reads

$$H = H_0 + \tfrac{1}{2} \sum_{i,j} v(r_{ij}) \ , \tag{3}$$

$$H_0 = \sum_i \left[\left[-\frac{\hbar^2}{2m} \right] \nabla_i^2 + \sum_l V(r_i, R_l) \right] \ , \tag{4}$$

where $V(r_i,R_l)$ is the potential produced by the lth ion at R_l and exerted on the ith electron at r_i. Since $\Delta E(U,\beta)$ has a fixed dimerization, the elastic energy is a constant and is omitted in the Hamiltonian (3).

Following the Jastrow-Feenberg ansatz,[20] the wave function for a system with repulsive interaction can be expressed as

$$\Psi(1,2,\ldots,N) = D[\phi_\kappa] \exp[u(1,2,\ldots,N)] \ , \tag{5}$$

where $D[\phi_\kappa]$ is a Slater determinant consisting of occupied orbits ϕ_κ, which are the eigenfunctions of H_0, and $u(1,2,\ldots,N)$ is a correlation factor which can be determined by the variational principle. For the repulsive interaction (2), there is no condensation. And, in the half-filled system, each cell only contains one electron; the density is not high. In such a case, the probability for three or more electrons gathering closely is small; then the two-body correlation is much more important than three-body or multibody ones. So, it is a good approximation to take only the two-body correlation,

$$u(1,2,\ldots,N)=\tfrac{1}{2}\sum_{i,j}u_{ij}\ . \tag{6}$$

Thus, the energy in the wave function (5) is

$$\begin{aligned}E_d(U,\beta)&=\frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle}\\&=\sum_k\varepsilon(\kappa)+\tfrac{1}{2}\int d1\int d2[P(1)-n_0]v(r_{12})[P(2)-n_0]+\tfrac{1}{2}\int d1\int d2\,P(1)v(r_{12})[g(1,2)-1]P(2)\\&\quad+\frac{\hbar^2}{8m}\int d1\int d2\,P(1,2)[\nabla_1u_{12}]^2+\frac{\hbar^2}{8m}\int d1\int d2\int d3\,P(1,2,3)[\nabla_1u_{12}]\cdot[\nabla_1u_{13}]\ ,\end{aligned} \tag{7}$$

where $\varepsilon(\kappa)$ is the eigenvalue of H_0, n_0 the average electron density, $P(1,2,\ldots,n)$ the n-particle distribution function, and $g(1,2)=P(1,2)/P(1)P(2)$ the electron correlation function. On the right-hand side of Eq. (7) the first term is the noninteracting energy, the second the electrostatic energy, the third the exchange energy, and the fourth and fifth the correlation energies.

According to the CBF method,[19] $P(1)$ and $P(1,2)$ can be obtained by solving the following equations,

$$\begin{aligned}P(1/\xi)=P(1|0)\exp\Bigg[&\int d\xi'\int d2\,u_{12}P(1,2|\xi')/P(1|\xi')\\&+\tfrac{1}{2}\int d\xi'\int d2\int d3\,u_{23}[P(1,2,3|\xi')/P(1|\xi')-P(1,2|\xi')]\Bigg]\ ,\end{aligned} \tag{8}$$

$$\begin{aligned}P(1,2|\xi)=P(1,2|0)\exp\Bigg[&\xi u_{12}+\int d\xi'\int d3(u_{12}+u_{23})P(1,2,3|\xi')/P(1,2|\xi')\\&+\tfrac{1}{2}\int d\xi'\int d3\int d4\,u_{34}[P(1,2,3,4|\xi')-P(1,2|\xi')P(3,4|\xi')]/P(1,2|\xi')\Bigg]\ .\end{aligned} \tag{9}$$

Since the two-body correlation is dominant, the convolution approximation[21] can be used to expand the three- and four-particle distribution functions in Eqs. (8) and (9) in terms of $g(1,2)$. Then, Eqs. (8) and (9) are closed, and the density $P(1)$ and correlation function $g(1,2)$ can be obtained by numerically solving the combined integral equations (8) and (9).

Substituting the obtained $P(1)$ and $g(1,2)$ into Eq. (7), the energy can be calculated. In this way, both $E_0(U,\beta)$ and $E_d(U,\beta)$, and then the energy gain $\Delta E(U,\beta)$, can be calculated.

III. RESULTS AND DISCUSSIONS

For the sake of simplicity, a cylindrical well with radius b and depth V_0 is taken as the potential $V(r_i,R_l)$ in H_0. By means of the Wannier wave function, the eigenvalue $\varepsilon(\kappa)$ and eigenfunction ϕ_κ of H_0 are easily determined. In the numerical calculation, the parameters are $a=2.56$ Å, $b=0.8$ Å, and $V_0=30$ eV. Then the hopping constant $t_0=0.35$ eV, the bandwidth $8t_0=2.8$ eV, and the dimerization $d=0.048$ Å. In this paper, two different polarized dimerizations are studied; one is along the diagonal direction and the other along the y axis.

In many-body theory, the key quantity is the correlation function $g(1,2)$. Once $g(1,2)$ is known, the energy $E_d(U,\beta)$ can be calculated from Eq. (7). In order to solve the combined integral equations (8) and (9), one needs to know the noninteracting distribution functions $P(1|0)$ and $P(1,2|0)$, which are determined by ϕ_k,

$$P(1|0)=2\sum_k^{\text{occ}}|\phi_k|^2\ , \tag{10}$$

$$P(1,2|0)=P(1|0)P(2|0)-2\left|\sum_k^{\text{occ}}\phi_k^*(1)\phi_k(2)\right|^2\ . \tag{11}$$

Substituting $P(1|0)$ and $P(1,2|0)$ into Eqs. (8) and (9), $g(1,2)$ can be obtained numerically. Three typical curves of the correlation function are shown in Figs. 2–4, in which the solid curves depict the correlation function before dimerization and the dashed curves depict it after dimerization. All these figures show $g(1,2)$ only along the y axis. Figure 2 has the origin at $r_1=0$; the solid curve is symmetrical to the origin. The origin of Fig. 3 is at $r_1=a/4$ and has no symmetry. The origin of Fig. 4 is at $r_1=a/2$ and the solid curve has symmetry.

Once the correlation function is in hand, the calcula-

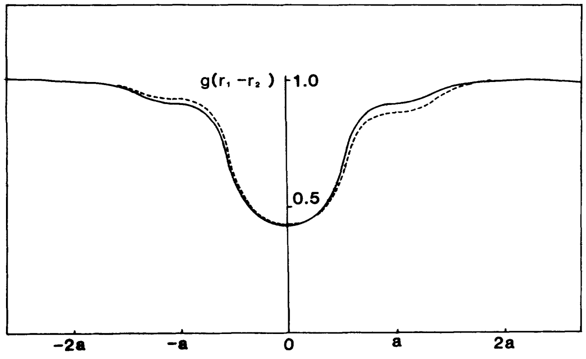

FIG. 2. The correlation function $g(1,2)$ with the origin at $(x_1,y_1)=(0,0)$. Solid line—before dimerization; dashed line—after dimerization.

tion of the energy gain $\Delta E(U,\beta)$ is straightforward. The results are shown in Fig. 5, where the solid lines denote the dimerization in the diagonal direction, the dashed lines denote it along the y axis. Both the solid and dashed lines have the same behavior. The lines in Fig. 5 demonstrate the dependence of the energy gain on the electron interaction. Each line has a fixed screening factor β. From these lines two conclusions can be drawn.

(1) The energy gain decreases with increasing interaction strength U. This means that the instability is reduced by the electron interaction.

(2) For the smaller β, the energy gain decreases more quickly. So, the interaction with the weaker screening is more effective in reducing the instability.

These two behaviors of the two-dimensional system are opposite from that of the one-dimensional case. It is known that,[14,16] for the usual screening ($\beta\sim 1$), the 1D dimerization is enhanced by the electron interaction. Furthermore, the weaker the screening, the larger the enhancement of 1D dimerization.

These conclusions are reasonable. As mentioned in the Introduction, the competition between the SDW and the BOW can suppress the Peierls instability. The electron interaction can establish long-range ferromagnetic order in a 2D system rather than a 1D system. Hence the 2D dimerization is reduced by the electron interaction. This causes the 2D systems to exhibit the normal behavior that the Coulomb repulsion resists the inhomogeneous distribution of charge following the dimerization. However, the behavior of the 1D system seems anomalous, and such a subtle property has been explained by the valence-bond approach.[22]

Finally, comparing our theory with existing ones, it is easy to see that the present work has two advantages: (1) it does not suffer from the finite-size effect, and (2) the effect comes from the full electron interaction rather than only on-site repulsion. Thus, the model in this paper is more physical and its results are more reliable.

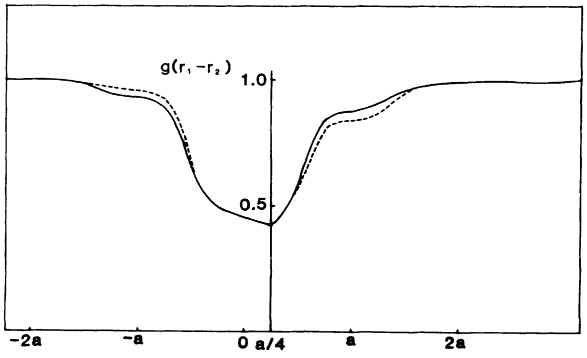

FIG. 3. The correlation function with the origin at $(x_1,y_1)=(0,a/4)$. Solid and dashed lines are before and after dimerization, respectively.

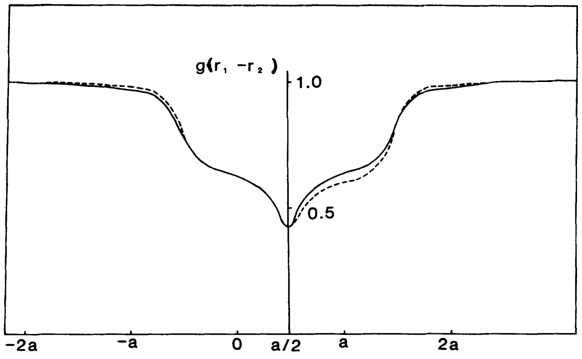

FIG. 4. The correlation function with the origin at $(x_1,y_1)=(0,a/2)$. Solid and dashed lines are before and after dimerization, respectively.

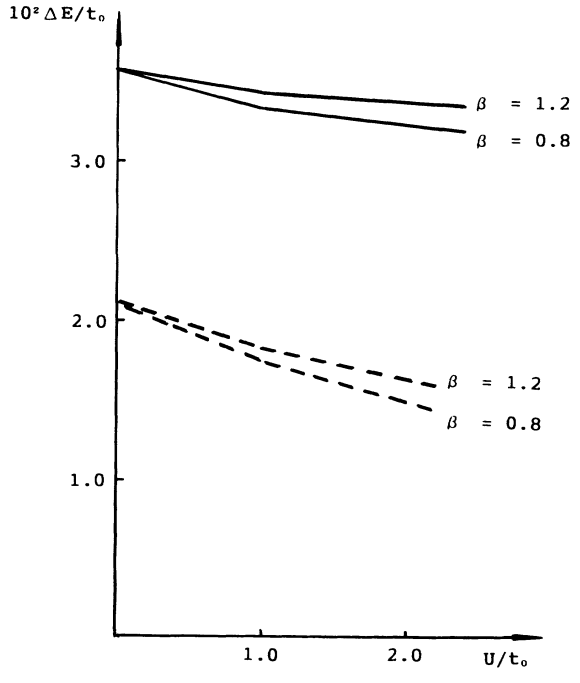

FIG. 5. The electron-interaction dependence of the energy gain. Solid line—dimerization along the diagonal direction; dashed line—y axis.

ACKNOWLEDGMENTS

J.L. and X.S. would like to thank Dr. Chang-qin Wu and Dr. Wei-guo Feng for helpful discussions. They are very grateful to the Institute for Molecular Science for hospitality extended during their visit. This work was partially supported by the Advanced Material Committee and by the National Science Foundation of China.

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[1] R. B. Noack, D. J. Scalapino, and R. T. Scalettar, Phys. Rev. Lett. **66**, 778 (1991).

[2] D. G. Hinks, D. R. Richards, B. D. Dabrowski, D. T. Marx, and A. W. Mitchell, Nature (London) **335**, 419 (1988); H. C. Zur Loye, K. J. Leary, S. W. Keller, W. K. Ham, T. A. Faltens, J. N. Michaels, and A. M. Stacy, Science **238**, 1558 (1987).

[3] J. E. Hirsch and S. Tang, Phys. Rev. Lett. **62**, 591 (1989); S. R. White, D. J. Scalapino, R. L. Sugar, E. Y. Loh, Jr., J. E. Gubernatis, and R. T. Scalettar, Phys. Rev. B **40**, 506 (1989).

[4] D. Vaknin *et al.*, Phys. Rev. Lett. **58**, 2802 (1987).

[5] D. Baeriswyl and K. Maki, Synth. Met. **17**, 13 (1987).

[6] E. J. Mele and G. M. Hayden, Synth. Met. **17**, 107 (1987).

[7] J. E. Hirsch, Phys. Rev. Lett. **51**, 296 (1983).

[8] S. Mazumdar and S. N. Dixit, Synth. Met. **28**, 463 (1989); G. W. Hayden and Z. G. Soos, Phys. Rev. B **38**, 6075 (1988).

[9] P. Tavan and K. Schulten, Phys. Rev. B **36**, 4337 (1987).

[10] D. K. Campbell, J. Gammel, and E. Loh, Phys. Rev. B **42**, 475 (1990).

[11] S. Mazumdar and D. Campbell, Phys. Rev. Lett. **55**, 2067 (1985).

[12] S. Kivelson, W. P. Su, J. R. Schrieffer, and A. J. Heeger, Phys. Rev. Lett. **58**, 1899 (1987); **60**, 72 (1988).

[13] A. J. Heeger, S. Kivelson, W. P. Su, and J. R. Schrieffer, Rev. Mod. Phys. **60**, 781 (1988).

[14] C. Wu, X. Sun, and K. Nasu, Phys. Rev. Lett. **59**, 831 (1987); **63**, 2535 (1989).

[15] X. Sun, R. Fu, Z. Shuai, C. Wu, and J. Li, Synth. Met. **27**, 1 (1988).

[16] X. Sun, J. Li, and C. Wu, in *Interacting Electrons in Reduced Dimensions*, edited by D. Baeriswyl and D. K. Campbell (Plenum, New York, 1989), p. 179.

[17] S. Tang and J. E. Hirsch, Phys. Rev. B **37**, 9546 (1988); **39**, 12 327 (1989).

[18] S. Mazumdar, Phys. Rev. B **39**, 12 324 (1989); **36**, 7190 (1987).

[19] E. Feenberg, *Theory of Quantum Fluids* (Academic, New York, 1969); S. Chakravarty and C. W. Woo, Phys. Rev. B **13**, 4815 (1976).

[20] R. Jastrow, Phys. Rev. **98**, 1479 (1955).

[21] F. Y. Wu and M. Chien, J. Math. Phys. **11**, 1912 (1970).

[22] S. Mazumdar and S. N. Dixit, Phys. Rev. Lett. **51**, 292 (1983); S. N. Dixit and S. Mazumdar, Phys. Rev. B **29**, 1824 (1984).