Coexistent States of Charge Density Wave and Spin Density Wave in One-Dimensional Systems with the Inter-site Coulomb Interaction under the Electron Filling Control

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The coexistent state of the spin density wave (SDW) and the charge density wave (CDW) in the one-dimensional systems is theoretically studied by the mean field approximation at $T=0$ in various electron-filling cases. We find that the coexistent state of SDW and CDW is stabilized when the on-site and the inter-site Coulomb interactions have the values estimated for the organic conductors. The ground state energies have cusp-like minima at $1/4$, $3/8$, $5/12$, $7/16$, $7/20$ and $9/20$-fillings.

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I. INTRODUCTION

(TMTSF)$_2$X and (TMTTF)$_2$X ($X$=ClO$_4$, PF$_6$, AsF$_6$, ReO$_4$, Br, SCN, etc.) have the quasi-one dimensional quarter-filled band, where superconductivity and the coexistent phase of charge density wave (CDW) and spin density wave (SDW) are observed. In (TMTSF)$_2$PF$_6$ at the ambient pressure, Pouget and Ravy observed the coexistence of $2k_F$-SDW and $2k_F$-CDW by the X-ray scattering measurement, where $k_F = \pi/4a$ is Fermi wave number and $a$ is the lattice constant. Under pressure (12 kbar), the superconducting phase appears at 0.9 K. In (TMTTF)$_2$Br, $4k_F$-CDW accompanied by $2k_F$-SDW is found in X-ray scattering measurements. Moreover, the superconductivity transition occurs at 0.8 K under 26 kbar.

These two kinds of the coexistent states ($2k_F$-SDW-$2k_F$-CDW and $2k_F$-SDW-$4k_F$-CDW) have been studied theoretically. In these studies, they considered the inter-site Coulomb interaction ($U$) in addition to the on-site Coulomb interaction ($U$). Mila has estimated $U/t \sim 5$ and $V/t \sim 2$, where $t$ is a transfer integral. The CDW-SDW coexistent state is understood as being caused by the interplay between $U$ and $V$.

Recently, it is found that the ground state in $X$-KOs changes from the charge order, which makes the stripe-type order, to the superconductivity under uniaxial pressure. Since, even in quasi-one-dimensional quarter-filled systems such as (TMTSF)$_2$X and (TMTTF)$_2$X, the coexistent state of CDW and SDW changes to the superconductivity under pressure, it is expected that the superconductivity appears near the coexistent state of CDW and SDW. In the high-$T_c$ cuprates such as La$_{1.6-x}$Nd$_x$Sr$_2$CuO$_4$, the stripe-type order is found when the rate of the doping is $x=1/8$ and the critical temperature of the superconductivity becomes the highest at $x \approx 1/8$. The superconductivity near the stripe-type order may be given by the fluctuation of the antiferromagnetism of the stripe-type order, because it is understood that the superconductivity in high-$T_c$ cuprates near the half-filling at which the antiferromagnetic state appears is due to the strong fluctuation of the antiferromagnetism.

In this paper, we study how the electron-filling ($f$) affects the coexistent state of SDW and CDW due to $V$ in the mean field theory. By calculating the condensation energy of the coexistent state, we find $f$ at which the coexistent state in one-dimensional systems is stabilized. The $f$-dependence of the condensation energy in the one-dimensional extended Hubbard model has never been studied, although the ground state energy as a function of $f$ has been calculated in the one-dimensional Hubbard model. Based on the result, we propose $f$ which favors the superconductivity in the strongly correlated one-dimensional systems with $V$.

We use the one-dimensional extended Hubbard model with $V$, where the dimerization is neglected for simplicity, because the coexistent states are stabilized without the dimerization.

II. MODEL

The one-dimensional extended Hubbard model is,
\[ \hat{H} = \hat{K} + \hat{U} + \hat{V}, \]
\[ \hat{K} = -t \sum_{i, \sigma} (c_{i, \sigma}^\dagger c_{i+1, \sigma} + h.c.), \]
\[ \hat{U} = U \sum_i n_{i, \uparrow} n_{i, \downarrow}, \]
\[ \hat{V} = V \sum_{i, \sigma, \sigma'} n_{i, \sigma} n_{i+1, \sigma'}, \]

where \( c_{i, \sigma}^\dagger \) is the creation operator of \( \sigma \) spin electron at \( i \) site, \( n_{i, \sigma} \) is the number operator, \( i = 1, \ldots, N_S \), \( N_S \) is the number of the total sites and \( \sigma = \uparrow \) and \( \downarrow \).

The interaction terms, \( \hat{U} \) and \( \hat{V} \), are treated in the mean field approximation as

\[ \hat{U}^M = \sum_{k_x} \sum_Q \{ \rho_{\uparrow \uparrow}(Q)C^\dagger(k_x, \downarrow)C(k_x - Q, \downarrow) 
+ \rho_{\downarrow \uparrow}(Q)C^\dagger(k_x - Q, \uparrow)C(k_x, \uparrow) \}, \]
\[ \hat{V}^M = \frac{V}{U} \sum_{k_x, \sigma, \sigma'} \sum_Q e^{-iQ\bar{a}} \{ \rho_{\sigma\sigma}(Q)C^\dagger(k_x, \sigma')C(k_x - Q, \sigma') 
+ \rho_{\sigma'\sigma}(Q)C^\dagger(k_x - Q, \sigma)C(k_x, \sigma) \}, \]

where \( I = U/N_S \). The self-consistent equation for the order parameter \( \rho_{\sigma\sigma}(Q) \) is given by

\[ \rho_{\sigma\sigma}(Q) = I \sum_{k_x} < C^\dagger(k_x, \sigma)C(k_x - Q, \sigma) >. \]

We do not consider the mean field, \( \rho_{\bar{\sigma}\sigma}(Q) \), where \( \bar{\sigma} \) is the opposite spin of \( \sigma \) for the simplicity. We consider the various electron-fillings, \( f = q/p \), where \( q \) and \( p \) are mutually prime numbers. We take the possible wave vectors of the order parameters as \( Q = nQ_0 \), where \( Q_0 = 2k_F = (2\pi/a) \cdot f \) and \( n = 1, \ldots, p \). The matrix size of the mean field Hamiltonian, \( \hat{K} + \hat{U}^M + \hat{V}^M \), is \( p \times p \). We calculate the self-consistent solutions by using eigenvectors obtained by diagonalizing \( \hat{K} + \hat{U}^M + \hat{V}^M \).

The ground state energy per site is

\[ E_g(\rho_{\sigma\sigma}(Q)) = \frac{1}{N_S} \sum_{j=1}^{N_s/2} \epsilon_j - \frac{1}{U} \sum_Q \rho_{\uparrow\uparrow}(Q, 0)\rho_{\downarrow\downarrow}^*(Q, 0) 
- \frac{V}{U^2} \sum_{Q, \sigma, \sigma'} e^{-iQ\bar{a}} \rho_{\sigma\sigma}(Q, 0)\rho_{\sigma'\sigma'}^*(Q, 0), \]

where \( \epsilon_j \) is the eigenvalue and the index \( j \) includes the degree of the spin freedom. The condensation energy, \( E_c \), is given by \( E_c = E_g - E_N \), where \( E_N \) is the normal state energy.

The electron density \( (n(j)) \) and the spin moment \( (S_z(j)) \) at site \( j \) are given by

\[ n(j) = \frac{1}{U} \sum_{Q, \sigma} \rho_{\sigma\sigma}(Q)e^{iQja} \]
\[ S_z(j) = \frac{1}{2U} \sum_Q (\rho_{\uparrow\uparrow}(Q) - \rho_{\downarrow\downarrow}(Q))e^{iQja}. \]

III. RESULTS AND DISCUSSIONS

We search the most stable self-consistent solutions by changing the initial values of order parameters. Since \( n(j) \), \( S_z(j) \) and \( E_c \) for \( f > 0.5 \) is the same as those for \( f < 0.5 \) due to the symmetry between an electron and an hole and we do not focus our attention on
the low electron-filling, we calculate at various fillings 
(2 ≤ p ≤ 20, 1 ≤ q ≤ 9) in the region of 0.2 ≤ f ≤ 0.5.

At f = 1/2, the stable state is 2kF-SDW, (↓,↑), 
(Sz(1) = -Sz(2) ≈ 1.0 and n(1) = n(2) ≈ 1.0) for 
2V ≤ U and the state is changed to 2kF-CDW, (0,↓↑), 
(Sz(1) = Sz(2) ≈ 0 and n(1) ≈ 0 and n(2) ≈ 2.0) for 
2V > U, where the arrows mean the spin moment, 0 
means small or zero electron density and ↑ represents 
that the up and down electrons exist in the same site. 
For 2V > U, the period of the CDW becomes two. Thus, 
when n = 2, the period of the CDW becomes two. As 
the order parameters have Q = (2π/a)·(1/2) dose not exist when 
p of f = q/p is odd number, the period of n dose not be 
come two. Thus, when p is odd number, the order of the 
CDW is not suitable for V.

At f = 1/3, the stable state is the coexistence of 
SDW and CDW, (↓,↓,↑), (|Sz(1)| = |Sz(2)| < Sz(3) and 
n(1) = n(2) < n(3)) for 0 ≤ V/t < 0.8, where the distor-
tion of the charge density is small and the coexistent state 
of SDW and CDW, (↓,0,↑) (Sz(1) = -Sz(3), Sz(2) = 0, 
n(1) = n(3) ≈ 1.0 and n(2) ≈ 0), is stabilized for 
V/t ≥ 0.8, as shown in Figs. 1 and 2. As the period 
of n in (↓,0,↑) is three, there is a frustration for V 
and the energy gap does not become large. Since the order 
parameters having Q = (2π/a)·(1/2) dose not exist when 
p of f = q/p is odd number, the period of n does not 
become two. Thus, when p is odd number, the order of the 
CDW is not suitable for V.

In the case of the quarter filling (f = 1/4), the stable 
state of 2kF-SDW, (↓,↓,↑) (Sz(1) = Sz(2) = -Sz(3) = 
-0.5, n(1) = n(2) = n(3) = n(4) = 0.5), is changed to the coexistent state of 2kF-SDW and 4kF-
CDW, (↓,0,↑,0) (Sz(1) = -Sz(3), Sz(2) = Sz(4) = 0, 
n(1) = n(3) ≈ 1.0 and n(2) = n(4) ≈ 0), for V/t > 0.39, 
as shown in Figs. 3 and 4. This result is consistent 
with the previous study by Seo and Fukuyama. For 
V/t > 0.39, as the period of the charge density is two, E_c 
becomes large due to the large energy gap, which will be 
shown in Fig. 7.

We show 2Sz and n at f = 3/8 in Figs. 5 and 
6, where Sz(1) = -Sz(5), Sz(2) = -Sz(6), Sz(3) = 
-0.5, Sz(4) = -0.5, n(1) = n(5), n(2) = n(6), 
n(3) = n(7) and n(4) = n(8). The stable coexis-
tent state of SDW and CDW is (↑,↑,↓,↑,↓) for 
V/t < 0.7, (↑,↑,↑,↑,↑,↓) for 0.7 ≤ V/t ≤ 3.0 
and (0,↑,↑,↑,↑,↓) (Sz(1) = Sz(3) = Sz(5) = 
Sz(7) = 0 and Sz(2) = Sz(4) = -Sz(6) = -Sz(8)) for 
V/t > 3.0. In particular, the period of n (n(1) = n(3) = 
n(5) = n(7) ≈ 0 and n(2) = n(4) = n(6) = n(8) ≈ 1.5) 
is two for V/t > 3.0, which gives the large gain of E_c, as 
will be shown in Fig. 7.
In the case of other fillings except the half-filling, the coexistent state of CDW and SDW is stabilized.

Next, we show $E_c$ in Fig. 7 as a function of $f$ for various $V$. At $V = 0$, $E_c$ monotonically decreases as $f$ increases, because $E_c$ is mainly determined by the density of states on the Fermi surface, $N(0) = N_S/(4\pi t \sin \alpha k_F)$, which decreases as $f$ increases. It is found that $E_c$ at $f = 1/4$ rapidly decreases as $V$ increases. In this filling, the localization of electrons occurs easily even at weak $V$. The reason is that the order of $(\downarrow, 0, \uparrow, 0)$ is favorable for the $4k_F$-CDW keeping the $2k_F$-SDW state. We can see that $|E_c|$ for $f = 1/2, 1/4, 3/8, 5/12, 7/16, 7/20$ and $9/20$ become large, compared to other fillings, upon increasing $V$. It is found that the cusp-like minima of the condensation energy in the coexistent state of CDW and SDW appear at $f = n/4m$, where $n$ and $m$ are integers. In these fillings, the period of $n$ accompanying the order of the SDW becomes two, resulting in the large energy gap. The local minimum at $f = 5/16$ may be too small to see in Fig. 7.

In the coexistent state of CDW and SDW, the commensurability of the electron-filling and the inter-site Coulomb interaction play the important role of the condensation energy. At $f = n/4m$, the coexistent state of CDW and SDW is compatible with the favored real-space order for both $U$ and $V$. On the other hand, $E_c$ at $f = 1/3$ changes little as $V$ increases. This feature can be understood by considering that the frustration occurs in the order of period three; double occupancy should be reduced by $U$ and electrons at nearest sites should be avoided for large $V$.

In the case of one-dimensional systems with $V$ where the superconductivity is attributable to the fluctuation of the antiferromagnetism, the superconductivity may appear at the fillings near $f = n/4m$. If the origin of the superconductivity of quasi-one-dimensional organic conductors such as $(\text{TMTTF})_2X$ and $(\text{TMTSF})_2X$ is so, the superconductivity will be obtained by changing electron-filling slightly from the quarter-filling.

IV. CONCLUSION

We study the coexistent state of CDW and SDW in the one-dimensional system with the inter-site Coulomb interaction by changing the electron-filling. We find that the coexistent state is stabilized at $f = n/4m$, for ex-
ample, 1/4, 3/8, 5/12, 7/16, 7/20 and 9/20-fillings due to the inter-site Coulomb interaction. Since the strong fluctuation of the antiferromagnetism is expected in the region close to the coexistent state, the superconductivity will appear near $f = n/4m$.

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