Theory of charge-density-wave superconductors

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It is shown theoretically that the superconducting state coexisting with charge-density wave (CDW, its wave vector $\vec{Q}$) is characterized by the spatially varying periodic order parameter $\Delta(Q)$ in addition to the ordinary uniform order parameter $\Delta(0)$. Perturbational calculation based on the linearized gap equation yields the depression of the transition temperature of this state. The upper critical field $H_{c2}(T)$ is derived from the Ginzburg-Landau (GL) equation modified so as to include the effect of the CDW, and shown to exhibit a positive curvature in $H_{c2}(T)$ vs T curve when applied magnetic field is perpendicular to $\vec{Q}$. The parallel $H_{c2}(T)$ follows the ordinary GL theory. Physical implication of this result is discussed in connection with highly anisotropic superconducting materials.

I. INTRODUCTION

Recently many experiments have been performed on charge-density waves (CDW) in highly anisotropic materials such as layered-type or quasi-one-dimensional systems. Among them systematic experiments on $2H$-type layered transition-metal dichalcogenides[1] have been done to show the existence of superconducting (SC) state at a transition temperature T_c lower than the CDW transition temperature T_{CDW}. It is natural to imagine that the CDW persists below T_c because the SC condensation energy (T_c^2/ϵ_F; ϵ_F is the Fermi energy) is much smaller than that of the CDW ($T_{\mathrm{CDW}}^2/\epsilon_F$) when $T_c < T_{\mathrm{CDW}}$. In fact the recent Raman scattering study on $2H$-$NbSe_2$ ($T_c = 7.3$ K, $T_{\mathrm{CDW}} = 33$ K) down to 2 K might be the first experiment[2] which confirms explicitly the coexistence of CDW and SC in such materials as far as the authors know.

In this respect, the recent upper critical-field measurement[3] on $Nb_{1-x}Ta_xSe_2$ raises an interesting question and gives a clue to the long-unsolved problem: The anomalous positive curvature in the $H_{c2}(T)$ vs T curve appears near T_c as x decreases or T_{CDW} increases. This strongly indicates some interplay between CDW and SC. It is reported that such anomalous positive curvature in the $H_{c2}(T)$ vs T curve near T_c also appears in other highly anisotropic materials, $NbSe_3$ (Ref. 4) and TaS_3 (Ref. 5), quasi-one-dimensional polymer $(SN)_x$ (Ref. 6), and the organic superconductor[7] $(TMTSF)_2PF_6$ at high pressure. $NbSe_3$ and $(TMTSF)_2PF_6$ exhibit a CDW transition at ambient pressure; TaS_3 and $(SN)_x$ do not. These experimental findings encourage us to investigate the correlation between SC and CDW and lead us to reexamine existing theoretical work. Note that no one has yet succeeded in explaining the anomalous positive curvature in the $H_{c2}(T)$ curve with reasonable physical grounds, although, in some layered compounds intercalated with organic molecules, some aspects of the anomalous behavior in $H_{c2}(T)$ can be explained[8] by the interlayer Josephson phase-coupling model.[9]

Recently Balseiro and Falicov[10] investigated theoretically the coexistence problem of CDW and SC in layered materials, and Bilbro and McMillan[11] have also studied a similar problem in connection with the martensitic transition in $A15$ type materials. Both authors assumed *a priori* BCS pairing with opposite momenta $\vec{k}$ and $-\vec{k}$ under periodic lattice distortion. In this paper we shall point out the possibility of a different SC state. In the presence of CDW, which strongly mixes up the conduction-electron states near the Fermi surface to open CDW gap in the energy spectrum, the stable SC state is such that, in addition to ordinary order parameter $\Delta(0)$, there appears spatially varying order parameter $\Delta(Q)$ to adjust itself with CDW of wave vector $\vec{Q}$. A similar possibility was investigated in the presence of ferromagnetism[12] and a spin-density wave.[13,14]

II. STABILITY PROBLEM

We consider the stability problem[15] of the superconducting state which coexists with a charge-density-wave state. The latter state gives rise to a spatially periodic lattice distortion which exerts a periodic potential on conduction electrons via electron-phonon coupling. Here we only investigate the case in which the superconducting transition temperature T_c is much smaller than that of CDW. Therefore we neglect the reaction of the CDW state due to the presence of superconductivity, and regard the CDW state as an external perturbation on the superconducting state. Thus the Hamiltonian we take is

$$H=\sum_{k\sigma}\xi_k C_{k\sigma}^{\dagger}C_{k\sigma}-V\sum_{k\sigma}(C_{k\sigma}^{\dagger}C_{k+Q\sigma}+\text{H.c.}) \; , \tag{2.1}$$

where we assume V as a given parameter although V is temperature dependent, of the order of T_{CDW} and proportional to the order parameter of CDW. We also assume that the wave number Q which characterizes the CDW state is equal to $2k_F$, where k_F is the Fermi momentum. As is seen later, if $Q\neq 2k_F$, CDW hardly affects on superconductivity.

Let us consider the stability problem of the superconducting state under such periodic potential, starting with the linearized gap equation for the spatially varying order parameter $\Delta(r)$:

$$\Delta(r)=gT\sum_{\omega_n}\int K(r,r',\omega_n)\Delta(r')dr' \; , \tag{2.2}$$

$$K(r,r',\omega_n)=G^{\uparrow}(r,r',\omega_n)G^{\downarrow}(r,r',-\omega_n) \; , \tag{2.3}$$

where $G^{\uparrow}(r,r',\omega_n)$ is the thermal Green's function for an up-spin electron. In the following we omit the spin index because the system is invariant with respect to spin inversion. g is the effective attractive interaction between conduction electrons. By the Fourier transformation, Eqs. (2.2) and (2.3) become

$$\Delta(q)=gT\sum_{q'}\sum_{\omega_n}K(q,q',\omega_n)\Delta(q') \; , \tag{2.4}$$

$$K(q,q',\omega_n)=\sum_{k_1\sim k_4}G_{k_1k_2}(\omega_n)G_{k_3k_4}(-\omega_n)\delta(k_1+k_3-q)\delta(k_2+k_4-q') \; . \tag{2.5}$$

Since relevant wave numbers we must take into account are $q=0$ and Q, it is enough to pick up two wave numbers in the sum of Eq. (2.4). Thus Eq. (2.4) is rewritten as

$$[1-gK(0,0)]\Delta(0)+gK(0,Q)\Delta(Q)=0 \; , \tag{2.6}$$
$$gK(Q,0)\Delta(0)+[1-gK(Q,Q)]\Delta(Q)=0 \; .$$

Then a nontrivial solution for $\Delta(0)$ and $\Delta(Q)$ is obtained when

$$\det\begin{vmatrix}1-gK(0,0) & gK(0,Q)\\ gK(Q,0) & 1-gK(Q,Q)\end{vmatrix}=0 \; , \tag{2.7}$$

which in turn determines the transition temperature T_c at which the superconducting state characterized by the two order parameters $\Delta(0)$ and $\Delta(Q)$ appears. We have defined $K(q,q')=T\sum_{\omega_n}K(q,q',\omega_n)$. This superconducting state is more stable than the ordinary BCS pairing state with the opposite momenta $\vec{k}$ and $-\vec{k}$ and must be energetically favorable if $T_c>T_c'$ where T_c' is the transition temperature of the ordinary BCS pairing state under the spatially periodic potential, and defined through

$$\left[1-gT\sum_{\omega_n}K(0,0,\omega_n)\right]\Delta(0)=0 \tag{2.8}$$

and

$$1-gT_c'\sum_{\omega_n}K(0,0,\omega_n)=0 \; . \tag{2.9}$$

In order to evaluate the matrix elements of the integral kernel $K(q,q',\omega_n)$, we take free electron spectrum with the Fermi sphere of radius k_F and $\vec{Q}=(0,0,Q=2k_F)$ in the cylindrical coordinate. Then the relevant electron Green's functions are given by

$$G_{kk}(\omega_n)=\frac{i\omega_n-\xi_{k\mp Q}}{(i\omega_n-\xi_k)(i\omega_n-\xi_{k\mp Q})-V^2} \; , \quad k_z \gtrless 0 \; , \tag{2.10}$$

$$G_{k,k\pm Q}(\omega_n)=\frac{V}{(i\omega_n-\xi_k)(i\omega_n-\xi_{k\mp Q})-V^2} \; . \tag{2.11}$$

The diagonal element $K(0,0,\omega_n)$ of the kernel is evaluated as

$$K(0,0,\omega_n)=\sum_k[G_{kk}(\omega_n)G_{-k,-k}(-\omega_n)+G_{k,k-Q}(\omega_n)G_{-k,-k+Q}(-\omega_n)+G_{k,k+Q}(\omega_n)G_{-k,-k-Q}(-\omega_n)] \; . \tag{2.12}$$

The other kernels are the following:

$$K(Q,Q,\omega_n)=\sum_k[G_{k,k+Q}(\omega_n)G_{-k+Q,-k}(-\omega_n)+G_{kk}(\omega_n)G_{-k+Q,-k+Q}(-\omega_n)] \; , \tag{2.13}$$

$$K(0,Q,\omega_n)=K(Q,0,\omega_n)=\sum_k[G_{kk}(\omega_n)G_{-k+Q,-k}(-\omega_n)+G_{k,k-Q}(\omega_n)G_{-k+Q,-k+Q}(-\omega_n)] \; . \tag{2.14}$$

We consider the effect of CDW perturbationally and restrict our discussion to the lowest order of V/ϵ_F. Within this approximation, it is easy to see that[16] $K(0,0)=K^{(0)}(0,0)-(V/\epsilon_F)^2K^{(2)}(0,0)$, $K(Q,Q)\propto(V/\epsilon_F)^2$ and $K(0,Q)=(V/\epsilon_F)K'(0,Q)$ when the order of T_c/ϵ_F is neglected. Then Eq. (2.7) is rewritten to the second order in V/ϵ_F as

$$\frac{1}{g}=K^{(0)}(0,0)-\left(\frac{V}{\epsilon_F}\right)^2[K^{(2)}(0,0)-gK'^2(0,Q)] \ . \tag{2.15}$$

This clearly shows $T_c > T_c'$ because of the presence of the off-diagonal term $K'(0,Q)$ as far as this has an appreciable value, that is, the superconducting state with $\Delta(0)$ and $\Delta(Q)$ is always more stable than the simple BCS state. Note that when the wave number Q differs from $2k_F$, the off-diagonal element $K(0,Q)$ simply vanishes because the mixing of wave functions of conduction electrons near the Fermi surface due to CDW formation does not become effective and hardly affects on superconductivity. Therefore the ordinary Cooper pairing becomes stable.

We evaluate explicitly the matrix elements of the integral kernel in the Appendix using three-dimensional Fermi sphere model. [Note that deviation from the spherical Fermi surface model further stabilizes this modified superconducting state because the anisotropy of the Fermi surface enhances the off-diagonal element $K(Q,0)$. Thus we can expect more favorable situation in actual highly anisotropic materials.]

Substituting Eqs. (A8) and (A11) into Eq. (2.15) we obtain

$$\frac{T_c-T_{c0}}{T_{c0}}=-\frac{V^2}{8\epsilon_F^2}\frac{1}{gN(0)}(1-\beta) \ , \tag{2.16}$$

$$\beta=\tfrac{1}{8}[gN(0)]^2\left(\sum_{n>0}^{\omega_D}\frac{1}{n+\frac{1}{2}}\ln\frac{n+\frac{1}{2}}{\epsilon_F/\pi T_{c0}}\right)^2 \ , \tag{2.17}$$

where ω_D is the Debye frequency and T_{c0} is the transition temperature for the unperturbed superconductor ($V=0$). A rough estimation yields $\beta=0.98$ when $\epsilon_F=3000$ K, $T_{c0}=5$ K and $gN(0)=0.2$ are employed.

Thermodynamic properties of this superconducting state with the two order parameters $\Delta(0)$ and $\Delta(Q)$ are not much different from the ordinary BCS state because the ratio $\Delta(Q)/\Delta(0)$ is of the order of (V/ϵ_F) which is assumed to be small. Therefore correction of thermodynamic quantities to the BCS state may be of this order at most. However in highly anisotropic materials such as layered-type compounds or quasi-one-dimensional systems, the ratio $\Delta(Q)/\Delta(0)$ should be enhanced enough to be observed in thermodynamic quantities by a careful measurement because in highly anisotropic materials appreciable portion of the Fermi surface is modified by the presence of CDW. Note also that the formation of superconducting energy gap associated with $\Delta(Q)$ is anisotropic with respect to $\vec{Q}$ even when starting with a spherical Fermi surface band. Thus the superconducting anisotropy is enhanced in low-dimensional materials even more.

III. LINEARIZED GL EQUATION AND UPPER CRITICAL FIELD

In order to elucidate physical implication of the modified pairing state, we now consider the upper critical field $H_{c2}(T)$ *semiphenomenologically* under the presence of magnetic field with different directions. The simplest argument to determine $H_{c2}(T)$ is to use the linearized Ginzburg-Landau (GL) equation[15] which is modified so as to be consistent with the above discussion given in Sec. II. We start with the linearized gap equation (2.2) to see what kind of terms come into play additionally in GL equation in the presence of CDW:

$$\Delta(r)=g\int K(r,r+R)\Delta(r+R)d^3R \ ,$$
$$K(r,r+R)=T\sum_{\omega_n}K(r,r+R,\omega_n) \ . \tag{3.1}$$

Expanding $\Delta(r+R)$ around R, and neglecting the higher-order term in $(V/\epsilon_F)^2$, we arrive at the following GL equation:

$$\frac{1}{6}\sum_{i=x,y,z}(a_i+2b_i\cos\vec{Q}\cdot\vec{r})\frac{\partial^2\Delta(r)}{\partial x_i^2}+[gK(0,0)-1]\Delta(r)-2gK(0,Q)\cos\vec{Q}\cdot\vec{r}\Delta(r)=0 \ , \tag{3.2}$$

where

$$a_i=\sum_q\int K(q,q)e^{-iqR}R_i^2d^3R=\tfrac{7}{8}\zeta(3)gN(0)\left(\frac{v_F}{\pi T_c}\right)^2+O\left(\frac{V^2}{\epsilon_F^2}\right) \ , \tag{3.3}$$

$$b_i=\sum_q\int K(q+Q,q)e^{-iqR}R_i^2d^3R\sim O\left(\frac{V}{\epsilon_F}\right) \ , \tag{3.4}$$

$$gK(0,0)-1=gN(0)\ln T_c/T \ . \tag{3.5}$$

v_F is the Fermi velocity and $\zeta(3)$ is the zeta function. Therefore up to the linear order in (V/ϵ_F) this equation reduces to the Mathieu-type differential equation, and differs from the ordinary GL equation. The new equation has an additional potential term of the form $K'\cos\vec{Q}\cdot\vec{r}$ which comes from the presence of the off-diagonal element $K(q,q+Q)$ in the integral kernel. This potential term is due to the presence of CDW.

Hereafter we only treat the following *semi-phenomenological gauge-invariant GL equation* with an anisotropic mass under a magnetic field

$$-(\vec{\nabla}-2ie\vec{A})\left(\frac{1}{2m}\right)^{\wedge}(\vec{\nabla}-2ie\vec{A})\Delta(r)+K'\cos\vec{Q}(\vec{r}-\vec{r}_0)\Delta(r)=\frac{1}{2m\xi^2(T)}\Delta(r)\ , \quad (3.6)$$

where $\xi(T)$ is the coherence length $[\xi^{-2}(T) \propto (T_c-T)]$, K' a constant of the order of $(V/\epsilon_F)/\xi^2(0)$, $\vec{A}$ the vector potential, $(1/m)^{\wedge}$ the effective-mass tensor, and $\vec{r}_0=(x_0,y_0,z_0)$ is chosen so as to select the lowest eigenvalue. When $K'=0$, Eq. (3.6) reduces to a conventional GL equation[17] with an anisotropic effective mass.

Let us consider a layered-type crystal with uniaxial symmetry, and assume

$$\left(\frac{1}{m}\right)^{\wedge}=\begin{pmatrix}1/M & 0 & 0\\ 0 & 1/m & 0\\ 0 & 0 & 1/m\end{pmatrix}\ . \quad (3.7)$$

Then we write Eq. (3.6) as

$$\left\{-\left(\frac{\partial}{\partial x}-i\frac{2\pi A_x}{\Phi_0}\right)^2-\epsilon^2\left[\left(\frac{\partial}{\partial y}-i\frac{2\pi A_y}{\Phi_0}\right)^2+\left(\frac{\partial}{\partial z}-i\frac{2\pi A_z}{\Phi_0}\right)^2\right]+K\cos Q(z-z_0)\right\}\Delta(r)=\frac{1}{\xi_\perp^2(T)}\Delta(r)\ , \quad (3.8)$$

with $\epsilon^2=M/m$, and $\Phi_0(=hc/2e)$ is the flux quantum. We have chosen the yz plane as the layer plane ($\vec{Q}\parallel z$), and $\xi_\perp(T)$ is the coherence length perpendicular to the layered plane.

A. H in xy plane: $H_{c2}(\phi)$

Denoting ϕ as the angle from x axis in the xy plane, we can choose the vector potential $\vec{A}$ as $\vec{A}=H(z\sin\phi,0,y\cos\phi)$. Then Eq. (3.8) reduces to

$$\left[-\left(\frac{\partial}{\partial x}-izh\sin\phi\right)^2-\epsilon^2\frac{\partial^2}{\partial y^2}-\epsilon^2\left(\frac{\partial}{\partial z}-iyh\cos\phi\right)^2+K\cos Q(z-z_0)\right]\Delta(r)=\frac{1}{\xi_\perp^2(T)}\Delta(r)\ , \quad (3.9)$$

with $h=2\pi H/\Phi_0$. In order to find out the lowest eigenvalue which gives the highest field H_{c2}, putting

$$\Delta(r)=\exp(ik_x x+ik_y y+ihyz\cos\phi)g(z) \quad (3.10)$$

we obtain

$$\left\{(k_x-zh\sin\phi)^2+\epsilon^2(k_y+zh\cos\phi)^2-\epsilon^2\frac{d^2}{dz^2}+K\cos Q(z-z_0)\right\}g(z)=\frac{1}{\xi_\perp^2(T)}g(z)\ . \quad (3.11)$$

Since the lowest eigenvalue occurs at $k_x=k_y=0$, it becomes

$$\left\{-\epsilon^2\frac{d^2}{dz^2}+(hz)^2(\epsilon^2\cos^2\phi+\sin^2\phi)+K\cos Q(z-z_0)\right\}g(z)=\frac{1}{\xi_\perp^2(T)}g(z)\ . \quad (3.12)$$

It is hard to solve the eigenvalue problem of this equation in general. We regard the cosine potential $K\cos Q(z-z_0)$ as a perturbation. A similar argument is given in Ref. 9. The unperturbed equation of Eq. (3.12) is nothing but a simple harmonic oscillator problem and hence the eigenvalue E_n is given by

$$E_n=(2n+1)\epsilon h(\phi)(\epsilon^2\cos^2\phi+\sin^2\phi)^{1/2} \quad (3.13)$$

and the eigenfunction is written in terms of the Hermite polynomials. The first order shift δE of the lowest eigenvalue ($n=0$) due to the cosine potential is easily calculated as

$$\delta E=-|K|\exp\left[-\frac{\epsilon Q^2}{4h(\epsilon^2\cos^2\phi+\sin^2\phi)^{1/2}}\right]\ , \quad (3.14)$$

where we have chosen z_0 to minimize the energy. Inserting the lowest eigenvalue, we obtain $h_{c2}(\phi)=2\pi H_{c2}(\phi)/\Phi_0$ as

$$\frac{1}{\xi_\perp^2(T)}=\epsilon h_{c2}(\phi)f(\phi)-|K|\exp\left[-\frac{\epsilon Q^2}{4h_{c2}(\phi)f(\phi)}\right]\ , \quad (3.15)$$

$$f(\phi)=(\epsilon^2\cos^2\phi+\sin^2\phi)^{1/2}\ .$$

It is noted that as long as $h_{c2}(\phi) < Q^2/8f(\phi)$ is fulfilled, $H_{c2}(\phi)$ has a positive curvature near T_c. In order to observe this anomalous temperature dependence of $H_{c2}(\phi)$, the exponential factor in Eq. (3.15) should have an appreciable value. This is possible when (1) $H_{c2}(\phi)$ is large enough because the wavelength of CDW ordering is of the order of lattice spacing in layered-type compounds, and/or (2) the wavelength Q^{-1} of CDW ordering is relatively long. Note that in $2H$-$NbSe_2$ ($T_c = 7.3$ K) the upper critical field $H_{c2}(T)$ parallel to layer plane reaches 100 kG at around $T/T_c = 0.5$. However we should remark that in such high field we might resort to a more sophisticated method to calculate $H_{c2}(T)$.

B. $\vec{H} \parallel z$; H_{c2}^z

Taking $\vec{A} = (0, Hx, 0)$, we rewrite Eq. (3.8) as

$$\left[-\frac{\partial^2}{\partial x^2} - \epsilon^2\left(\frac{\partial}{\partial y} - ihx\right)^2 - \epsilon^2\frac{\partial^2}{\partial z^2} + K\cos Q(z-z_0)\right]\Delta(r) = \frac{1}{\xi_1^2(T)}\Delta(r) \ . \quad (3.16)$$

We assume $\Delta(r) = \exp(ik_y y)g_1(x)g_2(z)$ and choose $k_y = 0$. Then the above equation reduces to

$$\left[-\frac{d^2}{dx^2} + (\epsilon h x)^2\right]g_1(x) = E_1 g_1(x) \quad (3.17)$$

and

$$\left[-\epsilon^2\frac{d^2}{dz^2} - K\cos Q(z-z_0)\right]g_2(z) = E_2 g_2(z) \ . \quad (3.18)$$

Therefore the lowest eigenvalue of the former equation gives $H_{c2}^z(T)$ as

$$H_{c2}^z(T) = \frac{\Phi_0}{2\pi\xi_1^2(0)}\frac{1}{\epsilon}\left|\frac{T-T_c}{T_c}\right| \ . \quad (3.19)$$

The upper critical field $H_{c2}^z(T)$ parallel to $\vec{Q}$ (or parallel to the layer plane) does not exhibit a positive curvature but follows the ordinary linear behavior near T_c as expected by the conventional GL theory. It should be noted that upon decreasing temperature the ratios $H_{c2}(\phi)/H_{c2}^z$ and H_{c2}^y/H_{c2}^x do increase, which is sharply contrasted to the prediction from the conventional GL equation where these ratios are temperature independent. The temperature dependence of $H_{c2}^{\perp}/H_{c2}^{\parallel}$, the ratio of perpendicular to parallel upper critical field, have been observed in layered compounds such as $2H$-$NbSe_2$.[18]

IV. CONCLUSION AND DISCUSSION

We have shown that in the presence of CDW with a wave number $Q(=2k_F)$ the stable SC state is characterized by the two order parameters: One is the spatially varying pairing $\Delta(Q)$ whose static wave is given by the wave number Q same as CDW, and other the ordinary Cooper pairing $\Delta(0)$. We show it by examining the linearized gap equation under a periodic lattice distortion due to CDW perturbationally, assuming a second-order phase transition. This stable SC state turns out to be easier to coexist with CDW compared with the ordinary BCS state.

It should be pointed out that the spin-density-wave (SDW) perturbation,[14] which is spatially periodic spin alignment, breaks the time-reversal symmetry. Superconductivity in such a case is heavily suppressed compared with the present CDW case where the time-reversal symmetry is not broken. Therefore superconductivity in a CDW can exist relatively easily. [We should remark that this modified pairing state is influenced by the presence of normal impurity scattering because $\Delta(Q)$ is not time-reversal pair. However since we only consider the system where CDW, which is also formed by non-time-reversal pairs, is fully developed, it is not unreasonable to assume that $\Delta(Q)$ is not suppressed by normal impurity scattering.] A similar calculation in SDW case shows that the stable superconducting state is nothing but the ordinary BCS state in which the effective attractive interaction $gN(0)$ is simply reduced by the SDW perturbation.

As is mentioned before, since this static spatially varying order parameter spontaneously breaks the spatial symmetry, it is expected that the Goldstone boson as a collective mode appears. This is because the spatially varying condensate wave function $\Delta(Q)$ can slide without energy loss just like the phase modes in CDW. We expect that this stable SC state might be detected by measuring various thermodynamic quantities in low-dimensional materials. However the most promising way is to measure the upper critical field. A qualitative difference in the temperature dependence of H_{c2} is expected, depending upon relative directions between the applied magnetic field and the wave vector Q. In this connection the recent experiment[3] of $H_{c2}(T)$ on the layered-type compound $Nb_{1-x}Ta_xSe_2$ is interesting, in which the anomalous positive curvature in H_{c2} parallel to layers near T_c is suppressed as x increases or T_{CDW} is lowered. This suggests importance of the interplay between CDW and superconductivity, and is qualitatively understood by the present theory. Therefore it is highly desirable to measure $H_{c2}(T)$ more carefully, especially when the applied magnetic field is in the layer plane where we expect the temperature dependence of H_{c2} different for parallel to Q and perpendicular to it. In $2H$-$NbSe_2$ CDW is characterized by the triple Q, therefore it may complicate the situation.

We do not consider in this paper the reaction of CDW state due to the onset of superconductivity, regarding CDW perturbation V as an external potential. This is valid as far as T_c is much smaller than T_{CDW} as the case in $2H$-$NbSe_2$. We also do not consider the possibility of a CDW state in the presence of superconductivity (the case $T_c > T_{\mathrm{CDW}}$). These problems remain for future work.

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APPENDIX: EVALUATION OF THE INTEGRAL KERNEL $K(q,q',\omega_n)$

1. Diagonal element $K(0,0,\omega_n)$

Substituting Eqs. (2.10) and (2.11) into Eq. (2.12), we can evaluate $K(0,0,\omega_n)$ in the form

$$K(0,0,\omega_n)=2\sum_{k_z>0}\frac{(i\omega_n-\xi_{k-Q})(-i\omega_n-\xi_{k-Q})}{[(i\omega_n-\xi_k)(i\omega_n-\xi_{k-Q})-V^2][(-i\omega_n-\xi_k)(-i\omega_n-\xi_{k-Q})-V^2]}$$
$$+2\sum_k\frac{V^2}{[(i\omega_n-\xi_k)(i\omega_n-\xi_{k-Q})-V^2][(-i\omega_n-\xi_k)(-i\omega_n-\xi_{k-Q})-V^2]}\;. \tag{A1}$$

If we subtract and add the term

$$2\sum_{k_z<0}\frac{1}{(i\omega_n-\xi_k)(-i\omega_n-\xi_{-k})} \tag{A2}$$

then, Eq. (A1) reduces to

$$K(0,0,\omega_n)=2\sum_k\frac{(i\omega_n-\xi_k)(-i\omega_n-\xi_k)+V^2}{[(i\omega_n-\xi_k)(i\omega_n-\xi_{k-Q})-V^2][(-i\omega_n-\xi_k)(-i\omega_n-\xi_{k-Q})-V^2]}$$
$$-2\sum_{k_z<0}\frac{1}{(i\omega_n-\xi_k)(-i\omega_n-\xi_{-k})}\;. \tag{A3}$$

We define the integral I_k of the first term of Eq. (A3) as

$$\begin{aligned}
I_k&=\sum_k\frac{2C+4V^2}{AA^*}\;,\\
A&=t^2-t(2i\omega_n-L^+-L^-)+(i\omega_n-L^+)(i\omega_n-L^-)-V^2\;,\\
A^*&=t^2-t(-2i\omega_n-L^+-L^-)+(i\omega_n+L^+)(i\omega_n+L^-)-V^2\;,\\
C&=\tfrac{1}{2}(A+A^*)-t(L^+-L^-)+2\omega_n^2-L^+L^-+(L^-)^2\;,
\end{aligned} \tag{A4}$$

where we have introduced the cylindrical coordinates (k_ρ,k_ϕ,k_z), $t=k_\rho^2/2m$, and $L^\pm=k_z^2/2m\pm k_zQ/2m$. After some manipulation we obtain

$$I_k=\frac{2\pi m}{(2\pi)^3}\int_{-\infty}^{\infty}dk_z\int_0^\infty dt\left\{\frac{1}{A}+\frac{1}{A^*}+4\left[\omega_n^2+\left(\frac{k_zQ}{2m}\right)^2+V^2\right]\frac{1}{AA^*}\right\}\;. \tag{A5}$$

We evaluate it perturbationally to the second order of (V/ϵ_F), that is,

$$\begin{aligned}
I_k&=I_1+I_2\;,\\
I_1&=\frac{2\pi m}{(2\pi)^3}2\int_0^\infty dx\left(\frac{m}{2}\right)^{1/2}\frac{1}{\sqrt{x}}\frac{1}{2i\omega_n}\ln\left(\frac{x^2-4\epsilon_Fx-\omega_n^2+2i\omega_nx}{x^2-4\epsilon_Fx-\omega_n^2-2i\omega_nx}\right)\;,\\
I_2&=\frac{2\pi m}{(2\pi)^3}4V^2\int_0^\infty dx\left(\frac{m}{2}\right)^{1/2}\frac{\sqrt{x}}{(x^2-4\epsilon_Fx-\omega_n^2)^2+4\omega_n^2x^2}\;,
\end{aligned} \tag{A6}$$

where $x = k_z^2/2m$. In view of the fact that ω_n/ϵ_F is very small these integrations are performed as

$$I_1 = \frac{2\pi N(0)}{|\omega_n|} \quad , \quad I_2 = -\frac{\pi N(0)}{|\omega_n|}\frac{V^2}{8\epsilon_F^2} \quad , \tag{A7}$$

where $N(0) = m^{3/2}\epsilon_F^{1/2}/\sqrt{2}\pi^2$ is the density of states at the Fermi energy. Therefore we obtain

$$K(0,0,\omega_n) = \frac{\pi N(0)}{|\omega_n|}\left(1 - \frac{1}{8}\frac{V^2}{\epsilon_F^2}\right) \quad . \tag{A8}$$

2. Off-diagonal element $K(0,Q,\omega_n)$

Substituting Eqs. (2.10) and (2.11) into Eq. (2.14), we evaluate $K(0,Q,\omega_n)$ as

$$K(0,Q,\omega_n) = \sum_k \frac{-2V}{AA^*}\left(t + \frac{k_z^2}{2m}\right) = -2V\frac{2\pi m}{(2\pi)^3}\int_{-\infty}^{\infty} dk_z \left(\frac{x}{4y(y^2+\omega_n^2)}\ln\frac{\xi_1\xi_1^*}{\xi_2\xi_2^*} - \frac{1}{8i\omega_n y}\ln\frac{\xi_1^*\xi_2}{\xi_1\xi_2^*}\right) \quad , \tag{A9}$$

where

$$\xi_{1,2} = i\omega_n - x \pm y, \quad y = [(k_z Q/2m)^2 + V^2]^{1/2} \quad . \tag{A10}$$

Neglecting the order of ω_n/ϵ_F and the terms higher than the second order of (V/ϵ_F), we obtain

$$K(0,Q,\omega_n) = \frac{\pi N(0)V}{8\epsilon_F|\omega_n|}\ln\frac{|\omega_n|}{2\epsilon_F} \quad . \tag{A11}$$

3. $K(Q,Q,\omega_n)$

It is straightforward to show in a similar way from Eq. (2.14) that

$$K(Q,Q,\omega_n) = \pi N(0) O\left(\frac{V^2}{\epsilon_F^2}\right) + \sum_k \frac{1}{AA^*}\left[(t+L^-)^2 + \omega_n^2 - \frac{1}{2}\left(\frac{k_z Q}{m}\right)^2\right] \quad . \tag{A12}$$

The second term is of the order of T_c/ϵ_F smaller than the diagonal element $K(0,0,\omega_n)$ and can be neglected.

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[16] Note that in the previous SDW case (Ref. 14) for the three-dimensional-Fermi sphere $K(0,0) = K^{(0)}(0,0) - (V/\epsilon_F)K^{(1)}(0,0)$ and $K(0,Q) = 0$. Thus SDW perturbs severely superconductivity and reduces the transition temperature drastically because of the time-reversal symmetry-breaking perturbation.

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