# Coexistence of charge-density waves and magnetic order

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The ground state of a simple model which includes a periodic lattice distortion and a local electron-electron Coulomb interaction is studied. In the absence of magnetic order, the Coulomb repulsion tends to suppress the Peierls transition, but ferromagnetism may induce a periodic lattice distortion, giving rise to a phase in which the ferromagnetic order is modulated by a spin-density wave and coexists with a charge-density wave. The interplay of magnetism and lattice distortion depends strongly on the number of conduction electrons. The variation of the order parameters is also calculated as a function of the coupling parameters and of temperature.

## I. INTRODUCTION

Systems exhibiting competition between different kinds of order have been investigated experimentally and theoretically for a long time. The largest interest has probably been devoted to the problem of coexistence of superconductivity and magnetism.[1] The magnetism breaks the time-reversal symmetry required to build up the Cooper pairs and consequently magnetism and superconductivity tend to exclude each other. Recently, the interplay of superconductivity with charge-density waves has been discussed in context with layered compounds.[2] Also in this case the presence of superconductivity tends to reduce the charge-density wave and vice versa. Since charge-density waves have time-reversal symmetry it is of interest to analyze whether the subsequent periodic lattice distortion (PLD) can coexist with ferromagnetism.

At first sight the coexistence of ferromagnetism and PLD seems contradictory. The origin of ferromagnetism is a strong Coulomb *repulsion* between electrons, whereas, on the other hand, a charge-density wave (CDW) and the subsequent PLD is originated by an *attractive* phonon-mediated electron-electron interaction. By this argument, however, ferromagnetism and CDW do not exclude each other necessarily, since ferromagnetism requires a repulsive electron-electron interaction for small momentum transfer, whereas for the appearance of a CDW an attractive interaction for the momentum transfer corresponding to the nesting of the Fermi surface is needed.[3,4] The instability conditions for both ferromagnetism and CDW involve the electrons near the Fermi energy only.

The purpose of this paper is to study the interplay between CDW and ferromagnetism. We analyze the broken-symmetry ground state of a simple model within the Hartree-Fock approximation. Its ground state can be paramagnetic, ferromagnetic, charge-symmetry broken (CDW), spin-symmetry broken (SDW), or a phase in which ferromagnetism, CDW, and SDW coexist. The coexistence of ferromagnetism and CDW always gives rise to the presence of a spin-density wave (SDW) with the same periodicity as the CDW, which modulates the ferromagnetic order.

In this mixed charge ordered magnetic phase the interplay of the order parameters is constructive. Assume that in the absence of magnetism the nesting condition is not satisfied and a CDW is not stable. Here ferromagnetic order may change the population of the spin subbands such that the nesting condition is fulfilled for either the minority or the majority subband. In this case a PLD is possible and charge order and magnetism can coexist to give a lower-energy ground state.

This mechanism has recently been suggested[5] to explain the observed reconstruction of a Co monolayer absorbed at the (100) Cu surface. The reconstruction is interpreted as due to a PLD induced by the Co ferromagnetism. A calculation of the elec-

 

tronic structure of the Co-Cu (100) system shows that there is nesting of the minority spin Fermi surface of ferromagnetic Co, which will not exist if Co were paramagnetic.

The rest of this paper is organized as follows. Our model is described in Sec. II. In Sec. III we calculate the phase diagram at $T=0$ and study the variation of the order parameters with the coupling parameters and temperature. We close the paper with a summary and a brief discussion of the results.

## II. THE MODEL

We consider a model of electrons in Bloch states in the presence of a static lattice distortion and interacting via the Coulomb repulsion. The Hamiltonian of the system is given by

$$H = H_0 + H_1 + H_E \ , \tag{2.1}$$

$H_0$ being essentially the Hubbard Hamiltonian

$$H_0 = \sum_{\vec{k}\sigma} \epsilon_{\vec{k}} C^{\dagger}_{\vec{k}\sigma} C_{\vec{k}\sigma} + \sum_{\vec{k}\vec{k}'\vec{q}} U C^{\dagger}_{\vec{k}+\vec{q}\uparrow} C_{\vec{k}\uparrow} C^{\dagger}_{\vec{k}'-\vec{q}\downarrow} C_{\vec{k}'\downarrow} \ , \tag{2.2}$$

where $C^{\dagger}_{\vec{k}\sigma}(C_{\vec{k}\sigma})$ creates (destroys) an electron in a Bloch state with momentum $\vec{k}$, spin $\sigma$, energy $\epsilon_{\vec{k}}$, and $U$ is the Coulomb repulsion between electrons at the same site. $H_1$ is the electron-phonon coupling which leads to the Peierls instability[6]

$$H_1 = -\sum_{\vec{k}\sigma} \tau_{\vec{k}} C^{\dagger}_{\vec{k}+\vec{Q}\sigma} C_{\vec{k}\sigma} \ , \tag{2.3}$$

where $\tau_{\vec{k}}$ is a matrix element proportional to the lattice distortion and $\vec{Q}$ is half a vector of the reciprocal lattice. We consider only a commensurate Peierls distortion which doubles the periodicity of the original lattice. For simplicity we assume $\epsilon_{\vec{k}+\vec{Q}} = -\epsilon_{\vec{k}}$ and $\tau_{\vec{k}} = \tau$, independent of $\vec{k}$. The third term in Eq. (2.1) represents the elastic energy, which is proportional to the square of the distortion (or to $\tau^2$)

$$H_E = A\tau^2 \ . \tag{2.4}$$

Here $A$ is proportional to the corresponding elastic constant divided by the relevant electron-phonon matrix element squared.

The term $H_0$ is treated in the Hartree-Fock approximation to give

$$H_0 = \sum_{\vec{k}\sigma} \epsilon_{\vec{k}\sigma} C^{\dagger}_{\vec{k}\sigma} C_{\vec{k}\sigma} + U \sum_{\vec{k}\sigma} b_{-\sigma} C^{\dagger}_{\vec{k}+\vec{Q}\sigma} C_{\vec{k}\sigma} - U b_{\uparrow} b_{\downarrow} - U n_{\uparrow} n_{\downarrow} \ , \tag{2.5}$$

where

$$\epsilon_{\vec{k}\sigma} = \epsilon_{\vec{k}} + U n_{-\sigma} \ , \tag{2.6}$$

$$n_{\sigma} = \sum_{\vec{k}} \langle C^{\dagger}_{\vec{k}\sigma} C_{\vec{k}\sigma} \rangle \ , \tag{2.7}$$

$$b_{\sigma} = \sum_{\vec{k}} \langle C^{\dagger}_{\vec{k}+\vec{Q}\sigma} C_{\vec{k}\sigma} \rangle \ . \tag{2.8}$$

Here $\langle \cdots \rangle$ indicates thermodynamic average and $n_{\sigma}$ is the mean number of electrons per site with spin $\sigma$.

Within this approximation $H$ is reduced to a one-particle Hamiltonian given by

$$H = \sum_{\vec{k}\sigma} \epsilon_{\vec{k}\sigma} C^{\dagger}_{\vec{k}\sigma} C_{\vec{k}\sigma} - \sum_{\vec{k}\sigma} \gamma_{\sigma} C^{\dagger}_{\vec{k}+\vec{Q}\sigma} C_{\vec{k}\sigma} + A\tau^2 - U b_{\uparrow} b_{\downarrow} - U n_{\uparrow} n_{\downarrow} \ , \tag{2.9}$$

where

$$\gamma_{\sigma} = \tau - U b_{-\sigma} \ . \tag{2.10}$$

In the following we consider a band of width $W$ with a constant density of states. The condition $\epsilon_{\vec{k}} = -\epsilon_{\vec{k}+\vec{Q}}$ is equivalent to assuming that the Fermi surface for the half-filled band has perfect nesting. The details of the density of states are not essential for our study provided there is nesting.

There are three relevant parameters in our model: $n = n_{\uparrow} + n_{\downarrow}$, $U$ and $A$. Depending on the values of these parameters the ground state of the system can be:

(a) A paramagnetic and nondistorted state with $\tau = 0 (b_{\uparrow} = b_{\downarrow} = 0)$ and $n_{\uparrow} = n_{\downarrow} = \frac{1}{2} n$. This state will be referred to as the $P$ state.

(b) A paramagnetic Peierls or CDW state with $\tau \neq 0 (b_{\uparrow} = b_{\downarrow} \neq 0)$ and $n_{\uparrow} = n_{\downarrow} = \frac{1}{2} n$. This state will be called the CDW state.

(c) A ferromagnetic (F) state with $\tau = 0 (b_{\uparrow} = b_{\downarrow} = 0)$ and $n_{\uparrow} \neq n_{\downarrow}$.

(d) An antiferromagnetic (SDW) state with $\tau = 0$, $b_{\uparrow} = -b_{\downarrow} \neq 0$, and $n_{\uparrow} = n_{\downarrow} = \frac{1}{2} n$.

(e) A distorted or CDW state with some kind of magnetic order.

Throughout this work, since there is electron-hole symmetry, we consider only $1 \leq n \leq 2$. The value of the parameter $\tau$ is found by minimization of the free energy of the system. For $T=0$ we obtain

$$\tau = (1/2A)(b_{\uparrow} + b_{\downarrow}) \ . \tag{2.11}$$

## III. PHASE DIAGRAM

### A. The zero temperature phase diagram

First we analyze the interplay of the electron-phonon interaction and the Coulomb repulsion on the CDW state. In the pure CDW state $b_{\uparrow} = b_{\downarrow} = b_c$, $n_{\uparrow} = n_{\downarrow} = \frac{1}{2} n$ and $\tau \neq 0$. The gap induced by the CDW is given by $2\gamma = 2(\tau - U b_c)$, which shows that the Coulomb repulsion tends to destroy the CDW state. The condition of stability of the CDW state ($\tau \neq 0$) is given by

$$\frac{1}{AW} \geq \frac{U}{W} - \frac{1}{\ln|1-n|} \ . \tag{3.1}$$

Since $1 \leq n \leq 2$ no CDW can exist for $1/A \leq U$. In

Fig. 1 we show the region of stability[7] of the CDW state as compared with the $P$ state (absence of magnetic order).

However, if we consider the possibility of magnetic order for $\tau=0$, we have that the condition for ferromagnetism is $U/W \geq 1$ and that the SDW state is the most stable one if the band is nearly half-filled.

In order to study the interplay between CDW and magnetic order we introduce the parameters $m$, $b_c$, and $b_s$

$$n_\sigma = \tfrac{1}{2}n + \sigma m \ , \tag{3.2}$$

$$b_\sigma = b_c - \sigma b_s \ . \tag{3.3}$$

Here $\sigma$ takes the values $\pm 1$ according to the spin orientation, $m$ is the magnetization of the system, $b_c$ is the order parameter for the CDW state, and $2b_s=(b_\uparrow - b_\downarrow)$ determines the amplitude of the SDW. Notice that Eq. (2.11) shows explicitly that $b_c$ is proportional to $\tau$.

The one-electron energies are

$$\omega_{1\vec{k}\sigma} = -Um\sigma + (\epsilon_{\vec{k}}^2 + \gamma_\sigma^2)^{1/2} \ , \tag{3.4a}$$

$$\omega_{2\vec{k}\sigma} = -Um\sigma - (\epsilon_{\vec{k}}^2 + \gamma_\sigma^2)^{1/2} \ , \tag{3.4b}$$

where

$$\gamma_\sigma = (1/2A)(b_\uparrow + b_\downarrow) - Ub_{-\sigma} \ . \tag{3.5}$$

The one-particle Green's functions corresponding to Eq. (2.9) are given by

$$\langle\langle C_{\vec{k}\sigma}, C_{\vec{k}\sigma}^\dagger \rangle\rangle_\omega = \frac{1}{2\pi} \frac{\omega + \epsilon_{\vec{k}}}{(\omega - \omega_{1\vec{k}\sigma})(\omega - \omega_{2\vec{k}\sigma})} \ , \tag{3.6a}$$

$$\langle\langle C_{\vec{k}+\vec{Q}\sigma}, C_{\vec{k}\sigma}^\dagger \rangle\rangle_\omega = -\frac{1}{2\pi} \frac{\gamma_\sigma}{(\omega - \omega_{1\vec{k}\sigma})(\omega - \omega_{2\vec{k}\sigma})} \ . \tag{3.6b}$$

The parameters $n_\sigma$ and $b_\sigma$ are obtained from the imaginary part of Eqs. (3.6a) and (3.6b), respectively. The parameters $m$, $b_c$, and $b_s$ are the solutions of

$$n_\sigma = \tfrac{1}{2}n + \sigma m = \tfrac{1}{2}\sum_{\vec{k}} [f(\omega_{1\vec{k}\sigma}) + f(\omega_{2\vec{k}\sigma})] \tag{3.7}$$

and

$$b_\sigma = b_c - \sigma b_s = -\gamma_\sigma \sum_{\vec{k}} \tfrac{1}{2}(\epsilon_{\vec{k}}^2 + \gamma_\sigma^2)^{-1/2} [f(\omega_{1\vec{k}\sigma}) - f(\omega_{2\vec{k}\sigma})] \ , \tag{3.8}$$

where $f(\omega)$ is the Fermi distribution function. The chemical potential $\mu$ is fixed by the number of particles, $n = n_\uparrow + n_\downarrow$.

The integrated expressions for $n_\sigma$ and $b_\sigma$ at $T=0$ are

$$n_\sigma = \tfrac{1}{2} + (X_\sigma / W)\,\mathrm{sgn}(Um\sigma + \mu) \ , \tag{3.9a}$$

$$b_\sigma = \frac{\gamma_\sigma}{W}\left[\operatorname{arcsinh}\frac{W}{2|\gamma_\sigma|} - \operatorname{arcsinh}\frac{X_\sigma}{|\gamma_\sigma|}\right] \ , \tag{3.9b}$$

where

$$X_\sigma = \begin{cases} [(Um\sigma + \mu)^2 - \gamma_\sigma^2]^{1/2} & \text{if } |Um\sigma + \mu| \geq |\gamma_\sigma| \ , \\ 0 & \text{otherwise.} \end{cases} \tag{3.9c}$$

An important result is that if we choose $m$ and $\tau$ different from zero (i.e., coexistence of the F and CDW states) Eq. (3.8) gives $b_s \neq 0$. This indicates that in the presence of a PLD a uniform magnetization cannot exist, but is always modulated by an SDW.

In Fig. 2 the phase diagram $1/AW$ versus $U/W$ is shown for different values of $n$. The full lines represent transitions with a continuous change in the order parameters, whereas the broken ones denote discontinuous transitions. Depending on $n$ the CDW and the magnetic order can interfere in a constructive or destructive way.

For $n=1.5$ the ferromagnetism induces a PLD for $U/W \geq 1$. In this case the F state is stable with $n_\uparrow = 1$ and $n_\downarrow = \frac{1}{2}$. As a consequence of the ferromagnetic order the minority spin band is half-filled and its Fermi surface has perfect nesting giving rise to a PLD.

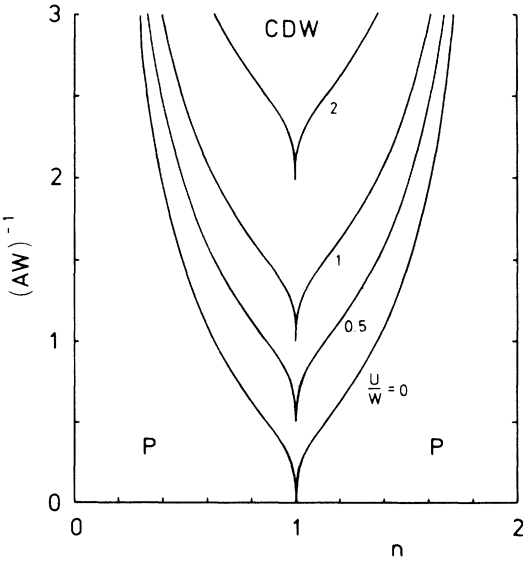


FIG. 1. Phase diagram $(AW)^{-1}$ against $n$ for the CDW in absence of magnetic order [see Eq. (3.1)]. The different curves correspond to different values of $U/W$ as indicated.

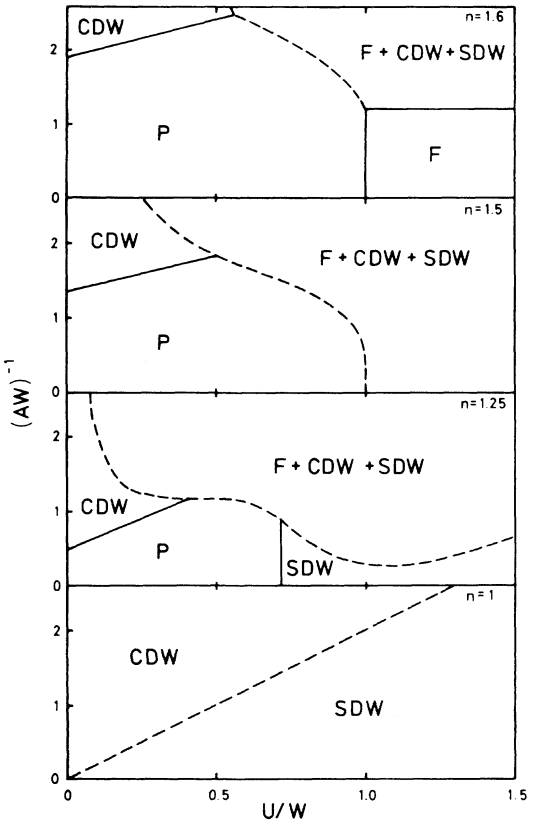


FIG. 2. Phase diagram $(AW)^{-1}$ vs $U/W$ for different occupation numbers $n$. The broken lines represent transitions where the order parameters jump at the transition and the full lines represent transitions where the order parameters are continuous. In general, for $n > 1$ the CDW and the magnetic order interfere in a constructive way.

If $U/W < 1$ and depending upon $1/AW$ it may be energetically favorable to have a PLD which splits the bands. There is a region in the phase diagram where neither the CDW nor the F state takes place alone but the state where both coexist is stable. As we mentioned above, when PLD and ferromagnetism coexist the magnetization is modulated. This is easily understood since in the minority band only the bonding states are occupied whereas in the majority band both bonding and antibonding states are occupied. This gives rise to a modulated magnetization governed by the electrons in the minority spin band with the same periodicity as the PLD.

For $n = 1.6$ (see Fig. 2) the phase diagram is similar to that of $n = 1.5$ but in the F state the minority spin Fermi surface does not have perfect nesting and a minimum value of $1/AW$ is necessary to stabilize the CDW.

In the case $n = 1.25$ the SDW state is more stable than the F state which cannot exist alone. For $n = 1$ either pure CDW or SDW states are stable. For large values of $U/W$ the SDW state is the stable one, whereas for large values of $(AW)^{-1}$ the CDW state is the more stable. The boundary between the two phases is given by $A^{-1} = 2U$. This result was previously derived by Chan and Heine.[8]

### B. Variation of the order parameters

In Fig. 3 we show the variation of the order parameters $m$, $b_c$, and $b_s$ as a function of the model parameters $(AW)^{-1}$ and $U/W$ for $n = 1.5$ and 1.25. For $n = 1.5$ the magnetization takes its maximum allowed value $(m = 1 - \frac{1}{2}n)$ and $b_c = b_s$. Here the modulation of the charge involves only electrons in the minority band. For $n = 1.25$ the magnetization corresponds to the magnetization required to have $n_\downarrow = \frac{1}{2}$ (i.e., perfect nesting in the minority spin Fermi surface). On the other hand $b_c$ may be smaller or larger than $b_s$ depending on the value of $U$. For small $U/W$ $b_c > b_s$ and for large $U/W$ $b_c < b_s$.

In order to study the temperature dependence of

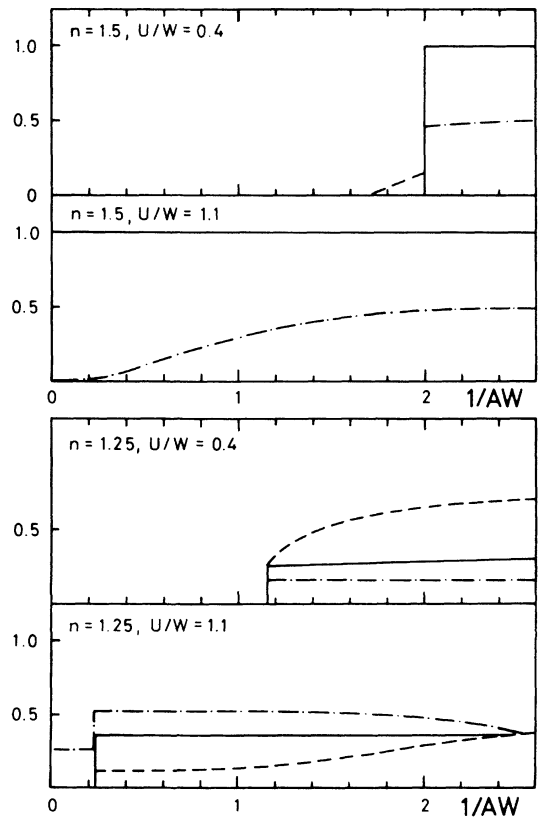


FIG. 3. Order parameters $m/(1 - \frac{1}{2}n)$ (full line), $b_c$ (dashed line), and $b_s$ (dashed-dotted line) as a function of $(AW)^{-1}$ for different values of $U/W$ and $n$. For $n = 1.5$, if $m \neq 0$ $b_s = b_c$ and only $b_s$ is drawn.

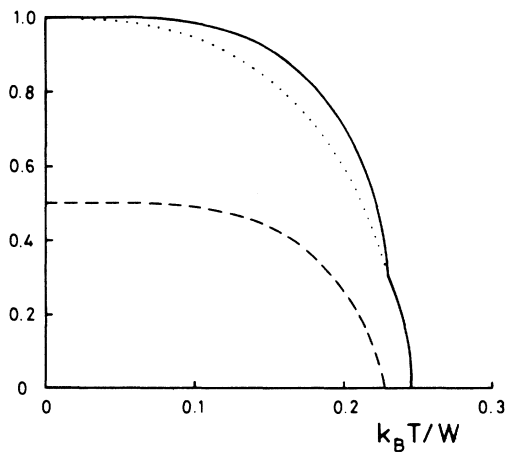


FIG. 4. Order parameters $m/(1-\frac{1}{2}n)$ (full line) and $\tau/W$ (dashed line) as a function of the temperature for $U/W=1.2$, $(AW)^{-1}=2$, and $n=1.5$. The dotted line represents the magnetization for $\tau=0$.

the order parameters we have to consider the free energy of the system given by

$$F=-k_BT\sum_{\vec{k}\sigma\alpha}\ln(1-e^{-(1/k_BT)(\omega_{\alpha\vec{k}\sigma}-\mu)}) +n\mu+A\tau^2-U(n_\uparrow n_\downarrow+b_\uparrow b_\downarrow)\ , \tag{3.10}$$

where $k_B$ is the Boltzmann constant. The label $\alpha$ can take the values 1 or 2 and $\omega_{\alpha\vec{k}\sigma}$ are the one-particle energies given by Eq. (3.4).

By minimizing the free energy with respect to $\tau$ and with Eqs. (3.7) and (3.8) we find the dependence of the order parameters $\tau$ and $m$ with the temperature. As an example in Fig. 4 we have plotted $\tau$ and $m$ vs $T$ for $(AW)^{-1}=2$, $U/W=1.2$, and $n=1.5$. At low temperatures the magnetization is larger for $\tau\neq 0$ than for $\tau=0$ (dotted line). Here the system gains energy with the CDW due to the nesting of the Fermi surface. For the parameters indicated in Fig. 4 we see that the critical temperature of the CDW is eight percent lower than the ferromagnetic critical temperature.

## IV. SUMMARY AND DISCUSSION

We considered a simple model consisting of Bloch states interacting via a Hubbard-like Coulomb repulsion and coupled linearly to a periodic lattice distortion. The model is characterized by three parameters: the Coulomb repulsion $U/W$, the elastic constant and the electron-phonon matrix element contained in $1/AW$ and the total number of electrons. Depending on these parameters we show within the Hartree-Fock approximation that there are five possible phases for the ground state of the system. The phases of the system are described by three order parameters, corresponding to the total magnetization, the CDW amplitude and the SDW amplitude. The possible states are the P state (all order parameters are equal to zero), the F, CDW, and SDW states (only one nonvanishing order parameter) and the mixed state (all order parameters are nonzero).

The interesting new phase is the mixed state where magnetism coexists with a PLD. The interference between ferromagnetism and the CDW may be constructive, in the sense that the mixed state can exist even if the simple ordered phases, characterized by a single order parameter, are not stable. The condition of stability of the pure CDW state is that of nesting of the Fermi surface. If this condition is not satisfied in the absence of magnetism, the ferromagnetism may repopulate the spin subbands such that one of them meets the nesting condition and lowers the energy of the system.

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