PAULI AND ORBITAL EFFECTS OF MAGNETIC FIELD ON CHARGE DENSITY WAVES

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Abstract. Taking into account both Pauli and orbital effects of external magnetic field we compute the mean field phase diagram for charge density waves in quasi–one–dimensional electronic systems. The magnetic field can cause transitions to CDW states with two types of the shifts of wave vector from its zero–field value. It can also stabilize the field–induced charge density wave. Furthermore, the critical temperature shows peaks at a new kind of magic angles.

1. INTRODUCTORY REMARKS

Although the charge and spin density waves [C(S)DWs] are resembling in many physical aspects, they behave differently in the external magnetic field. The reason is that the Pauli coupling probes different contents of order parameter spaces for two cases. The SDW order parameter is of complex vectorial form, in contrast to simple complex parameter space for CDWs. We write four complex S/CDW amplitudes in a compact form

\[ M_i = \Psi_\uparrow \rho_i \sigma_i \Psi_\uparrow + \Psi_\downarrow \rho_i \sigma_i \Psi_\downarrow, \]

where \( \Psi_\uparrow \) and \( \Psi_\downarrow \) are Pauli matrices in respective (+, −) and (↑, ↓) two-dimensional spaces, with \( \sigma_4 = I \). \( M_1, M_2 \) and \( M_3 \) are three components of SDW, with \( M_3 \) chosen along the direction of the magnetic field \( H \), while \( M_4 \) is the CDW amplitude. The Pauli coupling affects only components \( M_{3,4} = \Psi_{\uparrow \uparrow} \Psi_{\downarrow \downarrow} \pm \Psi_{\downarrow \downarrow} \Psi_{\uparrow \uparrow}, \) i.e. the linear combinations of two DWs with spins \( \uparrow \) and \( \downarrow \) and with wave numbers \( 2k_F \pm 2q_P \). Here \( q_P \equiv \mu_B H/v_F \) is the characteristic wave number for the Pauli coupling (\( \mu_B \) - Bohr magneton, \( v_F \) - longitudinal Fermi velocity). Due to this splitting and the mismatch of two Peierls wave numbers, the critical temperature for the resulting hybridized combination of \( M_3 \) and \( M_4 \) is suppressed with respect to its value at \( H = 0 \).

The systems with the SDW order avoid this suppression by orienting its magnetization perpendicularly to the magnetic field. The Pauli coupling therefore influences only the spectrum of collective modes. It also may introduce a spin flop transition if the magnetic field is oriented along the easy axis in systems with internal magnetic anisotropy.[1] The magnetic field influences the SDW phase diagram only through the another, orbital coupling, characterized by the wave number \( q_0 = ebH \cos \theta \), where \( b \) is the transverse lattice constant, and \( \theta \) is the inclination of the magnetic field with respect to the normal to the conducting \((a, b)\) plane. As is well known, this coupling has a general tendency to suppress the effects of imperfect nesting and to enhance the critical temperatures.[2]

Since both types of couplings are effective in CDW systems, and the ratio of characteristic scales \( \eta \equiv q_0/q_P \) may pass through a wide range of values (particularly by varying the orientation \( \theta \)), the resulting phase diagrams may well be more complex than that for SDW systems. In the present paper we discuss this problem within a mean field, random phase approximation (RPA), assuming also only sinusoidal modulations.[3] The extension to non-sinusoidal modulations, but with the Pauli coupling only, was considered elsewhere.[4]
2. PHASE DIAGRAM

The $2 \times 2$ susceptibility matrix for the $(M_3, M_4)$ DW response reads[3]

$$\chi_g \left( \frac{\sqrt{1 + \delta^2} + U_c \chi_g}{\delta} \delta \frac{\sqrt{1 + \delta^2} + \nu U_c \chi_g}{\chi_g} \right),$$

with $\chi_0 \equiv \sqrt{\chi_0^2}$, $\delta \equiv (\chi_0 - \chi_0)/(2 \chi_g)$, $f \equiv 1 + (1 + \nu) U_c \chi_g \sqrt{1 + \delta^2} + \nu U_c \chi_g^2$ and $\chi_0(q_x \pm 2 q_y, q_y)$. The contributions from the orbital coupling enter in the standard way through the bubble polarization diagram $\chi_0[2,3]$ The parameter $\nu$ is the ratio of SDW and CDW coupling constants, $\nu = U_s/(-U_c) = (2 g_1 - g_2)/g_2$, with the range of CDW stability defined by $U_c < 0$, $\nu < 1$. The critical temperature and the wave vector for the CDW in the magnetic field follow from the diagonalization of the matrix (1).

Let us at first assume that the Fermi surfaces are perfectly nested ($t_b \neq 0, t'_b = 0$ in the standard notation). As the phase diagram in Fig.1(a) shows, at weak enough fields $[h \equiv \mu_B H/(2\pi T) \leq h_c = 0.304]$, the systems keeps the perfect nesting wave vector $Q_0 = (2k_F, \pi/b)$ (i.e. $q_x = q_y = 0$ in eq.[4]), but the critical temperature $T_{c0}$ decreases with respect to its value at $h = 0$, $T_{c0} = (2\gamma E_F/\pi) \exp(-\pi v_F U_c)$. As the field passes the critical value $h_c$ (that weakly depends on parameters $\eta$ and $\nu$), this ordering is replaced by one of those with shifted wave vectors. Depending on the subtle relations [3] between the strength of the magnetic field, the interaction $U_c$, and the the values of parameters $\eta$ and $\nu$, two types of shifts, reflecting qualitatively different effects of Pauli coupling, appear possible.

The shift in the longitudinal direction, at some wave numbers $\pm q_x$ with respect to $2k_F$, is the direct consequence of the band Zeeman splitting, present already in the pure one-dimensional limit. With $q_x \neq 0$ we have a finite off-diagonal coupling of pure CDW and SDW$_z$ in the matrix (1). The resulting CDW$_x$ order is therefore a CDW-SDW hybrid, with the relative weight which, together with the critical temperature $T_{cx}$ and the wave number $q_x$, depends on the couplings $U_c, \nu$. Since CDW$_x$ does not involve the orbital coupling, it does not depend on the parameter $\eta$.

Another case is shown in the inset of Fig1(a). Between phases CDW$_0$ and CDW$_x$ a phase CDW$_y$ with $(q_x = 0, \pm q_y \neq 0)$ is stabilized. It appears for example if we suppress somewhat $T_{cx}$ by introducing a finite negative $\nu$. What remains as maximal critical temperature is $T_{cy}$ (itself independent on $\nu$), corresponding to the transition metal–CDW$_y$. CDW$_y$ does not involve SDW$_z$ [since $\delta = 0$ in (1)], but is a pure CDW with an effective imperfect nesting as a consequence of a finite (and large enough) value of $q_F$ in $\chi_g$. The properties of CDW$_y$ order follow from the lower diagonal element of the matrix (1). They are independent on the parameter $\nu$, since CDW channel is now not active. On the other hand they depend on the parameter $\eta$, since the “one-dimensionalization” of the corrugated Fermi surface due to the orbital coupling [2] helps in stabilizing this ordering. More precisely, the critical temperature $T_{y}$ is $\eta$-dependent and $t_b$-independent, while the wave number $q_y$ and the CDW amplitude at $T < T_y$ depend on $t_b$ as well.

In the phase diagram in Fig.1(a) all phase transitions $(T_{c0}, T_{cx},$ and $T_{cy})$ between metallic phase and three different CDW’s are of the second order. The transition between CDW$_0$ and CDW$_x$ is of the first order and is weaker and weaker (the meta-stability regime gets narrower) as one approaches $T_c$ from below. The transition between CDW$_0$ and CDW$_y$ is at the line $h = 0.304$ near $T_c$, and it deviates at low temperatures toward the point $\mu_B H \approx T_c[5]$, in figure denoted by $P$. In the inset of Fig.1(a), where intermediate phase CDW$_y$ comes into play, both transitions $CDW_0$–$CDW_y$ and $CDW_y$–$CDW_x$ are of the first order, and we expect similar meta-stable regimes around the transitions.

The perfect nesting–like phase diagram was found in the $\alpha - (ET)_2 KHg(CSN)_4$ compound[6,7], which indicates that the ordered state contains a CDW. The data are consistent with the case with one, CDW$_0$–CDW$_x$, transition in magnetic field. However, it is still not clear to what extent the phase diagram depends on the direction of magnetic field.[6,7] The anisotropy of $T_c$ in magnetic field would indicate that the orbital effects are also present, i.e. that the nesting is effectively imperfect.
The phase diagram for imperfectly nested case \((t_b' \neq 0)\) is shown in Fig.1(b). Note that for \(t_b'\) close to its critical value \(t_b'^*\) (the value of \(t_b'\) when \(T_c\) completely disappears for \(H = 0\)) the phenomenon of field induced CDW appears. The obvious difference with respect to FISDW system is that the Zeeman splitting eventually suppresses \(T_c\). We expect also a new kind of angular resonances involving the ratio between orbital and Pauli coupling. They are manifested as peaks in \(T_c\) at the “magic angles” given by \(\eta = 2/n\), \(n\) being integer.

3. CONCLUSIONS

We have studied the effects of a magnetic field on CDWs in Q1D systems. Both orbital and Pauli couplings are taken into account in the calculation the RPA response in CDW-SDW channel. At perfect nesting we explain quantitatively basic features of the phase diagram of \(\alpha\)-\(ET\) compounds. The field–driven phase transition [8] and the enhancement of the critical temperature in magnetic field [9] in \(NbSe_3\) are also possible experimental realizations of our theory. However, due to presumably badly nested Fermi surface in these materials, the theoretical analysis becomes more complicated and allow for various possible effects. More detailed experimental study would be also welcome. Finally, we emphasize the importance of studying the Q1D compounds of MX family in the magnetic field, since there the parameter \(\nu\) can be tuned by pressure.[10]

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