Imperfect nesting and scattering due to disorder in spin-density-waves

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As is well-known both imperfect nesting and scattering reduces the spin-density-wave transition temperature and the quasi-particle energy gap at $T = 0K$. We extend our earlier analysis to the condensate density f_1 and the pinning potential thus the threshold field, at both $T = 0K$ and $T = T_c$ when both imperfect nesting and scattering effect are present. At $T = 0K$, $f_1 = 1$ in the presence of both imperfect nesting and scattering until the quasi-particle energy gap is closed. Consequently, the threshold field E_T is almost constant until SDW is almost destroyed, where E_T suddenly moves up. We found that E_T exhibits a small peak just before T_c for small scattering rates. This result may help disentangle the mechanism behind the rapid cooling of $(TMTSF)_2ClO_4$.

Extending earlier models by Horowitz *et al.* [1] and Yamaji [2] we have shown recently [3] that the model with imperfect nesting can account for a number of features associated with SDW in Bechgaard salts like $(TMTSF)_2PF_6$ *etc.* and CDW's in $NbSe_3$ within mean field theory. For example the large ratio Δ_a/T_c observed in CDW's of $NbSe_3$ is accounted for in terms of imperfect nesting contrary to the prevailing but incorrect view based on the large fluctuation or strong coupling [4]. Here Δ_a is the apparent energy gap deduced from the activation energy of the electric resistance.

The impurity scattering is unavoidable in SDW (or CDW). Further in $(TMTSF)_2ClO_4$ the quenching of the anion disorder by rapid cooling will probably introduce an additional scattering due to the disorder for example. In this paper we discuss the threshold electric field when both imperfect nesting and scattering effect are present.

We limit ourselves to SDW for simplicity. – the results obtained here also apply to the quasi-one-dimensional CDW. We shall start with the Hamiltonian first introduced by Yamaji [2]:

$$H = \sum_{p,\alpha} \epsilon(p) c_{p\alpha}^\dagger c_{p\alpha} + U \sum_q n_{q\uparrow} n_{-q\downarrow} \quad (1)$$

with the quasiparticle energy:

$$\epsilon(p) = v(p_1 - p_F) - 2t_b \cos(bp_2) - \epsilon_0 \cos(2bp_2) \quad (2)$$

Here $c_{p\alpha}^\dagger$ and $c_{p\alpha}$ are the creation and annihilation operator of electrons with momentum p and spin α , and $n_{q\uparrow}$ and $n_{-q\downarrow}$ are the corresponding number operators. ϵ_0 is the parameter characterizing the imperfect nesting effect which is associated with the quasi-one dimensionality.

Within the mean field approximation, the quasiparticle Green's function in the spinor representation is given by:

$$G^{-1}(p, \omega_n) = i\omega_n - \epsilon_0 \cos(2bp_2) - \xi \rho_3 - \Delta \rho_1 \sigma_3 \quad (3)$$

where ρ_1 and ρ_3 are Pauli spin matrices operating on the spinor space formed by the left- and right-going electrons, ω_n is the Matsubara frequency, and

$$\xi = v(p_1 - p_F) - 2t_b \cos(bp_2) \quad (4)$$

The order parameter is determined self-consistently by

$$\Delta = UT \sum_n \int \frac{d^3p}{(2\pi)^3} \text{Tr}[\rho_1 G(p, \omega_n)] \quad (5)$$

We add the impurity scattering effect into the above model. Following the standard diagram approach [5], the impurity effect can be incorporated by replacing ω_n and Δ in Eq. (3) by $\tilde{\omega}_n$ and $\tilde{\Delta}$,

$$\tilde{\omega}_n = \omega_n + \frac{1}{2}(\Gamma_1 + \Gamma_2) \left\langle \frac{(\tilde{\omega}_n + i\varepsilon_0 \cos(\chi))}{\sqrt{(\tilde{\omega}_n + i\varepsilon_0 \cos(\chi))^2 + \tilde{\Delta}^2}} \right\rangle \quad (6)$$

and

$$\tilde{\Delta} = \Delta - \frac{1}{2}\Gamma_1 \left\langle \frac{\tilde{\Delta}}{\sqrt{(\tilde{\omega}_n + i\varepsilon_0 \cos(\chi))^2 + \tilde{\Delta}^2}} \right\rangle \quad (7)$$

where Γ_1 and Γ_2 are the forward and backward scattering rate respectively. $\chi = 2bp_2$ is the angle related to the second direction, and $\langle \dots \rangle$ denotes the angular average over χ .

The self-consistent equation Eq. (5) can be rewritten by substituting Eqs. (6) and (7) as:

$$\lambda^{-1} = 2\pi T \sum_{n=0}^{n_c} \frac{\tilde{\Delta}}{\Delta} \left\langle \frac{1}{\sqrt{(\tilde{\omega}_n + i\varepsilon_0 \cos(\chi))^2 + \tilde{\Delta}^2}} \right\rangle \quad (8)$$

where

$$\lambda = UN_0 \quad (9)$$

is the dimensionless coupling constant, and N_0 is the density of states at the Fermi surface.

We concentrate on calculating the threshold electric field E_T . In the strong pinning limit, the threshold field E_T^s is the ratio of the pinning potential F and the condensate density f_1 [3]:

$$E_T^s = \frac{F}{f_1} \quad , \quad (10)$$

and in the 3-D weak pinning limit,

$$E_T^w \propto (E_T^s)^4 \quad . \quad (11)$$

We compute E_T^s in the following and denote it simply by E_T .

In our earlier analysis [3], we calculated E_T as a function of temperature when only imperfect nesting ε_0 is present. We found that when T gets close to $T_c(\varepsilon_0)$, E_T moves up as ε_0 increases. In the presence of both imperfect nesting and scattering effect, F is given by:

$$F = 2\pi T \sum_{n=0}^{\infty} \tilde{\Delta}^2 \langle [(\tilde{\omega}_n + i\eta)^2 + \tilde{\Delta}^2]^{-\frac{1}{2}} \rangle^2 \quad , \quad (12)$$

and f_1 is given by:

$$f_1 = \frac{2\pi T}{\Delta} \sum_{n=0}^{\infty} \left(\langle \frac{\tilde{\Delta}^3}{R^3} \rangle + \frac{\Gamma_1}{2} \tilde{\Delta}^3 \Xi \right) \left(1 - \frac{\Gamma}{\Delta} \langle \frac{\tilde{\Delta}^3}{R^3} \rangle - \frac{\Gamma_1}{4} \Delta (\Gamma_1 + \Gamma_2) \tilde{\Delta}^3 \Xi \right)^{-1} \quad , \quad (13)$$

where

$$R = \sqrt{(\tilde{\omega}_n + i\eta)^2 + \tilde{\Delta}^2} \quad , \quad (14)$$

and

$$\Xi = \left\langle \frac{1}{R^3} \right\rangle \left\langle \frac{(\tilde{\omega}_n + i\eta)^2}{R^3} \right\rangle - \left\langle \frac{(\tilde{\omega}_n + i\eta)}{R^3} \right\rangle^2 \quad . \quad (15)$$

In order to understand the different role of the imperfect nesting ε_0 and the scattering Γ on E_T , we first calculate the temperature dependence of E_T when *only* Γ exists, i.e., $\varepsilon_0 = 0$. In this limit, F and f_1 are given respectively by:

$$F = 2\pi T \sum_{n=0}^{\infty} \frac{1}{u_n^2 + 1} \quad , \quad (16)$$

Figure 1: Threshold field E_T as function of temperature T for several Γ when $\varepsilon_0 = 0$: ($\circ$) $\Gamma = 0$; ($\square$) $\Gamma = 0.035\Delta_0$; ($\diamond$) $\Gamma = 0.15\Delta_0$. Δ_0 is the order parameter when $\Gamma = \varepsilon = T = 0$. E_T is normalized by $\pi\Delta_0/2$ the E_T value when $T = 0, \Gamma = 0$.

$$f_1 = \frac{2\pi T}{\Delta} \sum_{n=0}^{\infty} \frac{1}{(u_n^2 + 1)^{\frac{3}{2}}} \left[1 - \frac{\Gamma}{\Delta} \frac{1}{(u_n^2 + 1)^{\frac{3}{2}}} \right]^{-1}, \quad (17)$$

where u_n is obtained by solving:

$$\frac{\omega_n}{\Delta} = u_n \left(1 - \frac{\Gamma}{\Delta} (1 + u_n^2)^{-\frac{1}{2}} \right). \quad (18)$$

The order parameter Δ is obtained by:

$$-\ln\left(\frac{\Delta(T, \Gamma)}{\Delta_0}\right) = \begin{cases} \frac{\pi}{4}\zeta & (\zeta \leq 1) \\ \operatorname{arccosh}(\zeta) + \frac{1}{2}(\zeta \arcsin(\zeta^{-1}) - \sqrt{1 - \zeta^{-2}}) & (\zeta > 1) \end{cases} + 2 \int_{u_0}^{\infty} \frac{dE}{\Delta} \Re\left(\frac{1}{\sqrt{u^2 - 1}}\right) f(\beta E), \quad (19)$$

with

$$\zeta = \frac{\Gamma}{\Delta}. \quad (20)$$

At $T = 0K$, it can be shown that:

$$f_1 = \begin{cases} 1 & \text{for } \zeta \leq 1 \\ 1 - \sqrt{1 - \zeta^{-2}} & \text{for } \zeta > 1 \end{cases} \quad (21)$$

and

$$F = \Delta \begin{cases} \frac{\pi}{2} - \frac{2}{3}\zeta & \text{for } \zeta \leq 1 \\ \frac{\pi}{2} - \operatorname{arccos}\zeta^{-1} - \frac{\zeta}{3}(2 - (2 + \zeta^{-2})\sqrt{1 - \zeta^{-2}}) & \text{for } \zeta > 1 \end{cases} \quad (22)$$

A reference value of E_T at $\Gamma = 0$ can be calculated as

$$E_T^0 = E_T(T = 0, \varepsilon/\Delta_0 = 0, \Gamma/\Delta_0) = \frac{\pi}{2}\Delta_0 \quad (23)$$

Figure 2: Threshold field E_T as function of ϵ_0 at $T = T_c$ for several Γ ($\circ$) $\Gamma = 0$; ($\square$) $\Gamma = 0.035\Delta_0$; ($\diamond$) $\Gamma = 0.07\Delta_0$. $\Gamma_2 = \frac{1}{2}\Gamma_1$ is chosen. E_T is normalized by $\pi^3 T_{c0}/7\zeta(3)$ the E_T value when $T = T_c$, $\Gamma = 0$.

Near $T = T_c$, where T_c is determined by:

$$\ln\left(\frac{T_{c0}}{T_c}\right) = \psi\left(\frac{1}{2} + \frac{\Gamma}{2\pi T_c}\right) - \psi\left(\frac{1}{2}\right), \quad (24)$$

with ψ the Digamma function, E_T is given by:

$$E_T = \frac{\pi^3 T}{7\zeta(3)} \left\{ 1 + \left(\frac{\pi^4}{14\zeta(3)} - \frac{28\zeta(3)}{\pi^2} \right) \frac{\Gamma}{2\pi T} + \left(\frac{93\zeta(5)}{14\zeta(3)} - \frac{\pi^2}{3} + (310\zeta(5)\pi^{-2} - \frac{17\pi^6}{210\zeta(3)}) \frac{\Gamma}{2\pi T} \right) \left(\frac{\Delta}{2\pi T} \right)^2 \right\}. \quad (25)$$

From the above equation, one expects that E_T has a small peak when T gets very close to T_c for small Γ since the coefficient in front of Δ^2 would be positive. At exactly $T = T_c$, for small Γ ,

$$E_T = \frac{\pi^3 T_{c0}}{7\zeta(3)} \left(1 + \left(\frac{\pi^4}{14\zeta(3)} - \frac{28\zeta(3)}{\pi^2} - \frac{\pi^2}{2} \right) \frac{\Gamma}{2\pi T_{c0}} \right). \quad (26)$$

The coefficient before Γ is negative, therefore one expects that for $\epsilon_0 = 0$, at both $T = 0K$ (see Eqs. 22 and 21) and $T = T_c$, E_T decreases as Γ increases (see also Fig. 2 below). Fig. 1 shows E_T as function of T for several Γ . One clearly sees the small peak near T_c .

Including both imperfect nesting ϵ_0 and scattering rate Γ increases the complexity of the numerical computation. Instead of computing E_T for the whole range of temperatures from $0K$ to $T_c(\epsilon, \Gamma)$, we calculated E_T at $T = 0K$ and $T = T_c$. For $T = T_c$, analytical result exists, and Fig. 2 shows the result of E_T at $T = T_c$ for several Γ . F and f_1 are given by:

$$F = \Delta^2 2\pi T_c \sum_{n=0}^{\infty} \frac{1}{(\sqrt{\omega_n + \frac{\Gamma_1 + \Gamma_2}{2}})^2 + \epsilon_0^2 + \frac{\Gamma_1}{2}}^2}, \quad (27)$$

$$f_1 = \Delta^2 \pi T_c \sum_{n=0}^{\infty} \frac{1}{(\sqrt{(\omega_n + \frac{\Gamma_1 + \Gamma_2}{2})^2 + \epsilon_0^2 + \frac{\Gamma_1}{2}})^3} \left\{ \frac{2(\omega_n + \frac{\Gamma_1 + \Gamma_2}{2})^2 - \epsilon_0^2}{(\omega_n + \frac{\Gamma_1 + \Gamma_2}{2})^2 + \epsilon_0^2} - \frac{\Gamma_1}{2} \frac{\epsilon_0^2}{((\omega_n + \frac{\Gamma_1 + \Gamma_2}{2})^2 + \epsilon_0^2)^{\frac{3}{2}}} \right\} \quad (28)$$

On the other hand, no analytical expression exists at $T = 0K$ for general ϵ_0 and Γ , other than changing the summation over ω_n in the expressions of both F and f_1 into integration over continuous

Figure 3: Threshold field E_T as function of ϵ_0 at $T = 0K$ for several Γ ($\circ$) $\Gamma = 0$; ($\square$) $\Gamma = 0.035\Delta_0$; ($\diamond$) $\Gamma = 0.07\Delta_0$. $\Gamma_2 = \frac{1}{2}\Gamma_1$ is chosen. E_T is normalized by $\pi\Delta_s/2$ the E_T value when $T = 0, \Gamma = 0$.

variable ω . Fig. 3 shows the result of E_T for several Γ . One should notice that as ϵ_0 and Γ both come to play a role, f_1 is identically equal to unity until the quasi-particle energy gap is closed. It is similar to the case when Δ becomes smaller than Γ in the absence of ϵ_0 , but is more complicated when $\epsilon_0 \neq 0$. This is reflected in the sudden move-up in Fig. 3 as ϵ_0 becomes closer to its critical value of completely suppressing T_c . From Figs. 2 and 3, one notices that at both $T = 0K$ and $T = T_c$, E_T first decreases with Γ for small ϵ_0 , but later increases with Γ as ϵ_0 increases.

In conclusion, we have analyzed the impurity scattering in SDW (or CDW) with imperfect nesting. For all ϵ_0 the impurity scattering suppresses the order parameter, though the effect is more significant for larger ϵ_0 . On the other hand the effect on the density of states becomes less visible as ϵ_0 increases. The threshold field E_T in general is a complicated function of temperature when both ϵ_0 and Γ are present. ϵ_0 plays different role than Γ in changing E_T . The small peak near T_c may explain a recent experimental result obtained by Nomura *et al.* [6].

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