CDW in ZrTe5

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The coupling term for electrons and LA phonons is

$$\begin{aligned}\hat{H}_{e-\mathrm{ph},L} &= \sum_{\boldsymbol{k}} g_L V_{q_z} q_z \Big[\hat{X}_{L,q_z} \hat{C}^{\dagger}_{\boldsymbol{k}+\frac{q_z}{2}\boldsymbol{e}_z} \hat{C}_{\boldsymbol{k}-\frac{q_z}{2}\boldsymbol{e}_z} + h.c.\Big] \\ &= \sum_{\boldsymbol{k}} \left[g_L V_{q_z} q_z \sqrt{\frac{N_{\mathrm{ion}}\hbar}{2M\omega_{q_z}}}\right]\Big[(\hat{b}_{L,q_z} + \hat{b}^{\dagger}_{L,-q_z})\hat{C}^{\dagger}_{\boldsymbol{k}+\frac{q_z}{2}\boldsymbol{e}_z} \hat{C}_{\boldsymbol{k}-\frac{q_z}{2}\boldsymbol{e}_z} + h.c.\Big] \\ &\equiv \sum_{\boldsymbol{k}} \alpha_{L,q_z}\Big[(\hat{b}_{L,q_z} + \hat{b}^{\dagger}_{L,-q_z})\hat{C}^{\dagger}_{\boldsymbol{k}+\frac{q_z}{2}\boldsymbol{e}_z} \hat{C}_{\boldsymbol{k}-\frac{q_z}{2}\boldsymbol{e}_z} + h.c.\Big]\end{aligned} \tag{1}$$

where we used $\hat{X}_L(q_z) = (\hbar/2\rho\omega_{q_z})^{\frac{1}{2}}(\hat{b}_{q_z} + \hat{b}^{\dagger}_{-q_z})$, and

$$\alpha_{L,q} = \sqrt{\frac{N_{\mathrm{ion}}\hbar}{2M\omega_{L,q}}} q V_q \tag{2}$$

The mean-field Hamiltonian reads,

$$\hat{\hat{H}}_{e-\mathrm{ph},L} = \sum_{\boldsymbol{k}} |\Delta|(e^{i\phi}\hat{d}_{\boldsymbol{k}+k_F\boldsymbol{e}_z}\hat{\boldsymbol{d}}_{\boldsymbol{k}-k_F\boldsymbol{e}_z} + h.c.) \tag{3}$$

where $\Delta = |\Delta|e^{-i\phi} = \alpha_{2k_F}(\langle\hat{b}_{2k_F}\rangle + \langle\hat{b}^{\dagger}_{-2k_F}\rangle) \rightarrow 2\alpha_{2k_F}\langle\hat{b}_{2k_F}\rangle$ is the order parameter.

Then we will obtain the mean-field Hamiltonian for phonon,

$$\begin{aligned}\hat{H}_{\mathrm{ph}} &= \sum_{q_z} \hbar\omega_{L,q_z}\hat{b}^{\dagger}_{q_z}\hat{b}_{q_z} \longrightarrow 2\hbar\omega_{L,2k_F}\langle\hat{b}_{2k_F}\rangle^2 \\ &= \frac{\hbar\omega_{L,2k_F}|\Delta_L|^2}{2|\alpha_{2k_F}|^2}\end{aligned} \tag{4}$$

1 Gap Equation and Ground-state Energy

By standard RPA approach, effective dielectric constant at zero temperature for zeroth landau band $E^{(0+)}_{k_z}$ in long wavelength limit is

$$\begin{aligned}&\kappa^2(T=0) \\ =& \lim_{\omega_n\to 0, q\to 0} \frac{-e^2}{2\pi\epsilon l_B^2}\frac{1}{\beta}\sum_m \int_{-\infty}^{+\infty}\frac{dk_z}{2\pi}\frac{1}{\big[i\hbar\omega_m - \big(E^{(0+)}_{k_z} - E_F\big)\big]}\frac{1}{\big[i\hbar(\omega_m+\omega_n) - \big(E^{(0+)}_{k_z} - E_F\big)\big]} \\ \approx& \lim_{\omega_n\to 0, q\to 0} \frac{-e^2}{2\pi\epsilon l_B^2}\int_{-\infty}^{+\infty}\frac{dk_z}{2\pi}\frac{\partial f\big(E^{(0+)}_{k_z}\big)}{\partial E^{(0+)}_{k_z}} \\ =& \frac{e^2}{2\pi\epsilon l_B^2}\int_0^1 \frac{1}{2\pi\hbar v_F} d f\big(E^{(0+)}_{k_z}\big) \\ =& \frac{e^3 B}{4\pi^2\epsilon\hbar^2 v_F}\end{aligned} \tag{5}$$

,

and the electron-LA phonon coupling is followed:

$$|\alpha_{L,q}| = \sqrt{\frac{N_{\text{ion}}\hbar}{2M\omega_{L,q}}}q\frac{Ze^2}{\epsilon(q^2+\kappa^2)} \quad . \tag{6}$$

Mean field Hamiltonian of LA phonon is somehow simple,

$$\begin{aligned} H_{\text{ph},L} &= \sum_{\boldsymbol{q}} \hbar\omega_{L,\boldsymbol{q}}\langle\hat{b}^\dagger_{L,\boldsymbol{q}}\rangle\langle\hat{b}_{L,\boldsymbol{q}}\rangle \\ &= 2\hbar\omega_{L,2k_F}|\langle\hat{b}_{L,2k_F}\rangle|^2 \\ &= \frac{\hbar v_{s,L}}{2|\alpha_{L,2k_F}|^2}|\Delta_{L,2k_F}|^2 \\ &\equiv \frac{|\Delta_{L,2k_F}|^2}{g_{L,2k_F}} \end{aligned} \tag{7}$$

where coefficient for electron-LA phonon coupling is

$$g_{L,2k_F} = \frac{2|\alpha_{L,2k_F}|^2}{\hbar v_{s,L}} = \frac{N_{\text{ion}}Z^2e^4}{Mv_{s,L}^2\epsilon^2}\frac{q}{(q^2+\kappa^2)^2}|_{q=2k_F} \quad , \tag{8}$$

then Hamitonian valid in $[-k_F, k_F]$ and energy for ground-state reads

$$\begin{aligned} \bar{H}_g\,(k_z+k_F) &= \begin{pmatrix} E^{(0+)}_{k_z+k_F} & |\Delta_{L,2k_F}|e^{i\phi} \\ \dagger & E^{(0+)}_{k_z-k_F} \end{pmatrix} + \frac{|\Delta_{L,2k_F}|^2}{g_{L,2k_F}} \quad , \\ E_g(|\Delta_{L,2k_F}|) &= \int_{-k_F}^{+k_F}\Theta\big(E_F - E^{(0+)}_{g,k_z}\big)E^{(0+)}_{g,k_z}dk_z + \frac{|\Delta_{L,2k_F}|^2}{g_{L,2k_F}} \quad . \end{aligned} \tag{9}$$

The gap equation is straightforwardly obtained by self-consistant condition:

$$\frac{\partial E_g}{\partial|\Delta_{L,2k_F}|} = 0 \Rightarrow \ |\Delta_{L,2k_F}| = \left|(\hbar v_F k_F)\text{csch}\left(\frac{4\pi^2\hbar^2 v_F}{g_{2k_F}eB}\right)\right| \quad . \tag{10}$$

Note that k_F and v_F are also B-dependent:

$$\begin{aligned} k_F &= \frac{2\pi^2\hbar n_0}{eB} \quad , \\ v_F &= \frac{\partial E^{(0+)}_{k_z}}{\partial k_z}|_{k_z=k_F} \quad . \end{aligned}$$

2 Model Parameter and Reproduction

Dirac	v_x	v_y	v_z	M_0	M_1	M_z
Material	ε_r	n_0	a	N_{ion}	M	Z
Constant	e	ϵ_0	$\hbar$			

Table 1. Model parameters of ZrTe5.

The key results are reproduced as shown in Fig.(1).

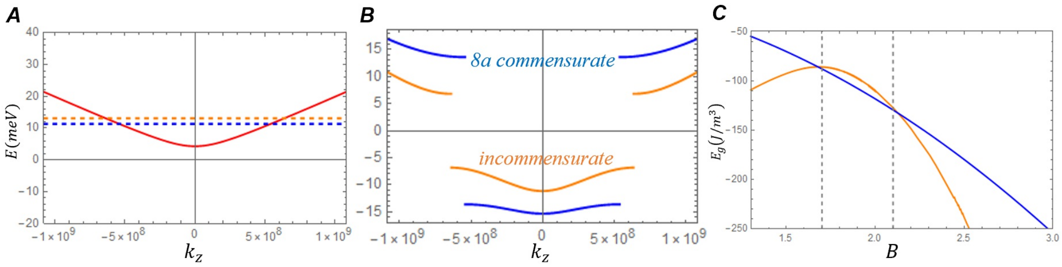

Figure 1. Incommensurate and $8a$-commensurate CDWs in $ZrTe_5$ when $B = 1.8T$.