Supplemental Material: A mechanism for weak itinerant antiferromagnetism: mirrored van Hove singularities

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Abstract –

Let us define a convenient notation. First, wavevectors k, q, Q will always be vectors unless denoted as magnitude $|k|$. Now, for any wavevector $k = (k_x, k_y, k_z)$, define $\bar{k} \equiv (k_x, -k_y, k_z)$, since the negative mass is for the k_y component. Also, the masses can be scaled out of the zone sum (integral over k) and we will suppose that has been done and use the same symbol k. The quadratic vHs dispersions at $Q/2$ and $-Q/2$ (spanned by vector Q) are ($m = 1 = \hbar$)

$$\begin{aligned} \varepsilon_{1,k} &= \frac{1}{2}(\bar{k} - \frac{\bar{Q}}{2}) \cdot (k - Q/2) = \frac{\bar{\kappa} \cdot \kappa}{2}, \\ \varepsilon_{2,k} &= \frac{1}{2}(\bar{k} + \frac{\bar{Q}}{2}) \cdot (k + Q/2) = \frac{\bar{\kappa} \cdot \kappa}{2}, \end{aligned} \tag{1}$$

in terms of the deviation $\kappa = k \pm \frac{Q}{2}$ from the vHs point,

The non-interacting susceptibility is

$$\chi_o(Q + q, \omega) = \sum_k \frac{f_k - f_{k+Q+q}}{\varepsilon_{k+Q+q} - \varepsilon_k - \omega - i\eta}. \tag{2}$$

Precisely at Q (*i.e.* $|q|$=0) (the eight values for TiAu are given in the main text), the energy difference in the denominator is zero in some *volume* Ω_{vHs} around the vHs points $\pm Q/2$ determined by the relative importance of third-order terms in the dispersion around the vHs. This equality is a consequence of the quadratic form of the dispersion and that all vHs have the same orientation. Of course, the numerator also vanishes, as the Fermi functions ($f_k \equiv f(\varepsilon_k)$) have identical arguments. Expansions in q and ω require some care. For small but nonzero $|q|$, the energy difference in the denominator is

$$v_{k+q} \cdot q = \bar{\kappa} \cdot q. \tag{3}$$

Since $v_{k+q} = \bar{\kappa}$, the first term in the expansion is finite, vanishing only at the vHs point. The denominator becomes $\bar{\kappa} \cdot q - \omega - i\eta$, familiar from conventional expressions. Here however $q \to 0$ indicates inter-vHs scattering rather than forward scattering on the Fermi surface.

Considering fluctuations around the spanning vector Q, the expressions for the low energy, small $|q|$ behavior are not so neatly tied to intraband scattering on the Fermi surface, so they are not as intuitive as for the FM Q=0 case. In addition, we are interested in the specific case where Q spans not only symmetry related but also co-oriented vHs as in TiAu. In the volume of the zone excluding Ω_{vHs}, $\chi_o(Q + q, \omega)$ is unaffected by the vHs. For k inside Ω_{vHs} the numerator expands as

$$\begin{aligned} f_k - f_{k+Q+q} &= [f_k - f_{k+Q}] - (\frac{df}{d\epsilon})_{k+Q} v_{k+Q} \cdot q \\ &= \delta(\varepsilon_{k+Q}) v_{k+Q} \cdot q. \end{aligned} \tag{4}$$

to lowest order in q, taking into account the equality of the argument of the Fermi factors and the zero temperature substitution $-df/d\varepsilon = \delta(\varepsilon)$ has been made, $\delta(\varepsilon)$ is the Dirac δ-function. The factors $v_{k+Q} \cdot q$ in numerator and denominator cancel, giving the vHs contribution to the real part of

$$\chi_o^{vHs}(Q = q, \omega) = \sum_k^{\Omega_{vHs}} \delta(\varepsilon_k) = N^{vHs}(\varepsilon_F) \tag{5}$$

and there is no linear in q term. With the density of states $N(\varepsilon)$ being much larger near the vHs than elsewhere, this term will contribute a local maximum in $\chi_o(Q + q, 0)$ whose magnitude depends on the relative importance of

$|q|^3$ terms and the effective masses. These local maxima at spanning vectors Q enhance the tendency of a finite Q Stoner-like instability: $I_Q\chi_o(Q) > 1$. We note in passing that the expressions above suggest significant, perhaps strong, frequency variation at small ω. We now look at the linear term in ω.

The imaginary part of the susceptibility at low frequency is $\chi_o^{''}(Q+q,\omega) = \pi\omega\xi(Q+q)$ in terms of the nesting function $\xi(p)$ that measures the phase space available for scattering from the Fermi surface at k to the Fermi surface at $k+p$, summed over all k. For the spanning vHs processes for which $\varepsilon_k = \varepsilon_{k+Q}$ so also $f(\varepsilon_k) = f(\varepsilon_{k+Q})$, in the limit of small $|q|$ the contribution from Ω_{vHs} becomes

$$\begin{aligned}
\xi_o''(Q+q) &= \sum_k^{\Omega_{vHs}} \delta(\varepsilon_k)\delta(\varepsilon_k - \varepsilon_{k+Q} - v_{k+Q}\cdot q) \\
&= \sum_k^{\Omega_{vHs}} \delta(\varepsilon_k)\delta(v_{k+Q}\cdot q) \\
&= \int_{\mathcal{L}_{vHs}} \frac{d\mathcal{L}_k}{|v_k||\nabla(v_{k+Q}\cdot Q)|} \\
&= \int_{\mathcal{L}_{vHs}} \frac{d\mathcal{L}_k}{|\bar{\kappa}\cdot q|}. \qquad (6)
\end{aligned}$$

The line integral is along the line $\mathcal{L}_{vHs}$ where the surface $\bar{\kappa}\cdot q = 0$ intersects the Fermi surface, a line of non-zero length since there are three components of $\bar{\kappa}$ to vary to satisfy the two constraints $\bar{\kappa}\cdot q = 0$ and ε_κ=0. Thus, neglecting $|k|^3$ terms in the vHs dispersion, the nesting function *diverges* as $1/|q|$ as $|q| \to 0$ at the spanning vector Q of two identically oriented vHs, as are all of the vHs in TiAu. This divergence arises from the coincidence (through second order) of areas of Fermi surface, as in the case of $\xi(q\to 0)$. The imaginary part of the critical susceptibility then has the form $\gamma\omega/|q|$, the same as for *ferromagnetic* fluctuations. This form is distinct from that of conventional AFM fluctuations used by Moriya and others, which has no $|q|^{-1}$ divergence. Thus the critical susceptibility maps onto that for ferromagnets, distinguishing TiAu from other wAFMs. The $|q|^{-1}$ divergence of $Im\chi_o$ will be modulated by thermal smearing and fluctuations of other degrees of freedom.

As an example of the implications, the phonon linewidth from electron-phonon (EP) coupling is given by the sum defining $\xi(q)$ but with EP matrix elements within the sum. The divergence of $\xi(Q+q)$ as $|q| \to$0 will lead to sharp Kohn anomalies in the phonon spectrum above the ordering temperature, below which they will vanish.