Van Hove singularities

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Abstract

We derive the van Hove singularities in every dimension and for every case of non-vanishing derivative.

1 Density of states

The density of states is defined as

$$J(\omega) = \int_{\mathrm{BZ}} \frac{d^2\mathbf{k}}{(2\pi)^2} \delta\left(\omega\left(\mathbf{k}\right) - \omega\right) \tag{1}$$

The general form of the dispersion relation at a critical point is

$$\omega\left(\mathbf{k}\right) = \omega_0 + Ak_x^l + Bk_y^m + Ck_z^n + O\left(k_x^{l+1}\right) + O\left(k_y^{m+1}\right) + O\left(k_z^{n+1}\right) \tag{2}$$

where $l, m, n \geq 2$. We let $\sigma_X = |X|/X$ for $X = A, B, C$ (σ_X is the sign of X). We first change coordinates to $q_X = X^{1/n_X} k_X$ (where $n_X = l, m, n$) so that we have

$$J(\omega) \propto \int \delta\left(\sigma_x q_x^l + \sigma_y q_y^m + \sigma_z q_z^n + \omega_0 - \omega\right) \, dq_x dq_y dq_z \tag{3}$$

The following formula for evaluating delta functions will be needed:

$$\int_a^b g(x)\delta\left(f\left(x\right)\right) \, dx = \sum_{x_0 : f(x_0)=0} g\left(x_0\right) \left|\frac{df}{dx}\right|_{x=x_0}^{-1} \tag{4}$$

1.1 Case $\sigma_x = \sigma_y = \sigma_z = 1$

$$J(\omega) \propto \int \delta\left(q_x^l + q_y^m + q_z^n + \omega_0 - \omega\right) \, dq_x dq_y dq_z \tag{5}$$

2 2D

2.1 Quadratic saddle

$$J(\omega) \propto \int \delta\left(q_x^2 - q_y^2 + \omega_0 - \omega\right) \, dq_x dq_y \tag{6}$$

Using Eq. (4), and integrating with respect to q_x,

$$J(\omega) \propto \int \sum_{q_{y_0}} \frac{1}{2\left|q_{y_0}\right|} \, dq_y \tag{7}$$

where

$$q_{y_0} = \pm\sqrt{q_y^2 - \omega_0 + \omega} \;\; \text{if} \;\; q_y^2 - \omega_0 + \omega > 0 \tag{8}$$

Using the unit step function $U(x)$,

$$J(\omega) \propto \int \frac{1}{\sqrt{q_y^2 - \omega_0 + \omega}} U\left(q_y^2 - \omega_0 + \omega\right) \, dq_y \tag{9}$$

If $\omega < \omega_0$, $U(\ldots) = 1$ if $q_y > \sqrt{\omega_0 - \omega}$, so

$$\begin{aligned}
J(\omega < \omega_0) &\propto \int_{\sqrt{\omega_0-\omega}}^{\sqrt{\omega_0-\omega}+R} \frac{1}{\sqrt{q_y^2 - \omega_0 + \omega}} \, dq_y && (10) \\
&= \log\left[\sqrt{\omega_0 - \omega} + R + \sqrt{\left(\sqrt{\omega_0 - \omega} + R\right)^2 - (\omega_0 - \omega)}\right] - \log\left[\sqrt{\omega_0 - \omega}\right] && (11) \\
&\approx \log\left[\sqrt{\omega_0 - \omega} + 2R\right] - \log\left[\sqrt{\omega_0 - \omega}\right] && (12) \\
&\approx -\log\left(\omega_0 - \omega\right) + O\left(\sqrt{\omega_0 - \omega}\right) && (13)
\end{aligned}$$

where we have used $R^2 \gg \omega - \omega_0$. If $\omega > \omega_0$, $U(\ldots) = 1$, so

$$\begin{aligned}
J(\omega > \omega_0) &\propto \int_0^R \frac{1}{\sqrt{q_y^2 - \omega_0 + \omega}} \, dq_y && (14) \\
&= \log\left[R + \sqrt{R^2 - (\omega_0 - \omega)}\right] - \log\left[\sqrt{\omega - \omega_0}\right] && (15) \\
&\approx -\log(\omega - \omega_0) + O\left(\sqrt{\omega_0 - \omega}\right) && (16)
\end{aligned}$$

2.2 Parabolic dispersion

$$J(\omega) \propto \int \delta\left(q_x^2 + q_y^2 + \omega_0 - \omega\right) \, dq_x dq_y \tag{17}$$

Using Eq. (4), and integrating with respect to q_x,

$$J(\omega) \propto \int \sum_{q_{y_0}} \frac{1}{2\left|q_{y_0}\right|} \, dq_y \tag{18}$$

where

$$q_{y_0} = \pm\sqrt{-q_y^2 - \omega_0 + \omega} \;\; \text{if} \;\; -q_y^2 - \omega_0 + \omega > 0 \tag{19}$$

Using the unit step function $U(x)$,

$$J(\omega) \propto \int \frac{1}{\sqrt{-q_y^2 - \omega_0 + \omega}} U\left(-q_y^2 - \omega_0 + \omega\right) \, dq_y \tag{20}$$

If $\omega < \omega_0$, $U(\ldots) = 0$ and $J(\omega < \omega_0) = 0$. If $\omega > \omega_0$, $U(\ldots) = 1$ if $q_y^2 < \omega - \omega_0$, and so

$$\begin{aligned}
J(\omega > \omega_0) &\propto \int_{-\sqrt{\omega-\omega_0}}^{\sqrt{\omega-\omega_0}} \frac{1}{\sqrt{\omega - \omega_0 - q_y^2}} \, dq_y && (21) \\
&= \pi && (22)
\end{aligned}$$

2.3 Mixed parabolic and quartic dispersion

$$J(\omega) \propto \int \delta\left(q_x^2 + q_y^4 + \omega_0 - \omega\right)\, dq_x dq_y \tag{23}$$

Using Eq. (4), and integrating with respect to q_x,

$$J(\omega) \propto \int \sum_{q_{y_0}} \frac{1}{2\left|q_{y_0}\right|}\, dq_y \tag{24}$$

where

$$q_{y_0} = \pm\sqrt{-q_y^4 - \omega_0 + \omega} \quad \text{if} \quad -q_y^4 - \omega_0 + \omega > 0 \tag{25}$$

Using the unit step function $U(x)$,

$$J(\omega) \propto \int \frac{1}{\sqrt{-q_y^4 - \omega_0 + \omega}} U\left(-q_y^4 - \omega_0 + \omega\right)\, dq_y \tag{26}$$

If $\omega < \omega_0$, $U(\ldots) = 0$ and $J(\omega < \omega_0) = 0$. If $\omega > \omega_0$, $U(\ldots) = 1$ if $q_y^4 < \omega - \omega_0$, and so

$$J(\omega > \omega_0) \propto \int_{-(\omega-\omega_0)^{1/4}}^{(\omega-\omega_0)^{1/4}} \frac{1}{\sqrt{\omega - \omega_0 - q_y^4}}\, dq_y \tag{27}$$

$$= \frac{2\sqrt{\pi}\Gamma(5/4)}{(\omega - \omega_0)^{1/4}\,\Gamma(3/4)} \tag{28}$$

2.4 Quartic dispersion

$$J(\omega) \propto \int \delta\left(q_x^4 + q_y^4 + \omega_0 - \omega\right)\, dq_x dq_y \tag{29}$$

Using Eq. (4), and integrating with respect to q_x,

$$J(\omega) \propto \int \sum_{q_{y_0}} \frac{1}{4\left|q_{y_0}\right|^3}\, dq_y \tag{30}$$

where

$$q_{y_0} = \pm\left(-q_y^4 - \omega_0 + \omega\right)^{1/4} \quad \text{if} \quad -q_y^4 - \omega_0 + \omega > 0 \tag{31}$$

If $\omega < \omega_0$, $U(\ldots) = 0$ and $J(\omega < \omega_0) = 0$. If $\omega > \omega_0$, $U(\ldots) = 1$ if $q_y^4 < \omega - \omega_0$, and so

$$J(\omega > \omega_0) \propto \int_{-(\omega-\omega_0)^{1/4}}^{(\omega-\omega_0)^{1/4}} \frac{1}{\left(\omega - \omega_0 - q_y^4\right)^{3/4}}\, dq_y \tag{32}$$

$$= \frac{2\Gamma(1/4)\Gamma(5/4)}{\sqrt{\pi}\sqrt{\omega - \omega_0}} \tag{33}$$