Problem set 6

Problem 1. Drude model

$\langle P(t)\rangle \rightarrow \bar{P}(t)$

$\langle \dot{P}(t)\rangle = -\gamma\langle P(t)\rangle + f(t)$, apply laplace transform on both sides, $\dot{\bar{P}}(t) + \gamma\bar{P}(t) = f(t)$.

$L.HS = s\cdot\bar{P}(s) - \bar{P}(0) + \gamma\cdot\bar{P}(s) = RHS = f(s)$

In s-domain, EOM is solved by $\bar{P}(s) = \frac{1}{s+\gamma}(\bar{P}(0) + f(s)) \xrightarrow{\mathcal{L}^{-1}} \bar{P}(t) = e^{-\gamma t}\bar{P}(0) + \int_0^t d\tau\, e^{-\gamma(t-\tau)} f(\tau)d\tau$

Let $f(t)$ be constant f,

$\bar{P}(t) = e^{-\gamma t}\bar{P}(0) + (-\frac{f}{\gamma})e^{-\gamma(t-\tau)}\Big|_0^t = e^{-\gamma t}\bar{P}(0) + \frac{f}{\gamma}(1-e^{-\gamma t})$,

When $t \gg \gamma^{-1}$ one get steady condition $\bar{P} = \frac{f}{\gamma} \xrightarrow{\gamma=\tau^{-1}} J = \frac{ne^2\tau}{m_e}E$

Let $f(t)$ be $f(t) = f\cdot e^{i\omega t}$, $f(s) = f\cdot\frac{1}{s-i\omega}$

$\bar{P}(s) = \frac{1}{s+\gamma}\bar{P}(0) + \frac{f}{(s+\gamma)(s-i\omega)}$

$\bar{P}(t) \overset{\mathcal{L}^{-1}}{=} e^{-\gamma t}\bar{P}(0) + \frac{f}{i\omega+\gamma}(e^{i\omega t} - e^{-\gamma t})$

Let $t \gg \gamma^{-1}$, $\bar{P}(t) = \frac{f(t)}{i\omega+\gamma}$

$\longrightarrow J(\omega) = \frac{ne^2\tau}{m_e}\cdot\overset{\frac{1}{i\omega\tau+1}}{\cancel{\frac{1}{i\omega+\gamma}}}E(\omega)$

* complex $\sigma_D(\omega)$ means a dynamical response to the oscillatory field. (current oscillating ~ field oscillating)

* when $\omega \gg \tau^{-1}$, $\sigma_D(\omega)$ becomes purely imaginary → only oscillation no damping → high frequency oscillation prevents collision

Problem 2. Hellmann-Feynman theorem

$\hat{H}_\lambda|\psi_\lambda\rangle = E_\lambda|\psi_\lambda\rangle$, $E_\lambda = \langle\psi_\lambda|\hat{H}_\lambda|\psi_\lambda\rangle$ $(\langle\psi_\lambda|\psi_\lambda\rangle = 1)$

$$\begin{aligned}\frac{\partial E(\lambda)}{\partial\lambda} &= \langle\tfrac{\partial}{\partial\lambda}\psi_\lambda|\hat{H}_\lambda|\psi_\lambda\rangle + \langle\psi_\lambda|\tfrac{\partial}{\partial\lambda}\hat{H}_\lambda|\psi_\lambda\rangle + \langle\psi_\lambda|\hat{H}_\lambda|\tfrac{\partial}{\partial\lambda}\psi_\lambda\rangle \\ &= E_\lambda\langle\tfrac{\partial}{\partial\lambda}\psi_\lambda|\psi_\lambda\rangle + \langle\psi_\lambda|\tfrac{\partial}{\partial\lambda}\hat{H}_\lambda|\psi_\lambda\rangle + E_\lambda\langle\psi_\lambda|\hat{H}_\lambda|\psi_\lambda\rangle \\ &= E_\lambda\underbrace{\tfrac{\partial}{\partial\lambda}\langle\psi_\lambda|\psi_\lambda\rangle}_{0} + \langle\psi_\lambda|\tfrac{\partial}{\partial\lambda}\hat{H}_\lambda|\psi_\lambda\rangle\end{aligned}$$

Problem 3 Van Hove Singularities

$$\varepsilon_{\vec{k}} = -2t\sum_{\mu=1}^{d}\cos(k_\mu a)$$

$$d\varepsilon = \frac{\partial\varepsilon}{\partial k_x}dk_x + \frac{\partial\varepsilon}{\partial k_y}dk_y + \frac{\partial\varepsilon}{\partial k_z}dk_z = \vec{\nabla}\varepsilon\cdot d\vec{k} = \vec{\nabla}\varepsilon\cdot(dk_\perp + dk_\parallel) = |\nabla\varepsilon|\,dk_\perp$$

$$N = \int_{1.BZ} g(\vec{k})\,d^3k = \frac{N}{\Omega_r}\int_{1.BZ} d^3k = \frac{N}{\Omega_r}\int_{1BZ} dk_\perp \int_{\partial\Omega} dS$$

$$= \frac{N}{\Omega_r}\int dE\int_{S_E}\frac{dS}{|\nabla E|} = \int d\varepsilon\, D(\varepsilon) \rightarrow D(\varepsilon) = \frac{N}{\Omega_r}\int_{S_\varepsilon} dS\,\frac{1}{|\nabla_k E|}$$

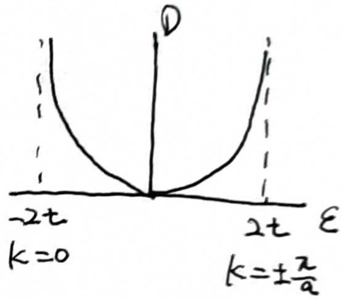
1-d case

$$\frac{\partial}{\partial k}\varepsilon = 2at\sin(ka) \xrightarrow{\text{H-F}} \langle v_k\rangle$$

$$= 0 \quad \Rightarrow k = 0, \pm\frac{\pi}{a}$$

$$|\nabla E| = 2at\,|\sin(ka)| = 2at\sqrt{1-\cos^2 ka} = 2at\sqrt{1-(\varepsilon/2t)^2}$$

$$D(\varepsilon) \propto \left[1-(\varepsilon/2t)^2\right]^{-\frac{1}{2}}$$



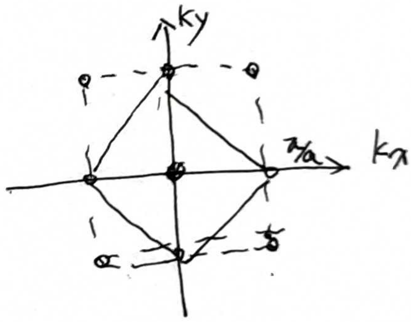
2-d case

$$\varepsilon(k_x,k_y) = -2t[\cos(k_x a) + \cos(k_y a)]$$

$$\frac{\partial}{\partial k_x}\varepsilon = 2ta\sin(k_x a), \quad \frac{\partial}{\partial k_y}\varepsilon = 2at\sin(k_y a)$$

$$\vec{\nabla}\varepsilon = 0 \rightarrow k_x = 0, \pm\frac{\pi}{a}, \quad k_y = 0, \pm\frac{\pi}{a}$$

$$\frac{\partial^2}{\partial k_x^2}\varepsilon = 2a^2t\cos(k_x a), \quad \frac{\partial^2}{\partial k_y^2}\varepsilon = 2a^2t\cos(k_y a)$$



maximum $(0,0)\ \frac{\partial^2}{\partial k^2} = 2a^2t$, minimum $(\pi/a, \pi/a)\ \frac{\partial^2}{\partial k^2} = -2at^2$.

saddle point $(\pi/a, 0)$, $\frac{\partial^2}{\partial k^2} = \pm 2a^2t$

vicinity of $(0,0)$, $x = \delta k_x$, $y = \delta k_y$, $A = 2at^2$

$$\varepsilon = \varepsilon_{min} + \frac{1}{2}A(x^2+y^2)$$

$$\cancel{\frac{2\delta\varepsilon}{A} = x^2+y^2} \quad \delta\varepsilon = \varepsilon - \varepsilon_{min} = \frac{1}{2}A(x^2+y^2) \rightarrow \begin{matrix} x = R\cdot\cos\theta \\ y = R\cdot\sin\theta \end{matrix} \quad \delta\varepsilon = \frac{1}{2}AR^2$$

$$\frac{\partial\varepsilon}{\partial x} = Ax, \quad \frac{\partial\varepsilon}{\partial y} = Ay, \quad |\nabla\varepsilon| = A\cdot\sqrt{x^2+y^2} = A\cdot R$$

$$D(\varepsilon) = \int_{S\varepsilon}\frac{ds}{|\nabla\varepsilon|} = \frac{2\pi R}{A\cdot R} = \frac{2\pi}{A} \rightarrow \text{constant}.$$

vicinity of $(-\frac{\pi}{a}, \frac{\pi}{a})$, $\varepsilon = \varepsilon_{max} - \frac{1}{2}A(x^2+y^2)$, $-\delta\varepsilon = \varepsilon - \varepsilon_{max} = -\frac{1}{2}A(x^2+y^2)$

Similarly, $D(\varepsilon) = $ constant.

vicinity of saddle point ~~$(\pi/a, 0)$~~ $(0, \pi/a)$

$$\delta\varepsilon = \varepsilon = 0 + \frac{1}{2}A(x^2-y^2) \longrightarrow \begin{matrix} x = R\cdot\cosh\alpha. \\ y = R\cdot\sinh\alpha. \end{matrix}$$

$$\frac{\partial\varepsilon}{\partial x} = Ax, \quad \frac{\partial\varepsilon}{\partial y} = -Ay, \quad |\nabla\varepsilon| = AR\sqrt{\cosh^2\alpha + \sinh^2\alpha}.$$

$$ds = R\,d\alpha\sqrt{\cosh^2\alpha + \sinh^2\alpha}$$

$$D(\varepsilon) \propto \int_{-\alpha_c}^{+\alpha_c} d\alpha = 2\alpha_c$$

Consider our truncation on $[-x_c, +x_c]$

$$x_c = R\cdot\cosh\alpha_c = \frac{R}{2}(e^{\alpha_c} + e^{-\alpha_c})$$

For large enough α_c, $x_c \approx \frac{R}{2}e^{\alpha_c}$ so $\alpha_c \approx \ln\frac{2x_c}{R}$

Note that $R^2 = \frac{2\delta\varepsilon}{A}$

$$D(\varepsilon) \propto 2\times\frac{1}{2}\ln\frac{2x_c^2A}{\delta\varepsilon} = \ln(2x_c^2A) - \ln\delta\varepsilon$$

Hence $D(\varepsilon)$ diverge logarithmically