Problem set 9.

Problem Sommerfeld expansion

(1.a) $f_\beta(z) = \frac{1}{e^{\beta z}+1}$

$$\frac{\partial}{\partial z} f_\beta(z) = -\frac{\beta e^{\beta z}}{(e^{\beta z}+1)^2} = f_\beta^{(1)}(z) ; \quad f_\beta^{(1)}(-z) = -\frac{\beta e^{-\beta z}}{(e^{-\beta z}+1)^2} = \frac{-\beta e^{-\beta z} \cdot e^{2\beta z}}{(e^{-\beta z}+1)^2 \cdot e^{2\beta z}} = \frac{-\beta e^{\beta z}}{(e^{\beta z}+1)^2} = f_\beta^{(1)}(z)$$

(1.b) Define $G_\omega(\varepsilon) \equiv \int_{-\infty}^{\varepsilon} dz\, H_\omega(z)$, $\frac{\partial}{\partial \varepsilon} G_\omega(\varepsilon) = H_\omega(\varepsilon)$.

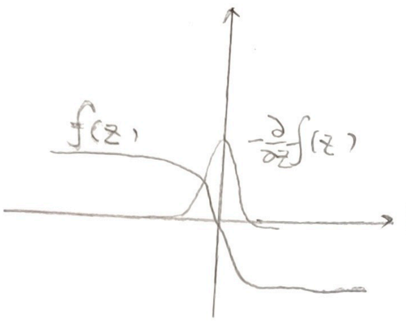
$$\omega = \int_{-\infty}^{\infty} d\varepsilon\, H_\omega(\varepsilon) f_\beta(\varepsilon-\mu)$$

Integrate by part

$$\omega = G_\omega(\varepsilon) f(\varepsilon-\mu)\Big|_{-\infty}^{+\infty} - \int_{-\infty}^{+\infty} d\varepsilon \cdot G_\omega(\varepsilon) \cdot \frac{\partial}{\partial \varepsilon} f_\beta(\varepsilon-\mu)$$

The first term vanishes when $\varepsilon \to \pm\infty$

$$-\quad \omega = \int_{-\infty}^{+\infty} d\varepsilon\, G_\omega(\varepsilon)\left(-\frac{\partial}{\partial \varepsilon} f_\beta(\varepsilon-\mu)\right)$$



$-f_\beta^{(1)}(z)$ decay rapidly away from 0, should be good approximation to evaluate near $\varepsilon = \mu$

(1.c) expand $G_\omega(\varepsilon)$ around μ

$$G_\omega(\varepsilon) = G_\omega(\mu) + G_\omega^{(1)}(\mu)(\varepsilon-\mu) + \frac{1}{2} G_\omega^{(2)}(\mu)(\varepsilon-\mu)^2 + \cdots + \frac{1}{k!} G_\omega^{(k)}(\mu)(\varepsilon-\mu)^k .$$

Insert into the integral gives

$$\omega = \sum_k \frac{1}{k!} \int_{-\infty}^{+\infty} d\varepsilon\, G_\omega^{(k)}(\mu)(\varepsilon-\mu)^k \cdot \left(-\frac{\partial f_\beta}{\partial \varepsilon}\right) = \sum_k \frac{1}{k!} G_\omega^{(k)}(\mu) \int_{-\infty}^{+\infty} d\varepsilon \left(-\frac{\partial f_\beta(\varepsilon-\mu)}{\partial \varepsilon}\right)(\varepsilon-\mu)^k$$

when k is an odd number, the integral vanishes

$$\omega = \sum_k \frac{1}{(2k)!} G_\omega^{(2k)}(\mu) \int_{-\infty}^{+\infty} d\varepsilon \frac{\beta e^{\beta(\varepsilon-\mu)}}{(e^{\beta(\varepsilon-\mu)}+1)^2}(\varepsilon-\mu)^{2k}$$

let $\beta(\varepsilon-\mu) = z$,

$$-\quad \omega = \sum_k \frac{1}{(2k)!} G_\omega^{2k}(\mu)(k_B T)^{2k} \cdot \int_{-\infty}^{+\infty} dz\, z^{2k} \frac{e^z}{(e^z+1)^2}$$

$$I = \int_{-\infty}^{\infty} dz\, z^{2k} \frac{e^z}{(e^z+1)^2}$$

$$= 2\int_0^{\infty} dz\, z^{2k} \frac{e^z}{(e^z+1)^2}$$

$$= 2\int_0^{\infty} dz\, z^{2k} \left(-\frac{\partial f}{\partial z}\right) \qquad f = \frac{1}{e^z+1}$$

$$= 2\left(-z^{2k} \cdot f(z)\Big|_0^{+\infty} + 2k\int_0^{\infty} dz\, z^{2k-1} \cdot f(z)\right)$$

$$= 4k\int_0^{\infty} dz\, z^{2k-1} \frac{1}{e^z+1}$$

Alternative derivation

$$w = I = \int_{-\infty}^{\infty} d\varepsilon\, H(\varepsilon)\, f_\beta(\varepsilon)$$

Let $\tau x = \varepsilon - \mu$, where $\tau = \beta^{-1}$

$$w = I = \int_{-\infty}^{\infty} \tau dx \cdot H(\tau x+\mu)\frac{1}{e^x+1} \quad \text{, using property of } \frac{1}{e^{-x}+1} = \frac{e^x}{1+e^x} = 1-\frac{1}{e^x+1}$$

$$= \overset{I_1}{\int_{-\infty}^{0} \tau dx\, H(\tau x+\mu)\frac{1}{e^x+1}} + \overset{I_2}{\int_{0}^{\infty} \tau dx\, H(\tau x+\mu)\frac{1}{e^x+1}}$$

$$I_1 = \int_{-\infty}^{0} \tau dx\, H(\tau x+\mu)\left(1-\frac{1}{e^{-x}+1}\right) = \int_{-\infty}^{0} \tau dx\, H(\tau x+\mu) - \int_{-\infty}^{0} \tau dx\, H(\tau x+\mu)\frac{1}{e^{-x}+1}$$

$$\overset{x\to -x}{=} \int_{-\infty}^{0} \tau dx\, H(\tau x+\mu) - \int_{0}^{+\infty} \tau dx\, H(-\tau x+\mu)\frac{1}{e^x+1}$$

$$w = I_1+I_2 = \int_{-\infty}^{0} \tau dx\, H_\omega(\tau x+\mu) + \int_{0}^{+\infty} \tau dx\, \frac{1}{e^x+1}\left[H_\omega(\mu+\tau x) - H_\omega(\mu-\tau x)\right]$$

Approximate $H(\mu+\tau x) - H(\mu-\tau x) \approx 2\tau x\, H'(\mu)$

$$w = \int_{-\infty}^{0} \tau dx\, H_\omega(\tau x+\mu) + 2\tau^2 \int_{0}^{+\infty} \frac{x\,dx}{e^x+1} \cdot H'(\mu)$$

Knowing $\int_{0}^{+\infty} \frac{x\,dx}{e^x+1} = \frac{\pi^2}{12}$

$$w = \int_{-\infty}^{\mu} d\varepsilon \frac{H_\omega(\varepsilon)}{e^{\beta(\varepsilon-\mu)}+1} + \frac{\pi^2}{6}(k_BT)^2 H'(\mu)$$

The "Knowing"

Remind $\int_{0}^{+\infty} \frac{x\,dx}{e^x-1} = \zeta(2)\cdot\Gamma(2)$ (In Debyemodel)

Let $\lambda = e^{-x}$, $\frac{1}{e^x-1} = \frac{\lambda}{1-\lambda} = \sum_{k=1} e^{-kx}$

$$\int_{0}^{+\infty} \frac{x\,dx}{e^x-1} = \sum_{k=1}\int_{0}^{+\infty} dx\, x\, e^{-kx} \overset{z=kx}{=} \sum_{k=1}\frac{1}{k^2}\int_{0}^{+\infty} dz\cdot z\cdot e^{-z} = \overset{1+\frac{1}{2^2}+\frac{1}{3^2}+\cdots}{\overset{\uparrow}{\zeta(2)}}\Gamma(2) = \frac{\pi^2}{6}$$

Now for $\int_{0}^{+\infty} \frac{x\,dx}{e^x+1}$, $\frac{1}{e^x+1} = \frac{\lambda}{1+\lambda} = (-1)\sum_{k=1}(-1)^k e^{-kx}$

Similarly, $\int_{0}^{+\infty} \frac{x\,dx}{e^x+1} = \sum_{k=1}\int_{0}^{+\infty} (-1)^{k+1} dx\, x\cdot e^{-kx} = \sum_{k=1}(-1)^{k+1}\frac{1}{k^2}\Gamma(2)$.

$$\sum_{k=1}(-1)^{k+1}\frac{1}{k^2} = 1-\frac{1}{2^2}+\frac{1}{3^2}-\frac{1}{4^2}+\cdots = 1+\frac{1}{2^2}+\frac{1}{3^2}+\frac{1}{4^2}+\cdots$$

$$-2\left(\frac{1}{2^2}+\frac{1}{4^2}+\cdots\right)$$

$$= \underbrace{\sum_{k=1}\frac{1}{k^2} - 2\sum_{k=1}\frac{1}{(2k)^2}}_{\text{converge series}} = \frac{\pi^2}{6} - \frac{1}{2}\cdot\frac{\pi^2}{6} = \underset{(\frac{1}{2}\zeta(2))}{\frac{\pi^2}{12}}$$

Similarly, one can get

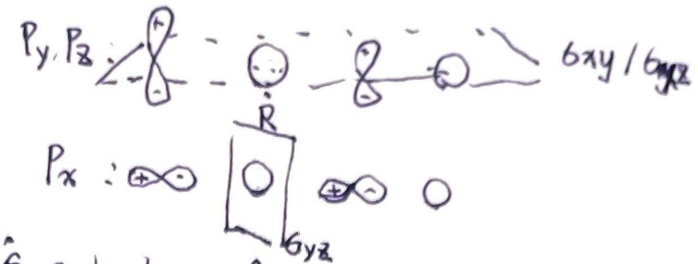
$$\int_{0}^{+\infty} \frac{x^{s-1}dx}{e^x+1} = \left\{\sum_{k=1}\frac{1}{k^s} - 2\sum_{k=1}\frac{1}{(2k)^s}\right\}\Gamma(s)$$

$$= \left\{1-\frac{1}{2^{s-1}}\right\}\zeta(s)\Gamma(s)$$

Problem 2. tight-binding with s, p

a)

$$P - \underbrace{S - P}_{a} - S - P \xrightarrow{x}$$



Consider reflection symmetry $\underset{(\mathbb{Z}_2)}{\hat{6}}$ such that $[\hat{h}, \hat{6}] = 0$, $h6 = 6h$

Suppose $\hat{6}|s\rangle = |s\rangle$, $\hat{6}|p\rangle = -|p\rangle$, transfer integral J

$$J = \langle p|\hat{h}|s\rangle = \langle p|\hat{h}\hat{6}|s\rangle = \langle p|\hat{6}\hat{h}|s\rangle \overset{6^{+}=6^{-1}=6}{=\!=} -\langle p|\hat{h}|s\rangle = 0$$

Therefore J_y, J_z vanishes since we can find $6_{xy}|P_z\rangle = -|P_z\rangle$, $6_{xz}|P_y\rangle = -|P_y\rangle$

For 6_{yz}, it still satisfies $[\hat{h}, 6_{yz}] = 0$

$$6_{yz}(R)|S(R)\rangle = |S(R)\rangle, \quad 6_{yz}(R)|p(R+a)\rangle = -|p(R-a)\rangle$$

$$J_x^R = \langle p(R+a)|h|s(R)\rangle = \langle p(R+a)|h6_{yz}|s(R)\rangle = +\langle p(R+a)|\hat{6}_{yz}\hat{h}|s(R)\rangle$$

$$= -\langle p(R-a)|h|s(R)\rangle = -J_x^L$$

b) $$\hat{H} = \sum_R J[c_s^{+}(R)\cdot c_{p_x}(R+a) + h.c.] - J[c_s^{+}(R)\cdot c_{p_x}(R-a) + h.c.] + \sum_R \varepsilon_s \hat{n}_s(R) + \sum_R \varepsilon_p[\hat{n}_{p_x}(R+a) + \hat{n}_{p_y}(R+a) + \hat{n}_{p_z}(R+a)]$$

$$\hat{C}_s(R) = \frac{1}{\sqrt{N}}\sum_k e^{ikR} c_s(k), \quad \hat{C}_p(R+a) = \frac{1}{\sqrt{N}}\sum_k e^{ik(R+a)} \hat{c}_p(R+a)$$

Knowing that ~~homogeneous~~ on-site $\varepsilon(R)$ will not have k dependency

$$\sum_R \varepsilon \hat{n}(R) = \sum_k \varepsilon \hat{n}(k).$$

hopping terms $= \sum_R \sum_{kk'} \frac{J}{N}[e^{-ikR} e^{+ik'(R+a)} c_s^{+}(k) c_{p_x}(k') - e^{-ikR} e^{+ik'(R-a)} c_s^{+}(k) c_{p_x}(k') + h.c.]$

using $\sum_R \frac{1}{N} \cdot e^{-i(k-k')R} = \delta(k-k')$

$$= \sum_k J(e^{ika} c_s^{+}(k) c_{p_x}(k') - e^{-ika} c_s^{+}(k) c_{p_x}(k) + h.c.]$$

$$= \sum_k J[2i\sin ka \; c_s^{+}(k) c_{p_x}(k) + h.c.]$$

$$\hat{H} = \sum_k \hat{\psi}^{+}_{(k)} \begin{pmatrix} \varepsilon_s & 2i\sin ka & & \\ -2i\sin ka & \varepsilon_p & & \\ & & \varepsilon_p & \\ & & & \varepsilon_p \end{pmatrix} \psi(k), \text{ where } \psi(k) = \begin{pmatrix} \hat{C}_s(k) \\ \hat{C}_{p_x}(k) \\ \hat{C}_{p_y}(k) \\ \hat{C}_{p_z}(k) \end{pmatrix}$$

Diagonalizing the matrix gives

$$(\varepsilon_s-\lambda)(\varepsilon_p-\lambda)-4J^2\sin^2(ka)=0 \Rightarrow \lambda=\frac{1}{2}\left(\varepsilon_s+\varepsilon_p\pm\sqrt{(\varepsilon_s+\varepsilon_p)^2-4(\varepsilon_s\varepsilon_p-4J^2\sin^2(ka))}\right).$$

$$=\frac{1}{2}\left(\varepsilon_s+\varepsilon_p\pm\sqrt{(\varepsilon_s-\varepsilon_p)^2+4J^2\sin^2ka}\right.$$

Obiviously, without off-diagonal part ε_{p_y}, ε_{p_z} remain dispersionless