Lecture 2. 自由电子气和费米液体

Motivation: 相互作用电子模型 = 自由电子模型 + 相互作用

$$\hat{H} = \underbrace{\hat{H}_0} + \hat{H}_I$$

$\hat{H}_0$ 单体 Hamiltonian. 二次型 (quadratic). 可严格求解.

(本次课内容).

$\hat{H}_I$, 相互作用, 如 $\hat{H}_I = \sum_{\sigma\sigma'} \int d\vec{r} \int d\vec{r}' \psi^+_\sigma(\vec{r}) \psi^+_{\sigma'}(\vec{r}') \frac{e^2}{|\vec{r}-\vec{r}'|} \psi_{\sigma'}(\vec{r}') \psi_\sigma(\vec{r})$

1. 能带理论回顾: 如何将电子能带模型写成二次量子化形式.

2. 费米液体理论: 在相互作用下, 电子往往表现为"修正"的自由电子气.

1) 能带理论:

* 王靖老师 固体物理 的内容. 本课程不再讨论.

* 实际科研中: 往往用DFT等第一性原理计算方法得到结果.

* 相互作用体系: 往往只考虑费米面附近的一条或多条能带; (低能有效理论).

简化模型. 因为还有更复杂的相互作用需要考虑.

*Bloch 波函数.

$\psi_{nk}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} u_{nk}(\vec{r})$. (Bloch 定理).

$\vec{k}$: 准动量. $u_{nk}(\vec{r})$ 有周期性 $u_{nk}(\vec{r}) = u_{nk}(\vec{r}+\vec{a})$

正交归一性: ~~$\int d\vec{r}$ ...~~.

$\int d\vec{r}\, \psi^*_{nk}(\vec{r}) \psi_{mk'}(\vec{r}) = \delta_{mn}\, \delta(\vec{k}-\vec{k}')$

当 $\vec{k}\neq\vec{k}'$ 时: 这是显然的. $\int d\vec{r}\, \psi^*_{nk}(\vec{r}) \psi_{mk'}(\vec{r}) = \frac{1}{N}\sum_a \frac{1}{V_{uc}} \int_{u.c.} d\vec{r}\, u^*_{nk}(\vec{r}) u_{nk'}(\vec{r})\, e^{-i(\vec{k}-\vec{k}')\cdot\vec{r}} e^{-i(\vec{k}-\vec{k}')\cdot a}$

当 $\vec{k}=\vec{k}'$ 时:

$$= \delta_{kk'} \frac{1}{V_{uc}} \int_{u.c.} d\vec{r}\, u^*_{nk}(\vec{r}) u_{mk'}(\vec{r})$$

$\Rightarrow \frac{1}{V_{u.c.}} \int_{u.c.} d\vec{r}\, u^*_{nk}(\vec{r}) u_{mk}(\vec{r}) = \delta_{nm}$

$\psi_{nk}(\vec{r})$ 为一组正交归一波函数. 相应的产生/湮灭算符为

$$C_{nk} = \frac{1}{\sqrt{V}} \int d\vec{r}\, \hat{\psi}(\vec{r}) \psi^*_{nk}(\vec{r}) = \frac{1}{\sqrt{V}} \int d\vec{r}\, \hat{\psi}(\vec{r}) u^*_{nk}(\vec{r}) e^{-i\vec{k}\cdot\vec{r}}.$$

$$\hat{\psi}(\vec{r}) = \frac{1}{\sqrt{V}} \sum_{nk} C_{nk} u_{nk}(\vec{r}) e^{i\vec{k}\cdot\vec{r}}$$

$\hat{H}_0 = \sum_{nk} C^+_{nk} \epsilon_{nk} C_{nk}$. (加入自旋自由度: $\hat{H}_0 = \sum_{nk\sigma} C^+_{nk\sigma} \epsilon_{nk} C_{nk\sigma}$).

自由度: 自由空间 $\vec{k} \in R^3$ $-\infty < k_{x,y,z} < \infty$.

晶格: $\vec{k} \in BZ$. $n \times BZ =$ 全空间.

$\vec{k} \to (n\vec{k})$ 相当于把 $\vec{k}$ 空间折叠进 B.Z. 但自由度不变.

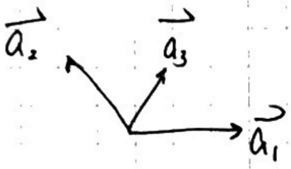
2) Wannier 波函数.

Bloch w.f. $\psi_{nk}(\vec r)$.

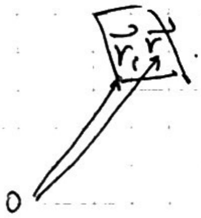
作 Fourier 变换: $\vec k\in B.Z. \to i\in \mathbb{Z}^3$.

记号: ~~$i=(i_x,i_y,i_z)$ $\vec r_i = i_x\vec e_x + i_y\vec e_y$~~

$i=(i_1,i_2[,i_3])$ $\vec r_i = i_1\vec a_1 + i_2\vec a_2 (+ i_3\vec a_3)$



$w_n(\vec r_i;\vec r)$ 或 $w_{ni}(\vec r)$. $i/\vec r_i$: label $\vec r$: 实空间坐标.



$$w_{ni}(\vec r)=\frac{1}{\sqrt N}\sum_k \psi_{nk}(\vec r)e^{-i\vec k\cdot\vec r_i}$$

$$=\frac{1}{\sqrt N}\sum_k u_{nk}(\vec r)e^{i\vec k\cdot\vec r-i\vec k\cdot\vec r_i}$$

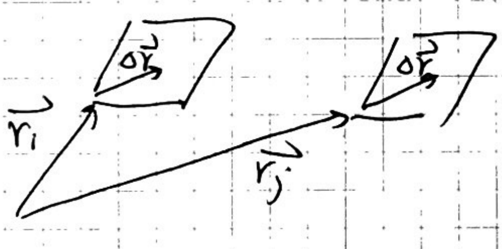
$$=\frac{1}{\sqrt N}\sum_k u_{nk}(\vec r-\vec r_i)e^{i\vec k\cdot(\vec r-\vec r_i)}.$$

归一化: $\sqrt{\frac{N}{V}}\,w_{ni}=\frac{1}{\sqrt{V_{uc}}}\,w_{ni}$

* 当 $|\vec r-\vec r_i|\to\infty$ 时, $e^{i\vec k\cdot(\vec r-\vec r_i)}$ 振荡很快, $w_{ni}(\vec r)\to 0$.

* $w_{ni}(\vec r_i+\Delta\vec r)=w_{nj}(\vec r_j+\Delta\vec r) = w_n(\Delta\vec r)$.

$w_{ni}(\vec r)=w_n(\vec r-\vec r_i)$.



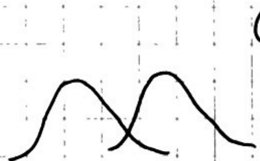
相应的二次量子化算符

$(V_0=V_{u.c.}=\frac{V}{N})$ $c_{ni}=\frac{1}{\sqrt{V_0}}\int d\vec r\,\hat\psi(\vec r)\,w^*_{ni}(\vec r)=\frac{1}{\sqrt{V_0}}\int d\vec r\,\hat\psi(\vec r+\vec r_i)\,w_n(\vec r)$

$$=\frac{1}{\sqrt{V_0}}\int d\vec r\,\hat\psi(\vec r)\frac{1}{\sqrt N}\sum_k\psi_{nk}(\vec r)e^{i\vec k\cdot\vec r_i}$$

$$=\frac{1}{\sqrt N}\sum_k c_{nk}e^{i\vec k\cdot\vec r_i}$$

$c_{ni}\leftrightarrow c_{nk}$ 离散 Fourier 变换.

3)  紧束缚模型 交叠很少:

$$\hat h_1=-\frac{\hbar^2\nabla^2}{2m}+V.$$

$$H=\sum_{nmij}\left[c^\dagger_{ni}\langle ni|\hat h_1|mj\rangle c_{mj}+h.c.\right]$$

$-t_{ni,mj} = \langle ni | \hat h_1 | mj \rangle$

$= \frac{1}{V_0}\int d\vec r\, w_{ni}^*(\vec r)\left(-\frac{\hbar^2\nabla^2}{2m}+\hat V\right) w_{mj}(\vec r)$.

$= \frac{1}{V_0}\int d\vec r\, w_n^*(\vec r-\vec r_i)\left(-\frac{\hbar^2\nabla^2}{2m}+\hat V\right) w_m(\vec r-\vec r_j)$.

$[\hat V(\vec r) = V(\vec r - \vec r_i + \vec r_j)]$

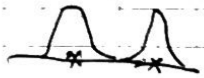
$= \frac{1}{V_0}\int d\vec r\, w_n^*(\vec r-\vec r_i+\vec r_j)\left[-\frac{\hbar^2\nabla^2}{2m}+V(\vec r)\right] w_m(\vec r)$.

单带模型， $n=m=1$.

$-t_{ij} = \frac{1}{V_0}\int d\vec r\, w^*(\vec r-\vec r_i+\vec r_j)\left[-\frac{\hbar^2\nabla^2}{2m}+V(\vec r)\right] w(\vec r)$.

d.f 轨道 $\vec r_i-\vec r_j$ 大时 t_{ij} 衰减很快.

$w(\vec r_0)$ 比较 localize,



只考虑最近邻 $t_{ij}\neq 0$.

$\hat H = \sum_{\langle ij\rangle}(-t_{ij}\, c_i^\dagger c_j + h.c.)$.

例: 正方晶格 紧束缚模型.

① 最近邻 (= nearest neighbor = n.n.): $t_{ij} = t$.

$\hat H = -t\sum_{\langle ij\rangle}(c_i^\dagger c_j + h.c.)$

Fourier 变换: $c_i = \frac{1}{\sqrt N}\sum_k c_k e^{i\vec k\cdot\vec r_i}$.

$\hat H = -t\sum_{\langle ij\rangle}\left(\frac{1}{\sqrt N}\sum_k c_k^\dagger e^{-i\vec k\cdot\vec r_i}\frac{1}{\sqrt N}\sum_{k'} c_{k'} e^{i\vec k'\cdot\vec r_j} + h.c.\right)$

$\left[\sum_{\langle ij\rangle} = \sum_i\sum_{\delta=x,y} \quad (w/\ \vec r_j = \vec r_i + \vec r_\delta)\right]$

$\hat H = -\frac{t}{N}\sum_{i\delta}\sum_{kk'}\left(c_k^\dagger c_{k'} e^{-i\vec k\cdot\vec r_i} e^{i\vec k'\cdot\vec r_i + i\vec k'\cdot\vec r_\delta} + h.c.\right)$

$= -t\sum_{kk'}\sum_{\delta=x,y}\left(c_k^\dagger c_{k'} e^{i\vec k'\cdot\vec r_\delta}\frac{1}{N}\sum_i e^{i(\vec k'-\vec k)\cdot\vec r_i} + h.c.\right)$

$\left[\frac{1}{N}\sum_i e^{i(\vec k'-\vec k)\cdot\vec r_i} = \delta_{\vec k,\vec k'}\right]$

$\hat H = -t\sum_{k\delta}\left(c_k^\dagger c_k e^{i\vec k\cdot\vec r_\delta} + h.c.\right)$

$= -t\sum_k c_k^\dagger c_k\left(e^{ik_x} + e^{ik_y} + e^{-ik_x} + e^{-ik_y}\right)$

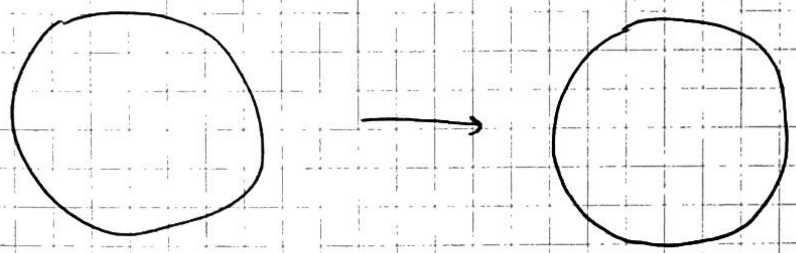
$= -2t\sum_k c_k^\dagger c_k(\cos k_x + \cos k_y)$

$\therefore\ \epsilon_k = -2t(\cos k_x + \cos k_y)$

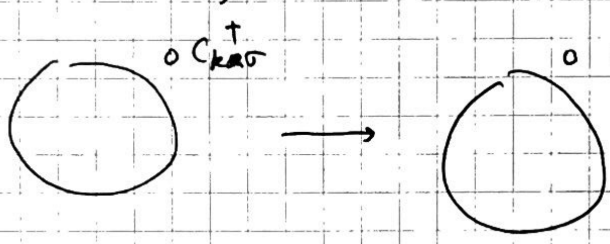
5) 费米液体 教材§12.5. + S. Sachdev 讲义 Fermi Liquid Theory.

绝热演化:

自由费米气体 费米液体.



基态→基态；激发态→激发态

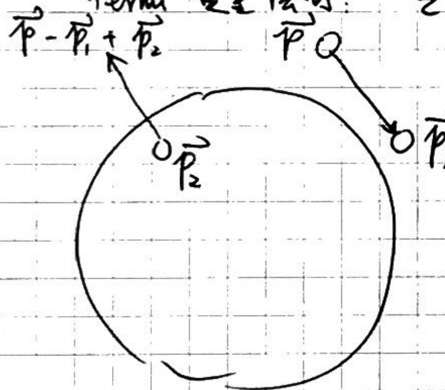


准粒子激发，也用 k, σ 标记.

$\tilde{c}^\dagger_{k\sigma} = \sqrt{Z}\, c^\dagger_{k\sigma} + \cdots$.

6) 准粒子寿命: $\frac{1}{\tau} \to \xi^2$ as $\xi \to 0$. $\xi_k = \epsilon_k - \mu$.

Fermi 黄金法则: $\frac{1}{\tau} \propto$ 相空间体积

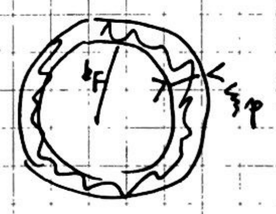


$T=0$:

$$\frac{1}{\tau} \propto |u|^2 \int d\vec{p}_1 d\vec{p}_2\, [1-f(\xi_{p_1})]\, f(\xi_{p_2})\, [1-f(\xi_{\vec{p}-\vec{p}_1+\vec{p}_2})].$$

$0 < \xi_{p_1} < \xi_p$

$0 < |\xi_{p_2}| < \xi_p - \xi_{p_1} < \xi_p$.

$\vec{p}_1 \in$ 

$\vec{p}_2 \in$ 

$\frac{1}{\tau} < [\cdots] \cdot \epsilon^2$.

7) 能量泛函；朗道参数:

$$\delta E = \sum_{k\sigma} \xi^0_k\, \delta n_\sigma(k) + \frac{1}{2V} \sum_{kk'\sigma\sigma'} f_{\sigma\sigma'}(\vec{k}, \vec{k}')\, \delta n_\sigma(\vec{k})\, \delta n_{\sigma'}(\vec{k}').$$

$\xi^0_k = \frac{k_F}{m^*}(k - k_F)$. 变分: $\delta n = n - n_0$

有效质量

$f(\vec{k}\uparrow, \vec{k}'\uparrow) = f^s(\vec{k}, \vec{k}') + f^a(\vec{k}, \vec{k}')$

$f(\vec{k}\uparrow, \vec{k}'\downarrow) = f^s(\vec{k}, \vec{k}') - f^a(\vec{k}, \vec{k}')$.

Legendre 展开: $f^{a,s}(\vec{k}, \vec{k}') = \sum_{l=0}^{\infty} f^{a,s}_l P_l(\cos\theta)$ —— 30.

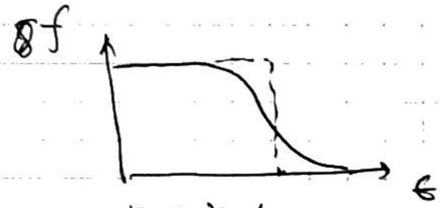
定义无量纲常数 $F^{a,s}_l = \frac{k_F m^*}{\pi^2} f^{a,s}_l$.

利用 Landau 参数可以计算 Fermi Liquid 的各项性质.

例1. $C_V = \frac{1}{3} m^* k_F k_B^2 T + O(T^2)$.

$$C_V = \frac{1}{V}\frac{\partial E}{\partial T} = \frac{1}{V}\frac{\partial}{\partial T}\left[\sum_{k\sigma}\epsilon_k^0\,\delta n_\sigma(k) + \frac{1}{2V}\sum_{kk'\sigma\sigma'} f(k,k')\,\delta n_\sigma(k)\,\delta n_{\sigma'}(k')\right]$$

有限温的 $\delta n_\sigma(k) = f\ \frac{1}{1+e^{\beta\epsilon_k}} - \theta(-\epsilon_k^0)$



$$\sum_k \delta n(k) \approx N(0)\int d\epsilon\,\delta n(\epsilon_k) = 0.$$

在此近似下: $\frac{1}{2V}\sum_{kk'} f(\theta)\,\delta n_\sigma(k)\,\delta n_{\sigma'}(k') = 0$.

只需考虑第一项.

$$C_V = \frac{1}{V}\frac{\partial}{\partial T}\, 2\sum_k \epsilon_k^0\left[\frac{1}{1+e^{\beta\epsilon_k}} - \theta(-\epsilon_k^0)\right]$$

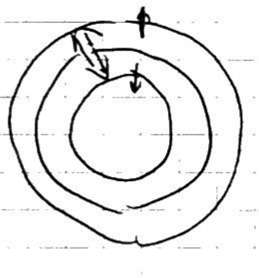
与自由费米子的计算形式相同, 只是 $m \to m^*$.

自由费米子 $C_V = \frac{1}{3} m k_F k_B^2 T$ (计算见教材 Chap.2).

费米液体 $C_V = \frac{1}{3} m^* k_F k_B^2 T$.

例2. (泡利)磁化率 $\chi = \frac{1}{1+F_0^a}\frac{\mu_B^2 k_F m^*}{\pi^2}$.

考虑在外加磁场下的均匀磁化: $\tilde{\epsilon}_{k\sigma}^0 = \epsilon_{k\sigma}^0 - \mu_B\sigma h$.



Spin-up 的 FS 变大/变小, 产生净磁化 M. $M = \mu_B(N_\uparrow - N_\downarrow)$

$\therefore\ \chi = \left(\frac{\partial^2 E}{\partial M^2}\right)^{-1}$.

热力学关系 $\chi = \frac{\partial M}{\partial h} = \frac{\partial^2 E}{\partial h^2}$.

线性区间, $\chi = \frac{M}{h}$ $\therefore\ \frac{\partial^2 E}{\partial M^2} = \frac{1}{\chi}$.

假设 $N_\uparrow \neq N_\downarrow$. $N_\uparrow + N_\downarrow = N$

$\therefore\ \delta N_\uparrow = -\delta N_\downarrow$, $\delta N_\uparrow = \sum_k \delta n_{k\uparrow}$.

考虑↑↓费米面的变化: $k_{F\uparrow} = k_F + \delta k_F$; $k_{F\downarrow} = k_F - \delta k_F$.

$$\delta N_\uparrow = \sum_{k_F<k<k_F+\delta k_F} 1 = V\int_{k_F<k<k_F+\delta k_F}\frac{d^3k}{(2\pi)^3} \approx V\cdot\frac{4\pi k_F^2\,\delta k_F}{8\pi^3}$$

$$M = \mu_B(\delta N_\uparrow - \delta N_\downarrow) = 2\mu_B\,\delta N_\uparrow = V\cdot\mu_B\frac{k_F^2}{\pi^2}\delta k_F.$$

or $\boxed{\delta k_F = \frac{\pi^2}{\mu_B k_F^2}\frac{M}{V}}$

下面计算 δE: 分两项计算.

$$\delta E_1 = \sum_{k\sigma}\epsilon_k^0(\delta n_{k\uparrow} + \delta n_{k\downarrow}) = 2\sum_k \epsilon_k^0\,\delta n_{k\uparrow} = 2V\int\frac{d^3k}{(2\pi)^3}\epsilon_k^0\,\delta n_{k\uparrow}$$

$$= 2V\cdot\frac{4\pi k_F^2}{8\pi^3}\int_{k_F}^{k_F+\delta k_F} dk\,\frac{k_F}{m^*}(k-k_F)$$

$$= V\frac{k_F^2}{\pi^2}\cdot\frac{k_F}{m^*}\frac{1}{2}(\delta k_F)^2 = \cancel{V}\,\frac{k_F^3}{2\pi^2 m^*}\cdot\frac{\pi^4}{\mu_B^2 k_F^4}\frac{M^2}{V^2} = \frac{\pi^2}{\mu_B^2 k_F m^*}\frac{M^2}{2V}$$

$$\delta \tilde{E}_2 = \frac{1}{2V} \sum_{kk'\sigma\sigma'} f_{\sigma\sigma'}(\vec{k}, \vec{k}') \, \delta n_{k\sigma} \, \delta n_{k'\sigma'}.$$

例: $\sigma = \sigma' = \uparrow$.

$$\frac{1}{2V} \sum_{kk'} f_{\uparrow\uparrow}(\vec{k}, \vec{k}') \, \delta n_{k\uparrow} \, \delta n_{k'\uparrow}$$

角度平均, ~~即~~ 得到 ~~与~~ $f_0 \propto 1$ 这一项.

$$= \frac{1}{2V} V^2 \int \frac{d\vec{k}}{(2\pi)^3} \int \frac{d\vec{k}'}{(2\pi)^3} f_{\uparrow\uparrow,0} \, \delta n_{k\uparrow} \, \delta n_{k'\uparrow}$$

$$= \frac{V}{2} \left(\frac{4\pi k_F^2}{8\pi^3} \right)^2 (\delta k_F)^2 f_{\uparrow\uparrow,0}.$$

$\sigma = \uparrow, \sigma' = \downarrow$:

$$\frac{1}{2V} \sum_{kk'} f_{\uparrow\downarrow}(\vec{k}, \vec{k}') \, \delta n_{k\uparrow} \, \delta n_{k'\downarrow}$$

$$= \frac{1}{2V} V^2 \int_{k_F}^{k_F+\delta k_F} \frac{d\vec{k}}{(2\pi)^3} \int_{k_F-\delta k_F}^{k_F} \frac{dk'}{(2\pi)^3} f_{\uparrow\downarrow,0} \, \cancel{\delta n_{k\uparrow}}^{+1} \, \cancel{\delta n_{k'\downarrow}}^{-1}$$

$$= -\frac{V}{2} \left(\frac{k_F^2}{2\pi^2} \right)^2 (\delta k_F)^2 f_{\uparrow\downarrow,0}$$

$$\therefore \delta \tilde{E}_2 = 2 \cdot \frac{V}{2} \left(\frac{k_F^2}{2\pi^2} \right)^2 (\delta k_F)^2 \, \cancel{(f_{\uparrow\uparrow,0} - f_{\uparrow\downarrow,0})}^{2 f_0^a}$$

$\uparrow\uparrow = \downarrow\downarrow$

$\uparrow\downarrow = \downarrow\uparrow$

$$= 2 V f_0^a \frac{k_F^4}{4\pi^4} \cdot \frac{\pi^4}{\mu_B^2 k_F^4} \frac{M^2}{V^2}$$

$$= \frac{M^2}{2V} \cdot \frac{f_0^a}{\mu_B^2}$$

$$= \frac{M^2}{2V} \cdot \frac{1}{\mu_B^2} \cdot F_0^a \cdot \frac{\pi^2}{k_F m^*}$$

$$= \frac{\pi^2}{\mu_B^2 k_F m^*} F_0^a \frac{M^2}{2V}$$

$$\delta E = \delta \tilde{E}_1 + \delta \tilde{E}_2 = (1 + F_0^a) \frac{\pi^2}{\mu_B^2 k_F m^*} \frac{M^2}{2V}.$$

$$\therefore \quad \chi = \left(\frac{\partial^2 \delta \tilde{E}}{\partial M^2} \right)^{-1} = \frac{1}{1 + F_0^a} \frac{\mu_B^2 k_F m^*}{\pi^2}.$$