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Chapter 2. 晶格费米子 (Altland. 钟寅. Bruus)

① 平均场论 (Part 2)

与其与粒子作用(V近邻)；不如与此些粒子构建平均场作用..

比如体系中有A.B两种粒子. A.B粒子间势能 $\int V_{\nu\mu\nu'\mu'} a^+_\nu b^+_\mu b_{\mu'} a_{\nu'}$

定义 $d_{\nu\nu'} = a^+_\nu a_{\nu'} - \langle a^+_\nu a_{\nu'} \rangle$ $e_{\mu\mu'} = e^+_\mu e_{\mu'} - \langle e^+_\mu e_{\mu'} \rangle$

我们忽略 $\int V_{\nu\mu\mu'\nu'} d_{\nu\nu'} e_{\mu\mu'}$ 项. 余下: $\hat{V} =$

$$\int V_{\mu\mu'\nu'} \left[(a^+a)\langle \quad \rangle + (b^+b)\langle \quad \rangle + \langle \quad \rangle\langle \quad \rangle \right]$$

对比原来: a^+ab^+b 项. 现在只留下了单粒子算符乘上均值. 去耦合.

这大大简化计算. 现在困难变成了求 $\langle \quad \rangle$. 什么是 $\langle a_\nu a^+_\nu \rangle$,

经典看为一个势 $V(0)$. 比如 $\sum_{kk'q} V a^+_{k+q} a^+_{k'-q} a_{k'} a_k = \sum V \cdot \underline{V(0)} \cdot a^+_k a_k$ $N(0)$

Actually $\langle a^+_\nu a_\nu \rangle$ 类似一个粒子数的平均场. $= \sum_i \langle \phi | a^+_\nu a_{\nu'} | \phi \rangle$

∴) 由于 $\langle A \rangle = Tr(\rho A)$ Now: $\langle a^+_\nu a_\nu \rangle = Tr[e^{-\beta H} a^+_\nu a_{\nu'}] \cdot \{Tr[\rho]\}^{-1}$

此中 H 也已是 $\hat{H}_{mean-field}$ $\beta = \frac{1}{kT}$ 要求随温度涨落平均场变化小。

∴) 最小化自由能, 当 $F = U - TS$; $F_{min} \Leftrightarrow S_{max}$ 平衡态

正则系综 $F = -k_T \ln Z$ $F_{min} \Rightarrow \frac{\partial F}{\partial N} = 0 \Rightarrow \frac{\partial}{\partial \langle \rangle}\left(-\frac{1}{\beta}\ln Z\right) = 0$

$$= Tr\left[\frac{e^{-\beta H}}{Z} \sum_{\mu\mu'} V (b^+_\mu b_{\mu'} - \bar{n})\right] = \sum_{\mu\mu'} V_{\nu\mu\nu'\mu'} \left(\langle b_\mu b_{\mu'} \rangle_{MF} - \bar{n}^b_{\mu\mu'} \right) = 0$$

上两法皆可求: $\langle \quad \rangle$

适用条件 ① (d, e) 小; 检验 $\langle d \rangle$. $\langle e \rangle$ 是否近 0. $\forall$ time. 系综

② 平衡态, F minimize and 正则系综

③ $\bar{n} = \langle a^+_\nu a_\nu \rangle = \begin{pmatrix} \ddots \end{pmatrix}_{m\times n}$ 体现一粒子数算符

PS: $\hat{N} = a^+_\nu a_\nu$ $\hat{\bar{N}} = \langle a^+_\nu a_\nu \rangle = \begin{pmatrix} \ddots \end{pmatrix}$ 仅对角元.

基底对角化.

③ 如果 N-dimension system $\sum_i \langle i | a_{j}^{+} a_{j'} | i \rangle = f(a_j^+ a_{j'})$
共 $N\times N = N^2$ 个 Equation 以确定 $a_j^+ = \begin{pmatrix} a \\ b \\ c \end{pmatrix}$ $a_{j'} = (一、二、三、四) = (\ )_{n\times n}$
过多. Now: assume 按③. $\langle a_k^+ a_{k'} \rangle = \delta_{k-k'} \langle n_k \rangle$
and $\langle \psi^+_{(r)} \psi^-_{(r')} \rangle = f(r-r')$，两者等价. 即:

$$a_k^+ a_{k'} = \iint e^{ikr} e^{-ik'r'} \psi^+(r)\psi(r') \frac{1}{V} \Rightarrow \langle a_k^+ a_{k'} \rangle = \int e^{(kr-k'r')} \frac{1}{V} f(r'-r)$$

$$= \frac{1}{V}\int dr\, e^{ikr} \int dr' e^{-ik'r'} f(r'-r) = \frac{1}{V}\int dr\, d(r-r')\, f(r-r')\, e^{-ik'r'+ik'r+ikr-ik'r}$$

$$= \frac{1}{V}\int dr\, du\, f(u)\, e^{iku} e^{i(k-k')r} = \frac{1}{V}\underbrace{\int_{R^+} dr\, e^{i(k-k')r}}_{V\,(\delta_{k,k'})} \underbrace{\int_{R^+} du\, e^{iku} f(u)}_{f(k)\,\sim\,\langle n_k\rangle}$$

故想要③近对角需系统有对称性.
在 r 处产生 r' 处湮灭只与 r'-r 距离有关，至少球对称，对于比如平面波 wave formation $\langle \psi^+(r)\psi(r') \rangle = h(r', r) \neq f(r'-r)$ 对称性破缺. $h(r,r') = h(r+R, r'+R)$ 不适用 $\Rightarrow \langle c_k^+ c_{k+Q} \rangle$ is finite
③ 检验有上文条件

Hartree Fock approximation:
Now. one particle: Hartree aproxiamation 联想到费米子波函数两体为满足 Pauli 不相容，常写作 $\psi(r_1, r_2) = \frac{1}{\sqrt{2}}[\chi_1(r_1)\chi_2(r_2) - \chi_1(r_2)\chi_2(r_1)]$
我们原本的 $V = i^+ j^+ L m$ 转化为 $V^{HF} = [i^+(r_i) j^+(r_j) i(r_i) j(r_j)$
以满足交换反对称. 在 V^{HF} 的意义下应用 $- i^+(r_i) j^+(r_j) i(r_j) j(r_i)]$
Mean-Field. 得到:

$$i^+_i j^+_j i_i j_j = j^+ j \langle i^+ i \rangle + \langle j^+ j \rangle i^+ i - \langle i^+ i \rangle \langle j^+ j \rangle$$ 二项.

$$i^+_i j^+_j i_j j_i = j^+ i \langle i^+ j \rangle + i^+ j \langle j^+ i \rangle - \langle i^+ j \rangle \langle j^+ i \rangle$$

其中第一项为 Hartree $V^{Hartree} = \sum_{\nu\nu'\mu\mu'} V_{\nu\nu'\mu\mu'} \bar{n}_{\mu\mu'} c_\nu^+ c_{\nu'} + \bar{n}_{\nu\nu'} c_\mu^+ c_{\mu'} - \bar{n}_{\nu\nu'} \bar{n}_{\mu\mu'}$
二项为 Fock 交换: $V^{Fock} = \sum_{\nu\nu'\mu\mu'} V_{\nu\nu'\mu\mu'} \bar{n}_{\nu\mu'} c_\mu^+ c_{\nu'} + \bar{n}_{\nu\mu} c_\nu^+ c_{\mu'} - \bar{n}_{\nu\mu'} \bar{n}_{\mu\nu'}$

$H^{HF} = H_0 + V^{Fock} + V^{Hartree}$

HF 近似与 HF 方程（又名自洽场方法 SCF）

比如现在仍讨论自由电子费米体系处于阳背景下，利用 Chapter 1 Hamiltonian

$$\hat{V}_{Hartree\text{-}Fock} = \frac{1}{2V}\sum_{\sigma\sigma' kk'q} V_q \{ k+q,\ k'-q,\ k',\ k \ \text{一堆} \}$$

$$\hat{H}_0 = \sum_{k\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma}$$

此模型电子密度也均匀，称 Jellium，由此 $V_{electron\text{-}lattice}$ 变为 $V_{electron\text{-}jellium}$ $= V(0) = const$ 电子/阳离子势能处处相同。

$$= \frac{1}{2V}\sum_{kk'q\sigma\sigma'} \bar{n}_{(k+q)\sigma\, k\sigma} c^\dagger_{k'-q\,\sigma'} c_{k'\sigma'} + \bar{n}_{(k'-q)\sigma'\, k'\sigma'} c^\dagger_{(k+q)\sigma} c_{k\sigma}$$

$$- \bar{n}_{(k+q)\sigma\, k\sigma} \bar{n}_{(k'-q)\sigma'\, k'\sigma'} + \bar{n}_{(k+q)\sigma\, k'\sigma'} c^\dagger_{(k'-q)\sigma'} c_{k\sigma}$$

$$+ \bar{n}_{(k'-q)\sigma'\, k\sigma} c^\dagger_{(k+q)\sigma} c_{k'\sigma'} - \bar{n}_{(k+q)\sigma\, k'\sigma'} \bar{n}_{(k'-q)\sigma'\, k\sigma}$$

$\bar{n}_{ij}$ 只有 $i=j$ 才非零，即一项：$q=0$ 二项：$q=0$ 三项不可能为0。

四项 $q=k-k'$ 五项 $q=k-k'$

$$\therefore \text{原式} = \frac{1}{2V}\sum_{kk'\sigma\sigma'} V(0)\, \underbrace{\bar{n}_{k\sigma} c^\dagger_{k'\sigma'} c_{k'\sigma'} + \bar{n}_{k'\sigma'} c^\dagger_{k\sigma} c_{k\sigma}}_{\text{相同}}$$

$$+ V(k'-k)\, \bar{n}_{k\sigma} c^\dagger_{k'\sigma} c_{k\sigma} + \bar{n}_{k'\sigma'} c^\dagger_{k\sigma} c_{k\sigma'}$$

$$= \frac{1}{V}\sum_{k} V(0)\, c^\dagger_{k\sigma} c_{k\sigma} \bar{n}_{k\sigma}$$

$$+ \sum_{k'k\sigma'\sigma} V(k'-k)\, \delta(\sigma'\sigma)\, \bar{n}_{k\sigma} c^\dagger_{k'\sigma} c_{k'\sigma} \rightarrow \sum_{k'k\sigma} \bar{n}_{k\sigma} c^\dagger_{k'\sigma} c_{k'\sigma}$$

$$\Rightarrow \boxed{H^{HF} = \sum_k \varepsilon_k^{HF} c^\dagger_{k\sigma} c_{k\sigma}} + const.$$

我们之后也可利用此HF近似得到 Hubbard Model 的 H^{HF}.

$$\varepsilon_k^{HF} = \varepsilon_k - \underbrace{\sum_{k'} V(k-k')\, \bar{n}_{k'\sigma}}_{\text{包括了 } k'=k\ V(0) \text{ 项}} \qquad V(q) = \frac{4\pi e^2}{q^2}$$

其中 $\bar{n}_{kk'} = \langle C_k^+ C_{k'} \rangle$ 电子并非局域晶格而为空间均匀分布，满足③.5 ∴ $\bar{n}_{kk'} = \delta_{kk'} \bar{n}_k$

? $\langle \hat{a}_k^+ \hat{a}_{k'} \rangle$ 究竟为何？ $\langle \psi^+(r)\psi(r') \rangle = f(r-r') \Leftrightarrow \langle a_k^+ a_{k'} \rangle = \delta_{kk'} \langle a_k$ 代表何义，为什么均匀分布成立. 晶格平移对称不成立 当考虑某一态为 $|1 \cdots 0 \cdots 1 . n \cdots 0 . 0\rangle$. 时，应该一致？

$\Downarrow$ 晶格不是这么写的.

Broken symmetry:

Recall: 平移不变性 ⇒ 动量守恒

$[H, T(R)] = 0$ for $\forall R \Rightarrow T(R) = e^{-\frac{iP\cdot R}{\hbar}}$ 即 P is const.

P is total momentum $P = \hbar \sum_k C_{ks}^+ C_{ks}$

此时：$\langle C_{ks}^+ C_{k+Q\sigma} \rangle \Rightarrow$ $C_{ks}^+ C_{k+Q\sigma}$ 相当于电子从 $k+Q$ 动量跑到 k 动量，一种"density wave"不会出现. 即.

$$\langle C_{ks}^+ C_{k+Qs} \rangle = \frac{Tr[e^{-\beta E_p} C_{ks}^+ C_{k+Q\sigma}]}{Z} = \frac{1}{Z}\sum_p \langle p | C_{ks}^+ C_{k+Q\sigma} | p \rangle e^{-}$$

$\cdots \to k+Q \to p \Rightarrow (p-Q)$ $\langle p | p-Q \rangle = 0$ 动量守恒表明 $e^{-\beta\hat{H}}$ 可用 $e^{-\beta E}$ 代表，对任一种总动量守恒体系. $\langle C_{ks}^+ C_{k+Q\sigma} \rangle = 0$.

然而：自发性对称破缺 比如晶格 energy barrier 使得序参量 $\sum_k \langle C$ 对应 Density Wave. 自由能随之改变，其它体系序参量有磁 Magentiza 等. 磁化性，超导 都依赖这些项的存在. Free electron Gas 仅为一特例.

续上 HF的 Free electron Gas V_{HF} when $T\to 0$ 全费米面下.

$$V_{HF}(k) = -\sum_{k'} \frac{4\pi e^2}{|k'-k|^2} \cdot \bar{n}_{k'\sigma} \to \begin{cases} 1\text{个电子} & k<k_F \\ 0\text{个电子} & k>k_F \end{cases} = -\sum_{k'} \frac{4\pi e^2}{|k'-k|^2}\theta(k-k_F)$$

$$= -4\pi e^2 \int_0^{k_F} \cancel{f(k)}\, k'^2 dk' \cdot \frac{1}{k^2+k'^2-2kk'\cos\theta}\, d\cos\theta\, d\phi \cdot \frac{1}{(2\pi)^3}$$

PS：~~此~~中引入了 $\sum_k f(k) \Leftrightarrow \int dk\, f(k) \cdot \frac{V}{(2\pi)^3}$

系：volume $\Delta k_x \Delta k_y \Delta k_z = \frac{2\pi}{L_x} \cdot \frac{2\pi}{L_y} \cdot \frac{2\pi}{L_z} = \frac{(2\pi)^3}{V}$

左边 Number × $V_{k_xk_yk_z}$ = 体积 × Number(f(k)).
右边：average = 体积 f(k) 求average in volume
对dv 甚小 两者等价

$$\Rightarrow V_{HF}(k) = -\frac{e^2}{\pi}\int \frac{k'^2}{k^2+k'^2-2kk'\cos\theta}\, dk'\, d\cos\theta$$

$$= \frac{-e^2 k_F}{\pi}\left(1+\frac{k_F^2-k^2}{2k_F k}\ln\left|\frac{k+k_F}{k-k_F}\right|\right)$$

还可以计算：E 之于 H^{HF} 发现 $E = E(\text{origin})$ 系均匀态对称后 $\langle de \rangle$ 即为零，但是，不可再用 $\sum_k \varepsilon_k^{HF} n(\varepsilon_k^{HF})$ ($\varepsilon \cdot n_\varepsilon$) 表示能量了.

平均场论处理相变有利，比如：

①. 铁磁海森堡模型.（下议）

② stoner 金属铁磁性（下议）.

② Hubbard 模型.

固体中电子处周期势场中，Bloch波函数可描述，Free electron Gas 用平面波展开 Hamiltonian 由于极好对称性多体 k, k', k'', k''' 部分2元描述 (k, q, k') 即可。Now use Bloch波函数展开 Hamiltonian。除了平面波(k) e^{ikx} 外，还有~~格点序号~~ n 部分 $\psi_{nk}(x)$，有：$e^{ikr}\underbrace{\phi_n(r)}_{周期}$.

能量

$$\hat\psi_\sigma(x) = \sum_{n,k} \psi_{nk}(x)\, \hat C_{n,k,\sigma}$$

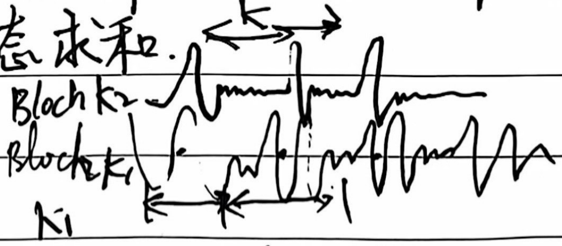
$$C_{nk\sigma} = \int dV_x\, \psi^*_{nk}(x)\, \hat\psi_\sigma(x)$$

，即：

$$\hat H = \sum_{n,k,\sigma} \varepsilon_{nk} C^\dagger_{nk\sigma} C_{nk\sigma} + \frac{1}{2}\sum_{n_1n_2n_3n_4}\sum_{k_1k_2k_3k_4}\sum_{\sigma\sigma'} V_{1234}\, C^\dagger_{n_1k_1\sigma} C^\dagger_{n_2k_2\sigma'} C_{n_3k_3\sigma'} C_{n_4k_4\sigma}$$

$$V_{1234} = \int dV_x\, dV_y\, V(x-y)\, \psi^*_{n_1k_1}(x)\, \psi^*_{n_2k_2}(y)\, \psi_{n_3k_3}(y)\, \psi_{n_4k_4}(x)$$

Free electron Gas 电子间 coloumb 势正好配合算符 e^{ikx} 决定了q的存在，此 $\psi_{nk}(x)$ 既对能带求和，又对动量态求和。

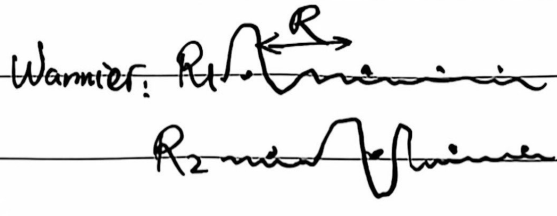


Wannier 波函数

我们看到Bloch在格点处高，余下稀疏特点，呈明显周期状。

Wannier 转至R空间一个 Fourier.

$$Wannier_{Rn}(x) = \frac{1}{\sqrt{N}}\sum_{k} e^{-ik\cdot R}\, Bloch_{kn}(x)$$



相当于Wannier处于k空间的"频域"上，对不同Bloch对应的k，有Wannier对应的R可以局域在某个R（频率ω）上，相当于Wannier局域在某个格点处，性质良好。

那么场算子 $\hat{\phi}_\delta(x) = \sum_{nk} \cancel{e^{ikr}\phi_n(r)}\ \mathrm{Bloch}_{nk}(r)\, C_{nk\delta}$

$$\mathrm{Bloch}_{nk}(r) = \sum_{nR} \frac{1}{\sqrt{N}} e^{ikR}\ \mathrm{Wannier}_{nR}(r)$$

$C_{nk\delta} = \sum_R \langle k|R\rangle C_{nR\delta} = \cancel{\sum_{nR}} \frac{1}{\sqrt{N}} = \sum_R e^{ikR} C_{nR\delta}$

$\Rightarrow \mathrm{Wannier}_{nR}(r-R) = \frac{1}{\sqrt{N}} \sum_k \mathrm{Bloch}_{kn}(r-R)\cdot e^{-ikR} = e^{ik(r-R)} u_n(r-R) e^{-ikR}$, $u_n(r-R) = u_n(r)$

$\Rightarrow \sum_R e^{ik(R-r)} u_n(r) \frac{1}{\sqrt{N}} \sum_k C_{nR\delta} = \sum_R e^{ik(r-R)} u_n(r-R)\, C_{nR\delta}$

$\therefore \hat{\phi}_\delta(x) = \sum_{nR} \mathrm{Wannier}_{nR}(r-R_i)\, C_{ni\delta}$ → 不同格点处产生一个.

Wannier 满足: ϕ_R 标准正交基. ✓

Fourier 分解

① $\lim_{V\to\infty} \frac{1}{V} \sum g(k) = \int_R \frac{d^d k}{(2\pi)^d} g(k)$.

② $\frac{1}{V} \int d^d x\, e^{i(k'-k)x} = \delta_{k'k}$ ↙ $\langle r|k\rangle$

③ $\psi^\dagger(r) = \frac{1}{\sqrt{V}} \sum_k \underset{\langle r|k\rangle^*}{e^{-ikr}} a_k^\dagger \quad \psi(r) = \frac{1}{\sqrt{V}} \sum_k e^{ikr} a_k$

④ 周期函数可作离散展开. $g(x) = \frac{1}{2T} \sum_k e^{ik_n x} G_k$

NOTES

把 Hamiltonian 代入 Wannier 部分：

$$\hat{H}_0=\sum_\sigma\int d^dx\ \psi_\sigma^+(x)\left[\frac{-\nabla^2}{2m}+u(x)\right]\psi_\sigma(x)$$

$$=\sum_{nR\sigma}\int d^dx\ W_{in}^*(r-R_i)\,C_{ni\sigma}^+\left(-\frac{\nabla^2}{2m}+u(x)\right)W_{jm}(r-R_j)\,C_{mj\sigma}$$

Wannier 有正交性 n=m 能是

$$=\sum_{nR\sigma}\left[-t_{jm}+\delta_{jm}\varepsilon_j\right]C_{j\sigma}^+C_{m\sigma}$$

其中 $t_{jm}=\int d^dx\ W^*(x-R_j)\left[\frac{-\nabla^2}{2m}+u(x)\right]W(x-R_m)\quad j\neq m$ 跃迁积分

$\varepsilon_j=\int d^dx\ W(x-R_j)\left[-\frac{\nabla^2}{2m}+u(x)\right]W(x-R_j)\quad j=m$

而 $\sum_j\varepsilon_j C_{j\sigma}^+C_{j\sigma}$ $(j\neq m)$ 纯粹自能格点处处相等. 先略.

故 $\hat{H}_0=-\sum_{jm}t_{jm}C_{m\sigma}^+C_{j\sigma}$ 描述不同格点电子跳跃

~~相互作用部分~~：　N: 4×4　一般电子仅在最近邻跳跃

对应矩阵：$\langle i|\hat{H}_0|j\rangle=\underset{\delta_{\text{正}}}{}(j\neq m)$ 对称性处处相等

为：$\begin{pmatrix}0&-t&0&0\\-t&0&-t&0\\0&-t&0&-t\\0&0&-t&0\end{pmatrix}:(H_0)$

此矩阵可对角化：ξ_n

$$\begin{pmatrix}0&-t&0&0\\-t&0&-t&0\\0&-t&0&-t\\0&0&-t&0\end{pmatrix}\underbrace{\begin{pmatrix}-0.3717&-0.6015&-0.6015&-0.3717\\-0.6015&-0.3717&0.3717&0.6015\\-0.6015&0.3717&0.3717&-0.6015\\-0.3717&0.6015&-0.6015&0.3717\end{pmatrix}}_{A}=\underbrace{\begin{pmatrix}-1.618&0&0&0\\0&0.618&0&0\\0&0&0.618&0\\0&0&0&1.618\end{pmatrix}}_{B}t$$

记本征态 $|n\rangle$ 为 $|1\rangle\quad|2\rangle\quad|3\rangle\quad|4\rangle$　　$C_n=|0\rangle\langle n|$

$|j\rangle:\begin{pmatrix}1\\0\\0\\0\end{pmatrix}\begin{pmatrix}0\\1\\0\\0\end{pmatrix}\begin{pmatrix}0\\0\\1\\0\end{pmatrix}\begin{pmatrix}0\\0\\0\\1\end{pmatrix}$

可以构造新的算符 $C_{nj}=\sum_j\underset{A_{nj}}{\langle n|j\rangle}C_n$

St：$\hat{H}_0=\sum_{\substack{jn\\ j'm}}A_{nj}A_{jn'}\,{-t_{jm}}\,C_{n'}^+C_n=\boxed{\sum_{n\sigma}B(n,n)\,C_{n\sigma}^+C_{n\sigma}}$

$n'=n$ 否则正交基为0　　$C_1^+C_1$

在新的基 $|n\rangle$. $C_n \equiv |0\rangle\langle n|$ 下. $\hat{H}_0$ 对角化.

V_{jljL}?

相互作用部分:

$$\hat{H}_{int} = \sum_{jklm\sigma\sigma'} V_{jklm} \frac{1}{2} C^+_{j\sigma} C^+_{k\sigma'} C_{l\sigma'} C_{m\sigma}$$

$$V_{jklm} = \int d^d(x,y)\, W^*(x-R_j)\, W^*(y-R_k)\, W(y-R_l)\, W(x-R_m)\, V(x-y)$$

$C^+_{j\uparrow} C^+_{j\downarrow} C_{j\downarrow} C_{j\uparrow}$ $\times(-1)\times(-1)=1$

比如① V_{jjjj} 代表 j 格点处两电子相互排斥的作用 $U(\hat{n}_{j\uparrow}\hat{n}_{j\downarrow})$ 同格点只能作1对.

② V_{jjLL} 代表 L 格点处两电子因相互作用跃迁至 j 格点处，多现于格点处有2电子时.

$U_p\, C^+_{j\uparrow} C^+_{j\downarrow} C_{L\downarrow} C_{L\uparrow}$ 跃迁

③ $V_{jLjL} \Rightarrow \sum_{\sigma\sigma'} V_{jLjL}\, C^+_{j\sigma} C^+_{k\sigma'} C_{L\sigma'} C_{m\sigma}$

$$= V_{jLjL}\Big[\underbrace{C^+_{j\uparrow} C^+_{L\uparrow} C_{j\uparrow} C_{L\uparrow} + C^+_{j\downarrow} C^+_{L\downarrow} C_{j\downarrow} C_{L\downarrow}}_{\hat{n}_j \hat{n}_L \text{ 排斥}} + C^+_{j\downarrow} C^+_{L\uparrow} C_{j\uparrow} C_{L\downarrow} + C^+_{j\uparrow} C^+_{L\downarrow} C_{j\downarrow} C_{L\uparrow}\Big]$$

定义自旋算符 $S = \frac{\hbar}{2} I$ $I =$ Pauli $(\sigma_x, \sigma_y, \sigma_z)$

二次量子化: $\hat{S} = \sum_{uu'\sigma\sigma'} \langle u'\langle\sigma|s|\sigma'\rangle u\rangle C^+_{u\sigma} C_{u\sigma'}$ 只对自己.

$$\Rightarrow \hat{S} = (\hat{S}^x, \hat{S}^y, \hat{S}^z) = \frac{\hbar}{2}\sum_u\Big([C^+_{u\downarrow} C_{u\uparrow} + C^+_{u\uparrow} C_{u\downarrow}],\ i[C^+_{u\downarrow} C_{u\uparrow} - C^+_{u\uparrow} C_{u\downarrow}],\ [C^+_{u\uparrow} C_{u\uparrow} - C^+_{u\downarrow} C_{u\downarrow}]\Big)$$

上式第二项可化作

$$V_{jLjL}\cdot 2\cdot \hat{S}^L\cdot \hat{S}^j$$

另外: $C^+_\uparrow C_\uparrow$ 相当于 $(\frac{\hbar}{2})$ $\hbar=1$ $\times(\frac{\hbar}{2}) = \frac{1}{4}$.

∴ ③项为 $[2\hat{S}^L\cdot\hat{S}^j + \frac{1}{4}\hat{n}_j\hat{n}_L]\, V_{jLjL} \times(-1)$

费米子交换了一次.

所有写出来. 总 Hamiltonian 不会再有其它了.

$= \hat{H}_0 + H_① + H_② + H_③$ 电子最多2格点. 分别之和

$$\hat{H}_{EH} = -\sum_{jm\sigma} t_{jm} c_{j\sigma}^{+} c_{m\sigma} + U\sum_{j} \hat{n}_{j\uparrow}\hat{n}_{j\downarrow} + \sum_{j} \frac{U}{2} c_{j\uparrow}^{+} c_{j\downarrow}^{+} c_{L\uparrow} c_{L\downarrow}$$

$$- V_{jLjL}\left[2\hat{S}^{L}\cdot\hat{S}^{j} + \frac{1}{4}\hat{n}_j\hat{n}_L \right]$$

当仅考虑最近邻跃迁，且仅自身格点处存在相互作用（jiii）时。得到了 Hubbard 的 Hamiltonian.

$$\boxed{\hat{H}_{Hubbard} = -t\sum_{\langle jm\rangle\sigma} c_{j\sigma}^{+} c_{m\sigma} + U\sum_{j} \hat{n}_{j\uparrow}\hat{n}_{j\downarrow}}$$

t: t_{jm}. 由对称性晶格内皆同 $=t$

U: V_{jjjj} 皆同 $=U$ $\quad \int |\omega^2(x-R_i)||\omega^2(y)||V(x-y)| d^3x d$

$R_i=0$

toy-model. 2格点系统.

$$\hat{H} = -t\sum_{\sigma} c_{1\sigma}^{+} c_{2\sigma} + c_{2\sigma}^{+} c_{1\sigma} + U(\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} + \hat{n}_{2\uparrow}\hat{n}_{2\downarrow})$$

total electron number $\hat{N} = \sum_\sigma \hat{n}_{1\sigma} + \hat{n}_{2\sigma}$ 对于 2-D. $[H, N]=0$.

总粒子必守恒. $|i,j\rangle$ 态 $\rightsquigarrow$ $|i+1, j-1\rangle$ N const

$|i,0\rangle$ 态 $\rightsquigarrow$ $0 + |i-1, 1\rangle$ N const.

用电子数 0~4 来表示系统. 比如 $N=2$ 时: 态 $|\uparrow\uparrow\rangle|\downarrow\downarrow\rangle|\uparrow\downarrow\rangle|\downarrow\uparrow\rangle|, \uparrow\downarrow\rangle$

6-D Hibert space $\langle S\rangle=1$ 除去因为 $\langle S\rangle = 1$ $\quad\langle S\rangle =$

$|\uparrow\uparrow\rangle$ 与 $|\downarrow\downarrow\rangle$ 对应三态 $E=0$, 系.

$\hat{S}_z = \frac{1}{2}\sum_j [c_{j\uparrow}^{+} c_{j\uparrow} - c_{j\downarrow}^{+} c_{j\downarrow}]$ (见上页). $\hat{S}_z|\uparrow\uparrow\rangle = 1 = -\hat{S}_z|\downarrow\downarrow\rangle$

$\hat{H} = -t\sum_\sigma c_{1\sigma}^{+} c_{2\sigma} + c_{2\sigma}^{+} c_{1\sigma}$ $\quad \hat{H}|\uparrow\uparrow\rangle = 0$

同理 之前电子 $|\uparrow\uparrow\rangle$ 态 ~~E = ...~~ $E=0$.

余下 4-D $|\phi\rangle = \begin{pmatrix} |\downarrow\uparrow\rangle \\ |\uparrow\downarrow\rangle \\ |, \uparrow\downarrow\rangle \\ |, \downarrow\uparrow\rangle \end{pmatrix}$

比如：$\langle\downarrow\uparrow|\hat{H}|,\uparrow\downarrow\rangle = \langle\downarrow\uparrow|\hat{N}|;\uparrow\downarrow\rangle$

方1：$+(-t)\times\langle\downarrow\uparrow|\,c_{1\uparrow}^\dagger c_{2\uparrow}+c_{2\uparrow}^\dagger c_{1\uparrow}+c_{1\downarrow}^\dagger c_{2\downarrow}+c_{2\downarrow}^\dagger c_{1\downarrow}\,|,\uparrow\downarrow\rangle$

$=\langle\downarrow\uparrow|\uparrow,\downarrow\rangle + 0 + \langle\downarrow\uparrow|\downarrow\uparrow\rangle + 0$

方2：$|0,\uparrow\downarrow\rangle = c_{2\uparrow}^\dagger c_{2\downarrow}^\dagger|0\rangle \Rightarrow \langle\downarrow\uparrow|\,c_{1\uparrow}^\dagger c_{2\uparrow}+c_{2\uparrow}^\dagger c_{1\uparrow}\; c_{2\uparrow}^\dagger c_{2\downarrow}^\dagger|0\rangle = -t$

$c_{1\uparrow}^\dagger c_{2\uparrow} c_{2\uparrow}^\dagger c_{2\downarrow}^\dagger$

$\therefore H = \begin{pmatrix} 0 & 0 & -t & -t \\ 0 & 0 & -t & -t \\ -t & -t & U & 0 \\ -t & -t & 0 & U \end{pmatrix}$ eigenvalue: eigenstate.

0. $\frac{1}{\sqrt{2}}(|\downarrow\uparrow\rangle+|\uparrow\downarrow\rangle)$ 符合知识 1

U. $\frac{1}{\sqrt{2}}(|d0\rangle-|0d\rangle)$ 高能双占据

$\frac{1}{2}\left(U\pm\sqrt{U^2+16t^2}\right)$ $|\psi\rangle = \frac{4t}{\sqrt{U^2+16t^2}-U}|\uparrow\downarrow\rangle + \frac{-4t}{\sqrt{U^2+16t^2}-U}|\downarrow\uparrow\rangle + |0d\rangle + |d0\rangle$

(利用 $-1/U$)

强耦合极限 $U\gg t$ 下： $E_3 = U+\frac{4t^2}{U}$ $\frac{1}{\sqrt{2}}\left(\cancel{|\downarrow\uparrow\rangle-|\uparrow\downarrow\rangle}\; \cancel{|0d\rangle}+|d0\rangle\right)$ $(|0d\rangle+|d\ldots$

$E_4 = -4t^2/U$ $\frac{1}{\sqrt{2}}(|\downarrow\uparrow\rangle-|\downarrow\uparrow\rangle)$

那么单占据态：$|\uparrow\uparrow\rangle$ $|\downarrow\downarrow\rangle$ $|\uparrow\downarrow\rangle+|\downarrow\uparrow\rangle$ $|\uparrow\downarrow\rangle-|\downarrow\uparrow\rangle$ 明朗了.

对有效自旋 $\langle S\rangle=\frac{1}{2}$ 的 $S_1\cdot S_2 = 3/4$ $-1/4$

$H_{effiecent} = J(\hat{S}_1\cdot\hat{S}_2-\frac{1}{4})$ $J = \frac{4t^2}{U}$ 对应E自旋为：0.0.0. $-\frac{4t^2}{U}$

半填满模型(N=2)低能4态对应 Hefficient 就是 Heisenberg 铁磁模型

H_2分子基态对应

也可用微扰论 $U\gg t$ 解本题

HF 用 $(\langle n_{i\uparrow}\rangle n_{i\downarrow} + n_{i\uparrow}\langle n_{i\downarrow}\rangle - \langle n_{i\uparrow}\rangle\langle n_{i\downarrow}\rangle)$ 替代U项

其中 $\langle n_{i\uparrow}\rangle = n+(-1)^i m$ 表磁性

$\langle n_{i\downarrow}\rangle = n-(-1)^i m$

DATE Chapter. 3. 格点间少跃迁. 单占 NOTES

⑩ t-J 模型. 近藤模型. 据态磁性掺杂.

Anderson model. 在格点系统中掺入一磁性杂质, Hamiltonian 此杂质的怎么写? 单能级量子点的 Hamiltonian 为: 设杂质为 d

$$H_D = \sum_\sigma \varepsilon_{d\sigma} c_{d\sigma}^\dagger c_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow}$$ 自能 + 相互作用自能 + 跃迁

Anderson: $+ \underbrace{\sum_{k,\sigma} t_k c_{d\sigma}^\dagger c_{k\sigma} + t_k^* c_{k\sigma}^\dagger c_{d\sigma}}_{H_T}$ 就是搞出了 d-项.

现在好奇的是单占据态情况, 也就是 $E_{单据} \ll E_{双据}, E_0$ 据态.

$E_1 = \varepsilon_{d\sigma} \ll (E_0 = 0.\quad E_2 = U + \underbrace{\varepsilon_{d\uparrow} + \varepsilon_{d\downarrow}}_{U+2\varepsilon})$

Schrieffer Wolff 变换矩阵 (漫长)

如果 H 可以 st. <单|H|单> = const 而: 双, 无

<双|H|双> ~→ 0 那么 H 易解此情形

就要找到 S, st. $H_S = e^{iS} H e^{-iS}$ H_S 满足上面要求 绘景变换.

$e^{iS} [H_D + H_T + H_{other\ particles}] e^{-iS}$

△ 要求 H_S 中 H_T 消失. 毕竟 $\langle \underset{k号}{\overset{(\sigma\uparrow\downarrow)}{1}}\ \underset{d}{\overset{(\sigma\uparrow\downarrow)}{1}} | t_k c_{d\sigma}^\dagger c_{k\sigma} | \underset{k号}{0}\ \underset{d}{2} \rangle$

$\Rightarrow \langle \uparrow\downarrow, \uparrow\downarrow | \ldots | \ldots \rangle = \begin{matrix} 2 & 0 \\ & 1 \end{matrix}$.

会存在 11 ~→ 0.2 的概率. 此项必要消失

$\Rightarrow e^{iS}[H_D + H_T + H_{other}] e^{-iS} = H_D + H_T + H_{other} + i[S, H_D + H_{other}] + i[S, H_T]$

要使之 $= H_D + H_{other} + O(t_k^2) = H_S$

$\Rightarrow i[S, H_D + H_{other}] = -H_T$

S 必然也是 $f(t_k)$ 的矩阵, 故 $[S, H_T]$ 就是 $O(t_k^2)$ 项.

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$$i[S, H_D + H_{LR}] = -H_T \qquad S = S^- + (S^-)^\dagger$$

$$\Rightarrow \sum_\sigma t_K c_{d\sigma}^\dagger c_{K\sigma} = \Big[S^-, \underbrace{\varepsilon_d}\, c_{d\sigma}^\dagger c_{d\sigma} + U \hat{n}_{d\uparrow}\hat{n}_{d\downarrow} + \sum_\beta \varepsilon_\beta n_\beta\Big] i \qquad \hat{H}_D$$

~~逐项分析~~ : $(\cdots)_{ij}$

$$S^- = \sum_{\alpha = L,R} \sum_{\gamma_\alpha \sigma} \Big[\frac{t_\alpha}{\varepsilon_{\gamma_\alpha} - E_2 + E_1} n_{d\sigma} c_{\gamma_\alpha\sigma}^\dagger c_{d\sigma} + \frac{t_\alpha}{\varepsilon_{\gamma_\alpha} + E_0 - E_1} (1 - \hat{n}_{d\bar\sigma}) c_{\gamma_\alpha\sigma}^\dagger c_{d\sigma} \Big]$$

比如: 验证 方1

$[S^-, H_D + H_{LR}] \Rightarrow$ 易(不证) $[S, H] = iH_T$.

故 $H_S \approx \underbrace{H_D + H_{LR}}_{H_S^{(0)}} + \underbrace{\frac{i}{2}[S, H_T]}_{H_S^{(2)}}$ $O(t_\alpha^2)$ 二阶项

$$H_S^{(2)} = \frac{i}{2}\Big([S^-, H_T^+] + [S^+, H_T^-] + [S^-, H_T^-] + [S^+, H_T^+]\Big)$$

H_D, H_{LR}

自旋(杂质 + 电子)跃迁

$c_d^\dagger c_K\, c_d \qquad c_K^\dagger c_d$

$\hat{n}_{d\downarrow}\ \hat{n}_{d\uparrow}$

$[S, H_T]$ Part 1:

$$\begin{cases} H_T^- = \sum t_\alpha c_{\alpha\sigma}^\dagger c_{d\sigma} & H_T^+ = \sum t_\alpha^* c_d^\dagger c_\alpha \\ S^- = A \cdot n_{d\sigma} c_{\alpha\sigma}^\dagger c_{d\sigma} + B(1 - \hat{n}_{d\bar\sigma}) c_{\alpha\sigma}^\dagger c_{d\sigma} \end{cases}$$

$\Rightarrow S^- H_T^- \Rightarrow c_{d\sigma} c_{d\sigma} \qquad S^+ H_T^+ \Rightarrow c_{d\sigma}^\dagger c_{d\sigma}^\dagger$

有: $(c_{d\uparrow} c_{d\uparrow})|\psi\rangle = 0$ 仅留下: $c_{d\uparrow} c_{d\downarrow}$ 与 $c_{d\uparrow}^\dagger c_{d\downarrow}^\dagger$ 项.

此二项表示从双占据态至空态跃迁, 与 Kondo 不符

Part 2.

☆计算: $[S^-, H_T^+]$

$$= \Big[\sum_{\alpha\sigma} \frac{t_\alpha}{\varepsilon_\alpha - E_2 + E_1} \hat{n}_{d\bar\sigma} c_{\alpha\sigma}^\dagger c_{d\sigma} + \frac{t_\alpha}{\varepsilon_\alpha + E_0 - E_1} (1 - \hat{n}_{d\bar\sigma}) c_{\alpha\sigma}^\dagger c_{d\sigma}\Big],$$

$$\sum_{\beta,\sigma} t_\beta^* c_{\beta\sigma}^\dagger c_{d\sigma} \Big]$$

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$$= \sum_{\alpha\beta\sigma} \frac{t_\alpha t_\beta^*}{\varepsilon_\alpha - E_2 + E_1} \left[n_{d\sigma} C_{\alpha\sigma}^+ C_{d\sigma},\ C_{d\sigma}^+ C_{\beta\sigma} \right]$$

$$+ \frac{t_\alpha t_\beta^*}{\varepsilon_\alpha + E_0 - E_1} \left[(1 - \hat{n}_{d\sigma}) C_\alpha^+ C_d,\ C_{d\sigma}^+ C_{\beta\sigma} \right]$$

$$= \sum_{\alpha\beta\sigma} A \cdot n_{d\sigma} \cdot \left\{ C_{\alpha\sigma}^+ [1 - \hat{n}_{d\sigma}] C_{\beta\sigma} - \hat{n}_{d\sigma} C_{\beta\sigma} C_{\alpha\sigma}^+ \right\}$$

$$+ B \cdot [1 - \hat{n}_{d\sigma}] \cdot \left\{ C_{\alpha\sigma}^+ [1 - \hat{n}_{d\sigma}] C_{\beta\sigma} = \hat{n}_{d\sigma} C_{\beta\sigma} C_{\alpha\sigma}^+ \right\}$$

= 性质：$[n_\alpha\ a_\alpha] = -a_\alpha \quad [a_\alpha^+ a_\beta\ \ a_\gamma^+ a_\theta] = a_\alpha^+ a_\theta \delta_{\alpha\theta}$

$[n_\alpha, a_\alpha^+] = a_\alpha^+$ 单占据 $\sum_\sigma n_{\sigma d} = 1 \quad a_\gamma^+ a_\beta \delta_{\gamma\beta}$

Therefore:

$$[S^-, H_T^+] = -i \sum_{\alpha\beta\sigma} \left(\frac{t_\alpha t_\beta^*}{\varepsilon_\alpha - E_2 + E_1} - \frac{t_\alpha t_\beta^*}{\varepsilon_\alpha + E_0 - E_1} \right) \times n_{d\sigma} C_{\alpha\sigma}^+ C_{\beta\sigma} - C_{d\bar\sigma}^+ C_{d\sigma} C_{\alpha\sigma}^+ C$$

$(\bar\sigma = -\sigma)$.

$$-i \sum_{\alpha\beta\sigma} \frac{t_\alpha t_\beta^*}{\varepsilon_\alpha + E_0 - E_1} C_{\alpha\sigma}^+ C_{\beta\sigma}$$

$\varepsilon_\alpha, \varepsilon_\beta \to 0$ 改写上式 当 $T \to 0$．电子自能区小，$<< E_2 - E_1$ 之于杂质．则．

$$[S^-, H_T^+] = \frac{i}{2} \sum_{\alpha\beta\sigma} \left(\frac{t_\alpha t_\beta^*}{E_2 - E_1} - \frac{t_\alpha t_\beta^*}{E_1 - E_0} \right) \times \left[(n_{d\bar\sigma} - n_{d\sigma}) C_{\alpha\sigma}^+ C_{\beta\sigma} - 2 C_{d\bar\sigma}^+ C_{d\sigma} C_{\alpha\sigma}^+ C_{\beta\bar\sigma} \right]$$

$$+ \frac{i}{2} \sum_{\alpha\beta\sigma} \left(\frac{t_\alpha t_\beta^*}{E_2 - E_1} - \frac{t_\alpha t_\beta^*}{E_1 - E_0} \right) \times C_{\alpha\sigma}^+ C_{\beta\sigma}$$

观察 Part 1.2．一部分表示 β位 −1．α位 +1．另一部分表示 β(−1)↓至 d(+1)↓，d(−1)↓至 α位的跃迁．系电子类似经"d"位自β向α的过程发生自旋反转．通过使杂质处自旋反转来实现

我们定义 $\hat{S}$（上文提及）$= \sum_{uu'\sigma\sigma'} \langle u\sigma | \frac{\hbar}{2}(\sigma_x, \sigma_y, \sigma_z) | u'\sigma' \rangle C_{u'\sigma'}^+ C_{u\sigma}$

$$\therefore \hat{S}_d \cdot \hat{S}_{\alpha\beta} = \sum_{x,y,z} \sum_{\sigma\sigma'\sigma_1\sigma_1'} (C_{d\sigma}^+ C_{d\sigma'} I_{\sigma\sigma'}^i) (C_{\alpha\sigma}^+ C_{\beta\sigma'} I_{\sigma\sigma'}^i)$$

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$$\varepsilon_d = E_1 - E_0$$

定义：$J_{\alpha\beta} = 2\left(\frac{t_\alpha t_\beta^*}{E_2-E_1} + \frac{t_\alpha t_\beta^*}{E_0-E_1}\right) = \frac{2U t_\alpha t_\beta^*}{(\varepsilon_d+U)(-\varepsilon_d)}$

$$W_{\alpha\beta} = -\frac{1}{2}\left(\frac{t_\alpha t_\beta^*}{E_2-E_1} + \frac{t_\alpha t_\beta^*}{E_1-E_0}\right) = \frac{(2\varepsilon_d+U)\,t_\alpha t_\beta^*}{2(\varepsilon_d+U)(-\varepsilon_d)}$$

$$[S^-, H_T^+] = -i\sum_{\alpha\beta} J_{\alpha\beta} S_d \cdot S_{\alpha\beta} - i\sum_{\alpha\beta\sigma} W_{\alpha\beta}\, C_{\alpha\sigma}^+ C_{\beta\sigma}$$

$S_d \cdot S_{\alpha\beta}$ 形式即 $\alpha \to d \to \beta$ 的自旋翻转。此项 $J_{\alpha\beta}$ 对应能量称交换散射能量，$C_\alpha^+ C_\beta$ 形式系单粒子受 $W_{\alpha\beta}(t_\alpha)$ 作用，受杂质的直接散射 $\alpha \to \beta$。称 $W_{\alpha\beta}$ 势能散射能量.

定义：$x = 1 + {}^{2\varepsilon_d}/_{U}$

$x=0$ when：$E_2-E_1 = E_1-E_0$. 等间距能级.

$x=\pm 1$. when. $E_0=E_1=E_2$ 简并时

$$\therefore J_{\alpha\beta} = \frac{8}{1-x^2}\frac{t_\alpha t_\beta^*}{U} \qquad W_{\alpha\beta} = \frac{2x}{1-x^2}\frac{t_\alpha t_\beta^*}{U}$$

when $x=0$ J极小. $W=0$ 空间 $\alpha \cdot \beta$ 关于 d 对称. 能量相等

$x=\pm 1$ J.W 发散、简并不接收能量 不跃迁. $E_{跃} \to \infty$

再利用：$[S^+, H_T^-] = -[S^-, H_T^+]^\dagger$，得到：

Finally：Kondo Hamiltonian

$$\boxed{\begin{aligned} H_S &= H_S^{(0)} + H_S^{(2)} \\ H_S^{(0)} &= \sum_\sigma \varepsilon_{d\sigma} C_{d\sigma}^+ C_{d\sigma} + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} + \sum_{\beta\sigma}\varepsilon_{\beta\sigma} C_{\beta\sigma}^+ C_{\beta\sigma} \\ H_S^{(2)} &= \sum_{\alpha\beta} J_{\alpha\beta}\,\hat{S}_d \cdot \hat{S}_{\alpha\beta} + \sum_{\alpha\beta\sigma} W_{\alpha\beta}\, C_{\alpha\sigma}^+ C_{\beta\sigma} \end{aligned}}$$

方2: $H|\psi\rangle = E|\psi\rangle$

H对应矩阵!

$$\begin{array}{cccc} & 0 & \text{单占据} & \text{双占据} \\ & \begin{pmatrix} H_{00} & H_{10} & H_{20} \\ H_{01} & H_{11} & H_{21} \\ H_{02} & H_{12} & H_{22} \end{pmatrix} \end{array}$$

若被电子占满要>1 $\hat{n}|\psi\rangle = N|\psi\rangle$, $N=1$

$\tilde{H}_{nm}$ 为投影算符的作用 $\hat{P}_n \hat{H} \hat{P}_m$ $\quad H_{3\times3} = \hat{P}_0 \hat{H} \hat{P}_m$

$\hat{P}_0 = (1-\hat{n}_{d\uparrow})(I-\hat{n}_{d\downarrow})$

$\hat{P}_1 = \hat{n}_{d\uparrow} + \hat{n}_{d\downarrow} - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}$ $\rightarrow n_\uparrow(1-n_\downarrow)+n_\downarrow(1-n_\uparrow)$

$\hat{P}_2 = \hat{n}_{d\uparrow}\hat{n}_{d\downarrow}$

$\psi = P_\psi|\psi\rangle + (1-P_\psi)|\psi\rangle$

① $(1-\hat{n}_d)$ 没有

② n_d 有

$H = H_D + H_T + H_{other}$

PS: 解投影算符 Second Quantization 投影至 $d=0.1.2$ 空间 不影响 R

$|0\rangle\langle 0| + |1\rangle\langle 1| + |2\rangle\langle 2| = I$

$P_0 = |0\rangle\langle 0| = I - |1\rangle\langle 1| - |2\rangle\langle 2|$

$\sum \langle 1|\,|1\rangle\langle 1|\,|1\rangle\, C^+C^-$

$\sum \langle 2|\,|2\rangle\langle 2|\,|2\rangle\, C^+C^+C^-C^-$

$\hat{P}_0 = I - C_\uparrow^+C_\uparrow - C_\downarrow^+C_\downarrow - C_\uparrow^+C_\downarrow^+C_\uparrow C_\downarrow$ $\quad$ exchange $\Leftrightarrow (-1)C_\uparrow^+C_\uparrow C_\downarrow^+C_\downarrow$

$= (I-\hat{n}_\uparrow)(I-\hat{n}_\downarrow)$

$\hat{P}_1 =$ ~~$(n_{d\uparrow} - n_{d\downarrow})(n_{d\uparrow} - n_{d\downarrow})$~~ $\quad P_2 := n_{d\uparrow} n_{d\downarrow}$

$\langle\uparrow|\,|1\rangle\langle 1|\,|\uparrow\rangle C_\uparrow^+C_\uparrow + \langle\uparrow|\,|1\rangle\langle 1|\,|\downarrow\rangle C_\uparrow^+C_\downarrow$

$P_0 . P_1 . P_2$ 满足: $P_0P_2 = P_2P_0 = 0 \quad P_0+P_1+P_2 = 1$

$P_0^2 = P_0$ 投影算符所有性质.

$H_D(\cdot) = \sum_\sigma \varepsilon C^+C^- + U n_\uparrow n_\downarrow = \varepsilon\, n_\uparrow + n_\downarrow + UP_2 = \varepsilon(\hat{P}_1 + 2\hat{P}_2) + UP_2$.

$\therefore \langle P_0|H_D|P_0\rangle = 0 \quad \langle P_1|H_D|P_1\rangle = \varepsilon \quad \langle P_2|H_D|P_2\rangle = 2\varepsilon + U$

$\langle P_0|H_D|P_1\rangle = \forall \langle P_i|H_D|P_j\rangle_{(i\neq j)} = 0$.

$$\therefore (H_D) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \varepsilon\hat{P}_1 & 0 \\ 0 & 0 & (2\varepsilon+U)\hat{P}_2 \end{pmatrix}$$

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② $H_T = \sum_{k,\sigma} t_k c_{d\sigma}^{+} c_{k\sigma} + t_k^{*} c_{k\sigma}^{+} c_{d\sigma}$

$\langle P_1 | H_T | P_0 \rangle = \sum_{k\sigma} \cancel{(1-n_\uparrow)(1-n_\downarrow)} \quad P_1 c_d^{+} P_0 c_k$

$= (1-n_\downarrow) n_\uparrow + (1-n_\uparrow) n_\downarrow \quad c_\uparrow^{+} \quad (1-n_\uparrow)(1-n_\downarrow)$

$\cancel{= c_\uparrow^{+} (1-n_\downarrow)(1-n_\downarrow) + n_\uparrow n_\downarrow)(1-n_\uparrow)(1-n_\downarrow)}$

$= c_\uparrow^{+} (1-n_\uparrow)(1-n_\downarrow) = \cancel{n_\uparrow c_\uparrow^{+} (1-n_\downarrow)} = (c_\uparrow^{+} - c_\uparrow^{+} \underbrace{c_\uparrow^{+}}_{=0} c_\uparrow)(1-n_\downarrow)$

$= c_\uparrow^{+} (1-n_\downarrow)$

$\therefore H_{10}^{T} = \sum_{k\sigma} \cdot V_k \, \hat{d}_\sigma^{+} (1-n_{-\sigma}) c_{k\sigma}$

同理 $H_{21} = \sum_{k\sigma} V_k \, d_\sigma^{+} n_{-\sigma} c_{k\sigma}$

$H_{00}^{T} = \langle P_0 | H^T | P_0 \rangle = H_{11}^{T} = H_{22}^{T} = 0$ 不可能不跃迁.

H_{20} H_{02} 从 k 至 d Max 1 电子 不可能 0→2. (皆 0)

③ $H^0 = EP_n$ ∀矩阵元 $(\langle P_n | H^0 | P_n \rangle = H^0 \langle P_n | P_n \rangle (P_n^2 = P_n) = H^0 P_n$.

综上所述: $\sum_{k\sigma} \varepsilon \, \sigma_k^{+} \sigma_k$

$$\hat{H} = \begin{pmatrix} H^0 \hat{P}_0 & \sum_k V_k \, c_k^{+} d_\sigma \, (1-n_{-\sigma}) c_{k\sigma}^{*} & 0 \\ H_{01}^{*} & (H^0 + \varepsilon_d) \hat{P}_1 & \sum_k V_k \, d_\sigma^{+} n_{-\sigma} c_{k\sigma} \\ 0 & H_{21}^{*} & (H^0 + 2\varepsilon_d + U) \hat{P}_2 \end{pmatrix}$$

$$\hat{H} \begin{pmatrix} \phi_0 \\ \phi_1 \\ \phi_2 \end{pmatrix} = E \begin{pmatrix} \phi_0 \\ \phi_1 \\ \phi_2 \end{pmatrix} \Rightarrow E\phi_0 = H_{00}\phi_0 + H_{01}\phi_1 + \underbrace{H_{02}}_{(0)}\phi_2$$

$(E - H_{00}) \phi_0 = H_{01} \phi_1$

$\phi_0 = (E - \hat{H}_{00})^{-1} H_{01} \phi_1 \qquad \phi_2 = (E - \hat{H}_{22})^{-1} H_{21} | \phi_1 \rangle$

$\cancel{\Rightarrow E\phi_1 = H_{01}\phi_0 + H_{11}\phi_1 + E_{21}\phi_2}$

$(E - H_{11}) \phi_1 = [H_{01} (E - H_{00})^{-1} H_{01}] \phi_1 + [H_{21}^{*} (E - H_{22})^{-1} H_{21}] \phi_1$.

约去 ϕ_1. Therefore: 第二项:

$\cancel{H_{12} (E - H_{22})^{-1} H_{12} =}$

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$$\sum_{kk'\sigma\sigma'} V_k V_{k'} C_{k\sigma}^+ d_\sigma n_{-\sigma} (E-H_{22})^{-1} d^+ C_k n_{-\sigma}$$

$$= \sum_{k'k\sigma\sigma'} V_k V_{k'} C_{k\sigma}^+ d_\sigma n_{-\sigma} (E-\hat{H}_0-2\varepsilon_d-U)^{-1} d_\sigma^+ C_{k\sigma} n_{-\sigma}$$

公式：$[\hat{H}_0, C_{k\sigma}] = -\varepsilon_k C_{k\sigma} \Leftrightarrow \frac{1}{E-H_0} C_{k\sigma} = C_{k\sigma} \frac{1}{\varepsilon_k+E+H_0}$

而：$\Rightarrow H_0 = \sum C_k^+ C_k \cdot \varepsilon$，$[H_0, C_{k\sigma}] = [C_{k\sigma}^+ C_{k\sigma}^- \varepsilon, C_{k\sigma}]$

$= [N\varepsilon, C_k] = -\varepsilon C_k$ 成立！

$$\Rightarrow \sum_{k'k\sigma'\sigma} V_k V_{k'} C_{k\sigma}^+ d_\sigma n_{-\sigma} d_\sigma^+ C_{k\sigma} n_{-\sigma} (E-\hat{H}_0-2\varepsilon_d-U+\varepsilon_k)^{-1}$$

与方1相似 E(单据) $= E^0+\varepsilon_d$ 代入 $\Rightarrow H^0 \approx E^0$

E(双据) $= E^0+2\varepsilon_d+U$ 此中取 $\tilde{E}=E$(单据) 𝑥 E单据最多，$\tilde{E}=E_{average}$ 由E单构成

$E-\hat{H}_0-2\varepsilon_d-U+\varepsilon_k = -(\varepsilon_d+U-\varepsilon_k)^{-1}$ 代入，

同理 $H_{01}(E-H_{00})^{-1}H_{01}$ 项亦可此表。

另外，关于项：$C_{k\sigma}^+ d_\sigma n_{-\sigma} d_{\sigma'}^+ C_{k\sigma'} n_{-\sigma'}$，单占据态 T.

$n_\uparrow + n_\downarrow = 1$　$n_\uparrow n_\downarrow = 0$，则：

$\sum_{kk'\sigma} C_{k\uparrow}^+ d_\uparrow d_\downarrow^+ d_\downarrow d_\uparrow^+ C_{k'\uparrow} d_\downarrow^+ d_\downarrow$　项1：$d_\uparrow(I-d_\uparrow^+ d_\uparrow) d_\uparrow^+ d_\downarrow d_\downarrow$.

$$C_{k\uparrow}^+ C_{k'\uparrow} d_\downarrow^+ d_\downarrow + C_{k\uparrow}^+ C_{k\uparrow} \underbrace{d_\uparrow^+ d_\uparrow d_\downarrow^+ d_\downarrow}_{u_0} + C_{k\uparrow} C_{k'\uparrow} d_\uparrow^+ d_\uparrow$$

$\Rightarrow$ 第三项：$\frac{V_k V_{k'}}{\varepsilon_d+U-\varepsilon_{k'}}$ $\hat{S}^z (C_{k\uparrow}^+ C_k - C_{k\downarrow}^+ C_k) + \hat{S}^+ (C_{k\downarrow}^+ C_{k\uparrow}) + \hat{S}^- (C_{k\uparrow}^+ C_{k\downarrow}) - \frac{1}{2}\sum_k C_{k\sigma}^+$

$\hat{S}^z$ 见 $\frac{1}{2}(d_\uparrow^+ d_\uparrow - d_\downarrow^+ d_\downarrow)$　$\hat{S}^+$: $d_\uparrow^+ d_\uparrow$　$\hat{S}^-$: $d_\downarrow^+ d_\uparrow$

第二项：$\frac{V_k V_{k'}}{\varepsilon_k-\varepsilon_d}$　不变

命：$J_{kk'} = V_k V_{k'} \left(\frac{1}{\varepsilon_d+U-\varepsilon_k} + \frac{1}{\varepsilon_k-\varepsilon_d}\right)$

$$W_{kk'} = V_k V_{k'} \left(-\frac{1}{\varepsilon_d+U-\varepsilon_k} + \frac{1}{\varepsilon_k-\varepsilon_d}\right)$$

DATE · 交换耦合 NOTE

$\therefore E - H_{11} = J_{kk'} [\hat{S}^z (C_{k\uparrow}^+ C_{k'\uparrow} - C_{k\downarrow}^+ C_{k'\downarrow}) + \hat{S}^+ C_{k\uparrow}^+ C_{k\downarrow} + \hat{S}^- C_{k\downarrow}^+ C_{k\uparrow}]$

$\left(\sum_{kk'}\right) + W_{kk'} C_{k\sigma}^+ C_{k'\sigma}$ (势能耦合).

$$\hat{S}^z \cdot S_{kk'}^z + \frac{(\hat{S}^x + i\hat{S}^y)}{2} \frac{S_{kk'}^x + S_{kk'}^y}{2} + \frac{\hat{S}^x - \hat{S}^y}{2} \frac{S^{kk'} - S}{2}$$

$$= \hat{S} \cdot \hat{S}_{kk'}$$

Again, we have Kondo Hamiltonian:

$$\underbrace{E - H_{11} = J_{kk'} \hat{S} \cdot S_{kk'} + W_{kk'} C_{k\sigma}^+ C_{k'\sigma}}$$

$\Rightarrow$ E单占据 = 上式 + H_{11} $\quad H_{11} = (H^0 + \varepsilon_d) P_1 =$ 上文三式

$\Downarrow 1 \quad n_\uparrow + n_\downarrow - 2n_\uparrow n_\downarrow = 1$.

Chapter 2 会后文再议.

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(续) Chapter 2. t-J Model

Interacting electrons and Quantum Magnetism (chapter 3)

Hubbard Hamiltonian:

$$\hat{H} = U\sum_{n_i} n_{i\uparrow} n_{i\downarrow} - \sum_{i,j,s} t_{ij} C_{is}^{+} C_{js}$$

when $U \gg t$ H_T 视微扰，用微扰论重写 $\hat{H}$.

H_U: $|$无双占据态$\rangle = |$基态$\rangle \overset{记}{=} |0\rangle^0$ $E=0$ ($n_{i\uparrow} n_{i\downarrow} |\psi\rangle$ 无双据 $) = 0$

一阶微扰能量: $E_0^{1阶}$ 基态: 用简并(基态大量简并)微扰论.

$$\det \left| \langle 0^0_{\alpha} | H_t | 0^0_{\alpha} \rangle - E_0^1 \right| = 0$$

α 简并

二阶微扰能量: 记 d 为双据态原子数

$$\sum_{d\neq 0,\beta} \frac{\langle 0^0_\alpha | H_t | d^0_\beta \rangle \langle d^0_\beta | H_t | 0^0_\alpha \rangle}{E_0^{(0)} - E_d^{(0)}} = E_0^{(2)}$$

Actually, 这n项即为 $U \gg t$ 之 t-J Model. 我们换一种记法:

单据投影算符: $P_{single} = \prod_i (\hat{I} - n_{i\uparrow} n_{i\downarrow})$ $P_{double} = \hat{I} - \hat{P}_s$

在 (P_s, P_d) 表象下写 H 矩阵，考虑到:

$H_U P_s |\psi\rangle = H_U |$基态$\rangle = 0$, we have:

$$H = \begin{pmatrix} P_s H_T P_s & P_d H_T P_s \\ P_s H_T P_d & P_d (H_U + H_T) P_d \end{pmatrix}$$

$E_0^1 |0\rangle\langle 0| = |0_\alpha\rangle \langle 0_\alpha | H_t | 0_\alpha \rangle \langle 0_\alpha | = P_s H_T P_s$ 二次量子化后

$\therefore H^{(1)} = P_s H_T P_s$

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$E_0^{(2)}$ = 同理 $P_S H_T$ (一堆) $H_T P_S$ ，此中有：

$$\sum_{d\neq 0,\beta} \frac{|d_\beta^0\rangle\langle d_\beta^0|}{E_0^{(0)}-E_d^{(1)}} = P_d \frac{1}{E_0^{(0)}-E_d^{(0)}} P_d$$

近半满时：$E_0^0 - E_d^0 \approx -U$. Therefore: (仅 $d=1$ 非零)

$$H_{eff} = P_S H_T P_S - P_S H_T \frac{P_d P_d}{U} H_T P_S$$

$(P_d P_d = P_d)$

即 $H^{t-J} = P_S [H_T - \frac{1}{U} (H_T P_d)(P_d H_T) P_S]$

$$= P_S (H_T - \frac{1}{U} \sum_{ijkss'} t_{ij} t_{jk} C_{is}^+ C_{js} n_{j\uparrow} n_{j\downarrow} C_{js'}^+ C_{ks'})$$

整理，for: $i=k$，$\hat{S}$ 定义 $\hat{S}_i = \sum_{\sigma\sigma'} C_{i\sigma}^+ I_{\sigma\sigma'} C_{i\sigma'} (\frac{1}{2})$

$$H^{QHM} = \frac{1}{2}\sum_{ij} J_{ij} (\hat{S}_i \cdot \hat{S}_j - \frac{n_i n_j}{4}) \quad J_{ij} = \frac{4t_{ij}^2}{U}$$

且 ~~$\sum_{\sigma\sigma',k_j} \langle\sigma| I^j_{\sigma\sigma'} I^k_{\sigma\sigma'} |\sigma'\rangle$~~ $j,k \in (x,y,z)$, and. $= T_r[I^j I^k] = (\frac{1}{4})$

$$\therefore H^{t-J} = P_S (H_T + H^{QHM} + J') P_S$$

$$J' = -\frac{1}{2U} \sum_{ijk} t_{ij} t_{jk} [\sum_s (C_{is}^+ C_{ks} n_j) - C_i^+ \vec{\sigma} C_k \, C_j \vec{\sigma} C_j]$$

当严格：Half-filling 时：J'，H_T 皆无 $\Rightarrow$ Mott-insulator

ie: Heisenberg Model.

Hubbard Model, Ground State: 变分法:

$$E^{\nu} = \frac{\langle \Psi^{\nu} | H | \Psi^{\nu} \rangle}{\langle \Psi^{\nu} | \Psi^{\nu} \rangle}$$

试探 Ψ: Fock state: $|\Psi\rangle$: $|n_1 \cdots n_m\rangle = \prod_i \frac{(a_i^\dagger)^{n_i}}{\sqrt{n_i!}} |0\rangle$

Fermi system: $|\Psi\rangle = \prod a_{k\sigma}^\dagger |0\rangle$

我们观察K空间中Hubbard Model.

$$H = \sum_{k,s=\uparrow\downarrow} \varepsilon_k C_{ks}^\dagger C_{ks} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

我们再观察: $\langle \Psi^{\nu} | H | \Psi^{\nu} \rangle$ 形式以决定参量的选取:

第一项比如: $\langle C_{i\uparrow}^\dagger C_{i\uparrow} C_{i\downarrow}^\dagger C_{i\downarrow} \rangle \overset{HF}{=} \langle C_{i\uparrow}^\dagger C_{i\uparrow} \rangle \langle C_{i\downarrow}^\dagger C_{i\downarrow} \rangle - \langle C_{i\uparrow}^\dagger C_{i\downarrow} \rangle \langle C_{i\downarrow}^\dagger C$

$$\langle U \sum_i n_{i\uparrow} n_{i\downarrow} \rangle = U \sum_i \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle - \langle S_{i\uparrow}^+ \rangle \langle S_{i\downarrow}^- \rangle$$

其中,在K-space中此项 $V = U \sum C_{k+q,\sigma}^\dagger C_{k'-q,\sigma'}^\dagger C_{k'\sigma'} C_{k\sigma}$

即定义了: $\langle S_i^+ \rangle = \underbrace{\frac{1}{N} \sum_{q'} e^{-iq' x_i}}_{\text{Fourier to Wannier-space}} \sum_k \langle C_{k\uparrow}^\dagger C_{k+q'\downarrow} \rangle$ (密度算符).

其它项类似,我们构造试探Fock态波函数的时候,需要 $|k_1 \cdots$

①每个K中的是否存在粒子,定义 θ_k, $\sin\theta_k = 1$ 代表存在, $=0$ 代表不存在,最小化每个 θ_k 见存在之比率; ②在K空间何处,定义q 代表去, ①+② 即存在否,大小为之参量. ③是否在费米面 Σ_F 内.

即可定义正则变换

$$\alpha_{k+}^\dagger = \cos\theta_k C_{k\uparrow}^\dagger + \sin\theta_k C_{k+q\downarrow}^\dagger \qquad \text{以 } \alpha_{k_1}\alpha_{k_2} \Rightarrow C_{k_1} C_{k_2}$$

$$\alpha_{k-}^\dagger = -\sin\theta_k C_{k\uparrow}^\dagger + \cos\theta_k C_{k+q\downarrow}^\dagger$$

则: $|\Psi\rangle = \prod_{\langle -\rangle} \alpha_{k\sigma}^\dagger |0\rangle$ $\Psi(q, \theta_k, \Sigma_F)$ 参量.

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在这组试探波Fock态下，我们计算第一项：

$$\langle S_i^+\rangle = \frac{1}{N}\sum_{q'} e^{-iq'x_i}\sum_K \langle C_{K\uparrow}^+ C_{K+q'\downarrow}\rangle$$

$$= \frac{1}{N}\sum_{q'} e^{-iq'x_i}\sum_K \sin\theta_{K+q-q'}\cos\theta_K\langle \alpha_{K+}^+\alpha_{K+q-q'+}\rangle$$

$$- \sin\theta_K\cos\theta_{K+q-q'}\langle\alpha_{K-}^+\alpha_{K+q-q'-}\rangle$$

$\Rightarrow \langle\alpha_{K_1}^+\alpha_{K_2}|\Phi\rangle$ 要求 $K_1=K_2$ 才非零，i.e. $q=q'$ 1 or 0 对 $[\xi_F^\pm]$

+与−：两类

$\therefore \langle S_i^+\rangle = m_q e^{-iqx_i}$， $m_q=\frac{1}{2N}\sum_K \sin(2\theta_K)(n_K^+-n_K^-)$ 费米面.

K-space 中波矢 q 代表一相位，示不同处之波矢产生之影响，"在K空间何处—布q" 示之。示xy平面上之自旋方向.

第二项：$\langle n_{i\uparrow}\rangle$ ~~将表示z方向之自旋，也即磁场方向~~，i.e.:

$\Rightarrow NU^{n^2}/4$

$$\langle C_{K\uparrow}^+C_{K+q'\uparrow}\rangle = \cos\theta_K\cos\theta_{K+q'}\langle\alpha_{K+}^+\alpha_{K+q'+}\rangle - \sin\theta_K\cos\theta_{K+q'}\langle\alpha_{K-}^+\alpha_{K+q'+}\rangle$$

(+)(−)不同费米面 $-\cos\theta_K\sin\theta_{K+q'}\langle\alpha_{K+}^+\alpha_{K+q'-}\rangle+\sin\theta_K\sin\theta_{K+q'}\langle\alpha_{K-}^+\alpha_{K+q'-}\rangle$

α_{-+}项必零 且要 $q'=0$，i.e.: $\cancel{\cos 2\theta_K}$ $[\cos^2\theta_K n_{K(+)}+\sin^2\theta_K n_{K(-)}]$

$$=(\cos^2\theta_K-\tfrac{1}{2})n_{K(+)}+\tfrac{1}{2}n_{K(+)}+h.c = -\cos(2\theta_K)(n_K^+-n_K^-)+(\tfrac{1}{2}n_K^+ + \ldots$$

$$\Rightarrow U\sum_i\langle n_{i\uparrow}\rangle\langle n_{i\downarrow}\rangle = \frac{1}{4}Nn^2U - NUm_z^2.$$

$n=\sum_{K\sigma=\pm} n_K^\sigma =$ 此项 $m_z=\frac{1}{2N}\sum_K(\cos2\theta_K)(n_K^+-n_K^-)$

故

$\Rightarrow V = \langle U \sum_i n_{i\uparrow} n_{i\downarrow} \rangle = NU\frac{n^2}{4} - NUm_z^2 - NUm_q^2$

其中: $n = \sum_{k\sigma=\pm} n_k^\sigma = \sum_k n_k^+ + n_k^-$

$m_z = \frac{1}{2N}\sum_k \cos(2\theta_k)(n_k^+ - n_k^-)$

$m_q = \frac{1}{N}\sum_k \sin(2\theta_k)(n_k^+ - n_k^-)$

第三项: $T = \langle \sum_{ks} \varepsilon_k c_{ks}^+ c_{ks} \rangle$

$= \cos^2\theta_k \langle \alpha_{k+}^+ \alpha_{k+} \rangle + \sin^2\theta_k \langle \alpha_{k-}^+ \alpha_{k-} \rangle - \sin\theta_k\cos\theta_k \langle \alpha_{k+}^+ \alpha_{k-} - \alpha_{k-}^+ \cdots$

$+ (\sin\theta_{k-q}\alpha_{k-q+}^+ + \cos\theta_{k-q}\alpha_{k-q-}^+)(\sin\theta_{k-q}\alpha_{k-q+} + \cos\theta_{k-q}\alpha_{k-q-} \cdots$

(+)(-) 不同时出现

$= (\cos^2\theta_k n_k^+ + \sin^2\theta_k n_k^- + \sin^2\theta_{k-q} n_{k-q}^+ + \cos^2\theta_{k-q} n_{k-q-}) \varepsilon_k$

$\Leftrightarrow \varepsilon_{k+q}(\sin^2\theta_k n_k^+ + \cos^2\theta_k n_k^-) + \varepsilon_k(\cos^2\theta_k n_k^+ + \sin^2\theta_k n_k^-)$

$= \sum_{\pm k}\left(\frac{\varepsilon_k + \varepsilon_{k+q}}{2} \pm \frac{\varepsilon_k - \varepsilon_{k+q}}{2}\cos(2\theta_k)\right) n_k^\pm$

综上: $E(q, \theta_k, \Sigma^\pm)$ (上两式相加).

$= \sum_{\pm k} \frac{\varepsilon_k + \varepsilon_{k+q}}{2} \pm \left[\left(\frac{\varepsilon_k - \varepsilon_{k+q}}{2} - m_z\right)\cos(2\theta_k) - U m_q \sin(2\theta_k)\right] n_k^\pm$

$+ NUm_z^2 + NUm_q^2 + NU\frac{n^2}{4}$

可做变分 $(n_K^+, n_K^-, q, \theta_K) \Rightarrow (q, \theta_K, m_q, m_z)$.

$\frac{\partial E}{\partial \theta_K} \Leftrightarrow \frac{\partial E}{\partial \cos(2\theta_K)} = 0 =$ 一堆. 得 θ_K 返代回, 得:

$$E_K^{\pm}(m_z, m_q) = \frac{\varepsilon_K + \varepsilon_{K+q}}{2} \pm \sqrt{\left(\frac{\varepsilon_K - \varepsilon_{K+q}}{2} + Um_z\right)^2 + U^2 m_q^2}$$

$$E_{All} = \underbrace{\sum_{\pm K} E_K^{\pm} n_K^{\pm}}_{E^0} + NUm_z^2 + NUm_q^2 + NUn^2/4 \quad (m_z, m_q).$$

$\frac{\partial E}{\partial m_K} = 0 \quad \frac{\partial E}{\partial m_q} = 0 \Leftrightarrow$ 变分参量 (n_K^+, n_K^-) 之变分,

ie. $\frac{\partial E^0}{\partial m_q} - 2NUm_q = 0$; $\frac{\partial E^0}{\partial m_z} - 2NUm_z = 0$

而比如: $\frac{\partial E^0}{\partial m_z} = \frac{1}{2} \frac{(\ )U + U^2 2m_z}{\sqrt{\ /////}}$ (对K求和).

数学上记它为:

$\frac{dE^0}{dm_z} = 4U^2 m_z \chi(0)$ where $\chi(0) = \frac{1}{2}\sum_K \frac{dn(\varepsilon_K)}{d\varepsilon_K}$ $n(\varepsilon) = (e^{\varepsilon/T}+1)^{-1}$

F-D 分布

则: $\Rightarrow 2U\chi(0) = 1$.

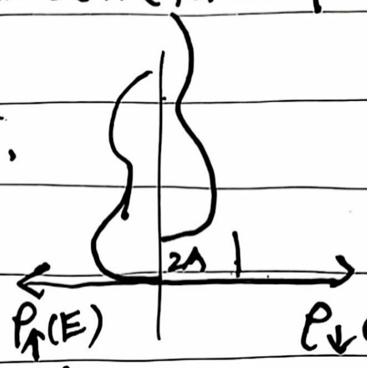
这就是 $q=0$ 情况之.

同理: $\chi(q) = \frac{1}{2}\sum_K \frac{n(\varepsilon_{K+q}) - n(\varepsilon_K)}{\varepsilon_K - \varepsilon_{K+q}}$ $2U\chi(q) = 1$

此二条件称 Stoner's criterion.

再议 Stoner's criterion, 变分法做了什么? $\chi(q)$ 由"双粒子关联函数"一节之结论, 正为极化率之形式。观察到 Stoner 判据实际表征$\boxed{\text{巡游电子在铁磁相变中所应满足之规律}}$, 曾经, 居里温度得出基于局域电子磁矩, 因为磁矩 $M = \frac{\partial}{\partial B} \ln Z \cdot \frac{n}{KT}$ 中: Z 为 $e^{\beta E}$ 而 E 为 $(m_q \mu_B B)$ 此中势能正比 B 之 μ_B 形式, 为整数, 即局域

之磁矩，而以之算 M　$M\to 0$ 得居里温度，现在考虑巡游电子时这(3d,4d)过渡金属体系中 Fe. Co. Ni 观察单粒子平均磁矩实验上非玻尔磁子(μ_B)整数倍。Actually，观察电子能带：d 电子双轨道能级由于此二电子交换作用产生劈裂，$d_\uparrow$ 与 $d_\downarrow$ 能量不同.(↑.本质是"分子场"自发磁化由于铁磁金属中存在交换相互作用在(↑.↓)中，$U\sum n_{i\uparrow}n_{i\downarrow}$，产生能级劈裂，如图：



交换作用大小 $H=\frac{U}{2N\mu_B^2}M$ 在外磁场 h 作用下，

总能带差为：$\delta\mu_B\left(h+\frac{U}{2N\mu_B^2}M\right)$.

现在利用能带论求解相变点满足条件，磁化强度为：

$$M(T)=N\mu_B\left(\langle n_\uparrow\rangle-\langle n_\downarrow\rangle\right)=\mu_B\sum_K\left[f(E_{k\uparrow})-f(E_{k\downarrow})\right]$$

$E_{k\uparrow}$, $E_{k\downarrow}$ 相差即 $\delta\mu_B\left(h+\frac{U}{2N\mu_B^2}M\right)=\Delta E$　f 为 F-D 分布，此式又为：

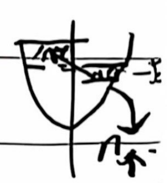
$$\sum_K\frac{f(\uparrow)-f(\uparrow)}{\Delta E}\cdot\Delta E\Rightarrow\sum_K\frac{\partial f}{\partial E}\Delta E=\Delta E\int\frac{\partial f}{\partial E}\underbrace{D(E)}_{\text{态密度}}dE$$，得到：

$\chi=\frac{M}{H}$

$U=0$ 时，为自由电子，$M(T)=\chi_p(T)h$　$\chi_p(T)$ 即极化率、

$M=\frac{1}{2}(\mu_B H$

$$\chi_p(T)=2\mu_B^2\int-\frac{\partial f}{\partial E}D(E)\,dE=\mu_B^2 g(\varepsilon_{F})$$



$=g($

即上文之式：χ_p 为自由电子 Pauli 磁化率 ($U=0$).

$U\neq 0$ 时，为巡游电子：定义 $M(T)=\chi_0(T)h$

称 χ_0 为顺磁静态极化率：

$$\chi_0(T)=\chi_p(T)\times\frac{1}{1-\frac{2U}{N}\frac{\chi_p(T)}{4\mu_B^2}}$$

or　$\chi_0^{-1}(T)=\chi_p^{-1}(T)-2\frac{U}{N}$

讨论T=0K情况，若 $2\frac{U}{N}\chi_p(T)=1$（即上文变分结论），$\chi_0(T)\to\infty$

※注意 χ_0 χ_p 记号与上文是相反的！$\chi_0(T)\to\infty$ 说明出现自发磁化，代表了顺磁至铁磁相变，$2\frac{U}{N}\chi_p(T)>1$ 代表稳定铁磁相。

$T\to0$，由 $\frac{\partial f}{\partial E}=\delta(E-E_F)$ ∴ $\chi_p(T=0)=\rho(E_F)$ 为费米能级处态密度。

即零温下形成铁磁相条件： $U\rho(E_F)>1$

称为 Stoner's criterion $\boxed{\text{零温也会因自发磁化相变！}}$

Ref：[姜寿亭. 凝聚态磁性物理；Kittel. 固体物理]

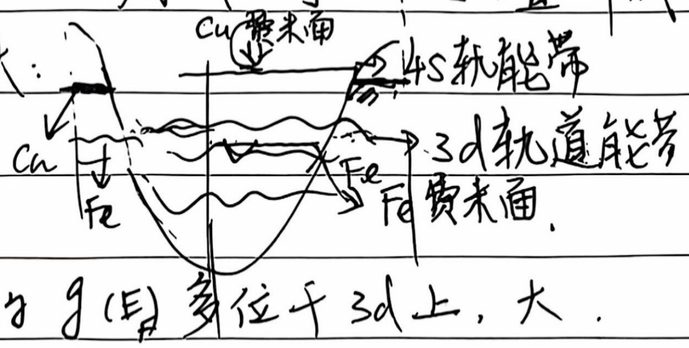
PS： $2\frac{U}{N}\chi=1$ （>1） 即 $1-Ug(E)<0$

即 $\Delta E=E_K:1+E_p:(-Ug(E))<0$

亦由之带来动、势能之和小于零。

对Fe、钴、Ni， U大：3d局域主导，无交叠降低势能。

g(E)大：



Fe的 $g(E)$ 多位于3d上，大。

Heisenberg Model. Ground state.

Heisenberg Antiferromagnetic describes superexchange.

$$\underset{i}{\downarrow}\overset{J}{\curvearrowright}\underset{i+1}{\uparrow} \Rightarrow - \overset{U}{\downarrow\uparrow} \Rightarrow \uparrow \underset{J}{\curvearrowleft} \downarrow$$

$$\hat{H} = J \sum_{\langle mn \rangle} \hat{S}_m \hat{S}_n \qquad \hat{S} = c_{i\sigma}^{+} \sigma_{,i\sigma'}$$

$$J = t^2/U$$

而: $S_i^z \overset{def}{=} c_{i\uparrow}^{+} c_{i\uparrow} - c_{i\downarrow}^{+} c_{i\downarrow} = (n_\uparrow - n_\downarrow)$ Eigenstate $|m_i\rangle$

eg $\uparrow\downarrow$ $1-1=0$ $m_i=0$ ∴ S_i^z 反映磁量子m. S反映S量子:

Eigenvalue: $\hat{S}^2 \Rightarrow S(S+1)$ ∴ 本征态: $|S\, m_1\rangle \otimes |S, m_2\rangle \cdots \otimes |S, m_N\rangle$

接下来. we proof classical antiferromagnet state is the so-called $\boxed{\text{Neel state}}$. 简单来说: 一半正一半负自旋 E_{min}, 精确一些. 达到分子格, 子格内自旋相同, 之间相反可达到反铁磁基

$$S^{stagg} = \sum_{i\in A子格} S_i^z - \sum_{i\in B} S_i^z$$

Maximize S^{stagg}: $\Psi^{neel}: \prod_i |S, \eta_i S|$ $\quad \eta_i = \begin{cases} 1 & i\in A \\ -1 & i\in B \end{cases}$

S^{stagg} 为反 order parameter 反铁下不为零. 这样才可以算.

~~Neel state~~ : $|S, \tilde{m}_i\rangle = \begin{cases} |S, m_i\rangle & i\in A \\ (-1)^{(S+m_i)} |S, m_i\rangle & i\in B \end{cases}$

$\boxed{\text{why } S\ ?}$ $(-1)^S$ 什么意思?

$S\in(0,1) = \{\downarrow, \uparrow\}$ B子格 spin-up 个数偶. B取正.

B子格 spin-up 奇 B取负

$\sum J_{ij} S_i S_j$ [illegible]

这么些 $|\uparrow\downarrow\rangle \otimes |\downarrow\uparrow\rangle \cdots$ 态的线性组合组合基态，i.e.

$$\Psi_0 = \sum_\alpha f_\alpha \Psi_\alpha \quad \Psi = |\uparrow\downarrow\rangle \otimes |\downarrow\uparrow\rangle \cdots$$ 取决于B中 spin-up 个数奇偶（见上页）

有定理：$\boxed{\text{Marshell's Theroem}}$：

$$\forall \alpha.\ f_\alpha > 0$$ （并非 $\Psi = \Psi_1 + \Psi_2 + \cdots +$，$\Psi = \Psi_1 + \Psi_2 - \Psi_3$ 是 $\tilde{\Psi} = \Psi_1 + \Psi_2 + \cdots$ 区别为是否反转 B

when subspace $A = B$ (in size) $\hat{S}_{All}|\Psi\rangle = 0$ （无磁矩）

pf: $\hat{S}_1\cdot\hat{S}_2$ 仅考虑最近邻，${}^{\forall} 1\in A\ 2\in B$. $\hat{H} = H^{zz} + H^{xy}$

$$\tilde{H}^{zz} = \sum_{i\in A\, j\in B} |J_{ij}| S_i^z S_j^z \quad J \to |J| \quad \text{系 } |\rangle \to (-1)^s |\rangle$$

$$\tilde{H}^{zz}|\tilde{\Psi}_\alpha\rangle = e_\alpha |\tilde{\Psi}_\alpha\rangle$$ $\boxed{\text{why ?}}$

注意到：H^{zz} 对角，若 $i_m . j_n$ $m\neq n$. 则无相互作用

命：$\langle\tilde{\Psi}|\tilde{H}^{xy}|\tilde{\Psi}_\beta\rangle = -|K_{\alpha\beta}|$ 核心！

$$\tilde{H}^{xy} = -\frac{1}{2}\sum |J|(S_i^+ S_j^- + S_i^- S_j^+) \quad \therefore \text{跃迁项必负}.$$

Now. 本征方程 $\hat{H}|\tilde{\Psi}\rangle = E|\tilde{\Psi}\rangle$

$$\Rightarrow -\sum_\beta |K_{\alpha\beta}| f_\beta + e_\alpha f_\alpha = E f_\alpha$$

我们运用"正定"思想，既然 $\Psi = \sum f_\alpha |\Psi\rangle$ 为本征态，$\Psi' = \sum |f_\alpha| |\Psi\rangle$ 呢？此态 $E_{\Psi'} = \langle\Psi'|\hat{H}|\Psi'\rangle = \sum e_\alpha |f_\alpha|^2 - \sum_{\alpha\beta} |K_{\alpha\beta}||f_\alpha||f_\beta|$

$$\leq \sum e_\alpha |f_\alpha|^2 - \sum_{\alpha\beta} |K_{\alpha\beta}| f_\alpha f_\beta = E$$

比本征能小，必亦为基态. 此二态本征方程为：

$(e_\alpha - E) f_\alpha = \sum_\beta |K_{\alpha\beta}| f_\beta$ 与 $(e_\alpha - E)|f_\alpha| = \sum_\beta |K_{\alpha\beta}||f_\beta|$

$(e_\alpha - E)|f_\alpha| = \sum_\beta |K_{\alpha\beta}||f_\beta|$ ← 连立！

$$\Rightarrow \left|\sum_\beta |K_{\alpha\beta}| f_\beta\right| = \sum_\beta |K_{\alpha\beta}||f_\beta| \Rightarrow \forall \beta.\ f_\beta \geq 0 \text{ 证毕}$$

我们直接举一个 4-particle Ground state as example

$J_{ij} = A$ $i.j$相邻 1 2 3 4 $H = -J_{ij} S_i \cdot S_j$ $i \in (1234)$ J_{ij}

H_{11} eg: $\langle \uparrow_1 | \hat{S}_1 \cdot \hat{S}_1 | \uparrow_1 \rangle \cdot (-J)$ $\quad I_{\sigma\sigma'}$

$S_i = (S_i^x, S_i^y, S_i^z) \Rightarrow \quad C^+_{i\sigma} \cdot C_{i\sigma'}$

$= \frac{\hbar}{2}[(C^+_{i\uparrow}C_{i\downarrow} + C^+_{i\downarrow}C_{i\uparrow}), i[C^+_{i\downarrow}C_{i\uparrow} - C_{i\uparrow}C_{i\downarrow}], C^+_{i\uparrow}C$

$\hat{S}_1 \cdot \hat{S}_1 \cdot |\uparrow_1\rangle = \hat{S}_1 \cdot \frac{\hbar}{2}[|\downarrow\rangle, i|\downarrow\rangle, |\uparrow\rangle]$

$= \frac{\hbar^2}{4} \cdot [|\uparrow\rangle + i^2|\uparrow\rangle + |\uparrow\rangle] = \frac{3}{4}\hbar^2 |\uparrow\rangle$

其它 J_{ij} 比如 $S_2 \cdot \hat{S}_1 |\uparrow_1\rangle$ $\quad \hat{S}_2 |\uparrow_1\rangle = 0$ 自然为零

$\therefore H_{11} = (-J)\, 3/4\, \hbar^2$

$\therefore H_{22} = H_{33} = H_{44} = (-J)\, 3/4\, \hbar^2$

同理 $H_{13}, H_{24}, \ldots = 0$

而: $H_{12} = \langle \uparrow_2 | \hat{S}_2 \cdot \hat{S}_1 | \uparrow_1 \rangle (-J)$

$= \langle \uparrow_1 \otimes |\downarrow\rangle_2, \uparrow_1 \otimes i|\downarrow\rangle_2, \uparrow_1 \otimes |\uparrow\rangle_2 \,\big|\, |\downarrow\rangle_1 \otimes \uparrow_2, i|\downarrow\rangle_1 \otimes \uparrow_2,$

$\uparrow_1 \otimes \uparrow_2 \rangle \frac{\hbar^2}{4}(-J)) = 0 + 0 + \frac{\hbar^2}{4} \Rightarrow H_{12} = \frac{\hbar^2}{4}$

$\therefore \hat{H} = \frac{1}{4}\hbar^2 \begin{pmatrix} 3 & 1 & 0 & 0 \\ 1 & 3 & 1 & 0 \\ 0 & 1 & 3 & 1 \\ 0 & 0 & 1 & 3 \end{pmatrix}$ 比如 2-D $\begin{pmatrix} 3 & 1 \\ 1 & 3 \end{pmatrix}$ $U^+ H U : U =$

$\therefore \frac{\text{Space1} \oplus \text{Space2}}{\sqrt{2}}$ E 激

$\frac{\text{Space1} \ominus \text{Space2}}{\sqrt{2}}$ E 基

同2粒子"单态"$S=0, m=0$ "三态"$S=1. m=\pm1.0$ 一样.
"单态"如上文即基态. 有最低能量. 非简并。Neel态非基态. 是一种表示反铁磁线性组合的方向. 比如 4格点基态,

$$|\uparrow\uparrow\downarrow\downarrow\rangle + |\uparrow\downarrow\downarrow\uparrow\rangle + |\downarrow\downarrow\uparrow\uparrow\rangle + |\downarrow\uparrow\uparrow\downarrow\rangle$$

A B A B

$$-2|\uparrow\downarrow\uparrow\downarrow\rangle - 2|\downarrow\uparrow\downarrow\uparrow\rangle$$ 有正. 负号之别.

space A. 不变. Space B. 前4项 $(-1)^{m_{B1}} \times (-1)^{m_{B2}} = (-1)^1 \cdot (-1)^0 = -1$

$\to S = S_B$ (2粒子). 后2项 $(-1)^{m_{B1}} \times (-1)^{m_{B2}} = (-1)^1 \cdot (-1)^1 = 1$

$(-1)^S$ $(S=1) = -1$ ∴ space B 正负号定. 定后 $f_\alpha|\tilde{\alpha}\rangle$ 的自然 f_α 就取正数了。真正基态是 Neel state 中 $S=0. m=0$ 的单非简并态.
但 Neel 态也并非唯一基态. 因其仅考虑基元沿z轴 $|\uparrow\rangle. |\downarrow\rangle$. 如 $|\nearrow\rangle$ $|\nwarrow\rangle$ 态也有回旋基态存在. $S_{tot}|\psi_0\rangle = 0$.

Half-Odd Integer Spin Chains.