6. 自由電子ガス・平面波基底

6.1 一電子軌道とk点積分

$$\left\{-\frac{\nabla^2}{2}+\cancel{v(r)}\right\}\varphi_{kj}(r)=\varepsilon_{kj}\varphi_{kj}(r)$$

もしくは定数

$$-\frac{\nabla^2}{2}\varphi_k(r)=\varepsilon_k\varphi_k(r) \Longrightarrow \varphi_k=\frac{e^{ikr}}{\sqrt{V}}\ ,\quad \varepsilon_k=\frac{k^2}{2}$$

$V \to N_{uc}V_{uc}$

$$u_k=\frac{1}{\sqrt{V_{uc}}}\ :\ 定数$$

$$\sum_k^{N_{uc}}\cdots \Rightarrow \int_{BZ}d^3k\,\frac{N_{uc}}{V_{BZ}}\cdots=\frac{V}{(2\pi)^3}\int_{BZ}d^3k\cdots$$

$$V_{BZ}=\|(b_1,b_2,b_3)\|=(2\pi)^3\|(a_1,a_2,a_3)^{t^{-1}}\|=\frac{(2\pi)^3}{V_{uc}}$$

自由電子系では、$V_{uc}\to 0$、$V_{BZ}\to\infty$ なので

$$\sum_k\cdots \longrightarrow \frac{V}{(2\pi)^3}\int_0^\infty dk\,k^2\int_0^\pi d\theta\sin\theta\int_0^{2\pi}d\phi\cdots$$

6.2 物理量とDOS

・エネルギー(単位体積あたり)

$$\frac{E}{V}=\frac{1}{(2\pi)^3}\int_0^\infty dk\,k^2\int_0^\pi d\theta\sin\theta\int_0^{2\pi}d\phi\,\frac{k^2}{2}\theta\Big(\varepsilon_F-\frac{k^2}{2}\Big)$$

$\varepsilon_F = \frac{k_F^2}{2}$

$$\frac{D(\varepsilon)}{V}=\frac{1}{(2\pi)^3}\int_0^\infty dk\,k^2\int_0^\pi d\theta\sin\theta\int_0^{2\pi}d\phi\,\delta\Big(\varepsilon-\frac{k^2}{2}\Big)$$

レポート課題

6.3 分極関数

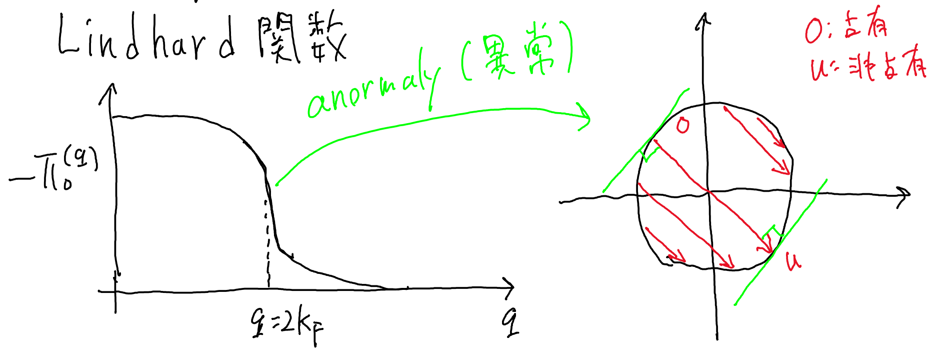
$$\Pi_0^{(q)}(r,r') \equiv \sum_{jj'} \int_{BZ} \frac{d^3k}{V_{BZ}} \frac{-f_{kj}(1-f_{k+qj'})}{\varepsilon_{k+qj'}-\varepsilon_{kj}} \rho_{kjk+qj}(r)\, \rho^*_{kjk+qj'}(r')$$

↓ r, r' 非依存　　　$u_k = \frac{1}{\sqrt{V_{uc}}}$ なので $\frac{1}{V_{uc}}$

$$\Pi_0^{(q)} = \frac{1}{V_{uc}} \int_{BZ} \frac{d^3k}{(2\pi)^3} \frac{-f_k(1-f_{k+q})}{\varepsilon_{k+q}-\varepsilon_k}$$

⇓

Lindhard 関数



6.4 平面波基底

一般のポテンシャル $v(r)$

$$\left(-\frac{(\nabla+ik)^2}{2} + v(r)\right) u_{kj}(r) = \varepsilon\, u_{kj}(r)$$ を解く
(数値的)

$$u_{kj}(r) = \sum_\alpha \tilde{u}_{kj}(\alpha)\, \chi_\alpha(r)$$ 基底展開

↳ $\chi_\alpha(r) = \delta(r_\alpha)$ → 実空間メッシュ
有限要素法

・平面波展開

$$u_{kj}(r) = \sum_G e^{iGr}\, \tilde{u}_{kj}(G)$$

G " 逆格子ベクトル $G = n_1 b_1 + n_2 b_2 + n_3 b_3$

$$\left(\frac{(G+k)^2}{2}+\hat{v}\right)\tilde{u}_{kj}(G)=\varepsilon\tilde{u}_{kj}(G)$$

$v(G,G')$ のような行列になってしまうが…

$$\hat{v}\tilde{u}_{kj}(G)\equiv\sum_{G'}v(G,G')\tilde{u}_{kj}(G')=\int_{uc}d^3r\frac{e^{-iGr}}{\sqrt{V_{uc}}}v(r)u_{kj}(r)$$

$O(N_{pw}^2)$

たたみこみ＋高速フーリエ変換

$O(N_{pw}\ln N_{pw})$

6.5 自由電子の生成・消滅演算子

$$\hat{\psi}_\sigma(r)=\sum_k\hat{c}_{k\sigma}\frac{e^{ikr}}{\sqrt{V}}=\frac{\sqrt{V}}{(2\pi)^3}\int d^3k\, c_{k\sigma}e^{ikr}$$

$$\mathcal{H}^{(1)}=\sum_\sigma\sum_{kk'}c^\dagger_{k\sigma}c_{k'\sigma}\int_V d^3r\frac{1}{V}e^{-ikr}\left\{-\frac{\nabla^2}{2}+v(r)\right\}e^{ik'r}$$

$$=\sum_\sigma\sum_{kk'}c^\dagger_{k\sigma}c_{k'\sigma}\left\{\frac{k'^2}{2}\underbrace{\int_V\frac{d^3r}{V}e^{i(k'-k)r}}_{\delta_{kk'}}+\underbrace{\frac{1}{V}\int_V d^3r\, v(r)e^{i(k'-k)r}}_{v_{k'k}}\right\}$$

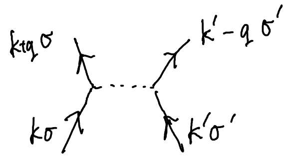
$$=\sum_\sigma\left(\sum_k\frac{k^2}{2}c^\dagger_{k\sigma}c_{k\sigma}+\sum_{kk'}v_{k'k}c^\dagger_{k\sigma}c_{k'\sigma}\right)$$

$$\mathcal{H}^{(2)} = \frac{1}{2}\sum_{\sigma\sigma'}\sum_{k_1k_2k_3k_4} c^\dagger_{k_1\sigma} c^\dagger_{k_2\sigma'} c_{k_3\sigma'} c_{k_4\sigma} \underbrace{\frac{1}{V^2}\int_V d^3r \int_V d^3r' \frac{e^{i(k_4-k_1)r}\, e^{i(k_3-k_2)r'}}{|r-r'|}}_{\substack{r-r' \to r \\ r \to r+r'}}$$

$$\frac{1}{V^2}\int d^3r \frac{e^{i(k_4-k_1)r}}{|r|} \int d^3r' e^{i(k_3+k_4-k_1-k_2)r'} \longrightarrow \begin{array}{l} k_3 \to k' \\ k_4 \to k \\ k_1 \to k+q \\ k_2 \to k'-q \end{array}$$

$$\longrightarrow 2\pi \int_0^\infty dr\, r^2 \int_{-1}^{1} dt\, \frac{e^{ikrt}}{r} = \frac{4\pi}{k^2}$$

$$= \frac{1}{2}\sum_{\sigma\sigma'}\sum_{kk'q} \frac{4\pi}{q^2} c^\dagger_{k+q\sigma} c^\dagger_{k'-q\sigma'} c_{k'\sigma'} c_{k\sigma}$$



・反交換関係

$$c_{k\sigma} = \frac{1}{\sqrt{V}}\int d^3r\, e^{-ikr} \psi_\sigma(r)$$

$$\{c_{k\sigma}, c^\dagger_{k'\sigma'}\} = \frac{1}{V}\int d^3r \int d^3r'\, e^{-ikr} e^{ik'r'} \underbrace{\{\psi_\sigma(r), \psi^\dagger_{\sigma'}(r')\}}_{\delta_{\sigma\sigma'}\delta(r-r')}$$

$$= \frac{1}{V}\int d^3r\, e^{i(k'-k)r} \delta_{\sigma\sigma'} = \delta_{kk'}\delta_{\sigma\sigma'}$$