9. グリーン関数、多体摂動論の基礎

9.1 大分配関数の摂動展開

グランドカノニカル集団の大分配関数

$$Z_G = \sum_n e^{-\beta(E_n - \mu N_n)} = \sum_n \langle n | e^{-\beta(\hat{\mathcal{H}} - \mu \hat{N})} | n \rangle$$

$$= \mathrm{tr}\left[e^{-\beta(\hat{\mathcal{H}} - \mu \hat{N})}\right] \quad \text{トレース（対角和）}$$

$$\hat{\mathcal{H}} = \underset{\text{非摂動項}}{\hat{\mathcal{H}}^{(1)}} + \underset{\text{摂動項}}{\hat{\mathcal{H}}^{(2)}}$$

グランドポテンシャル $F_G = -T \ln Z_G \longrightarrow Z_G = e^{-\beta F_G}$

非相互作用（非摂動）の場合

$$Z_{G0} = \mathrm{tr}\left[e^{-\beta(\hat{\mathcal{H}}^{(1)} - \mu \hat{N})}\right] \equiv e^{-\beta F_{G0}}, \quad F_{G0} = -T \ln Z_{G0}$$

$$\langle X \rangle_0 = \frac{1}{Z_{G0}} \sum_n e^{-\beta(E_{n0} - \mu N_{n0})} \langle n_0 | \hat{X} | n_0 \rangle$$

$\hat{\mathcal{H}}^{(1)}$の多体固有状態

$$\hat{\mathcal{H}}^{(1)} | n_0 \rangle = E_{n0} | n_0 \rangle$$

$$\hat{N} | n_0 \rangle = N_{n0} | n_0 \rangle$$

$$= \frac{1}{Z_{G0}} \mathrm{tr}\left[e^{-\beta \underbrace{(\hat{\mathcal{H}}^{(1)} - \mu \hat{N})}_{\text{以下 } \tilde{\mathcal{H}}_0 \text{ と書く}}} \hat{X}\right]$$

目的

Z_Gを$\mathcal{H}^{(1)}$の固有状態による何らかの量の期待値として書く

$$Z_G = \langle \hat{U}(\beta) \rangle_0 e^{-\beta F_{G0}} = \frac{\cancel{e^{-\beta F_{G0}}}}{\cancel{Z_{G0}}} \mathrm{tr}\left[e^{-\beta \mathcal{H}_0} \hat{U}(\beta)\right]$$

これは具体的にはどの様な演算子か？

tr[ ]の中身

$$e^{-\beta(\hat{\mathcal{H}} - \mu \hat{N})} = e^{-\beta \mathcal{H}_0} \hat{U}(\beta)$$

両辺をβで微分

$$-\underbrace{(\mathcal{H}-\mu N)}_{\mathcal{H}_0+\mathcal{H}^{(2)}}\underbrace{e^{-\beta(\mathcal{H}-\mu N)}}_{e^{-\beta\mathcal{H}_0}U(\beta)} = \mathcal{H}_0 e^{-\beta\mathcal{H}_0}U(\beta) + e^{-\beta\mathcal{H}_0}\frac{\partial U(\beta)}{\partial\beta}$$

$$\frac{\partial U(\beta)}{\partial\beta} = -\hat{\mathcal{H}}^{(2)}(\beta)\,\hat{U}(\beta)$$

$$\hat{\mathcal{H}}^{(2)}(\beta) = e^{\beta\hat{\mathcal{H}}_0}\hat{\mathcal{H}}^{(2)}e^{-\beta\hat{\mathcal{H}}_0}$$

$\hat{X}(\tau) \equiv e^{\tau\mathcal{H}_0}\hat{X}e^{-\tau\mathcal{H}_0}$ ：相互作用表示

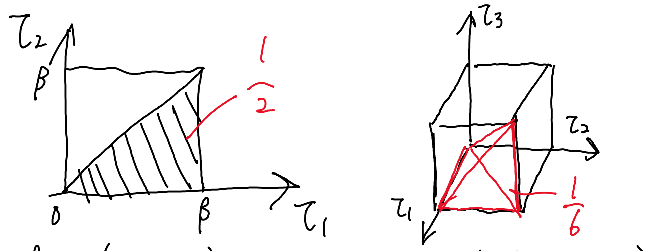
$U(0)=1$ より

τ：虚時間と呼ぶ

$$U(\beta) = 1 - \int_0^\beta d\tau\,\hat{\mathcal{H}}^{(2)}(\tau)\,\hat{U}(\tau)$$

$$= 1 - \int_0^\beta d\tau_1\mathcal{H}^{(2)}(\tau_1) + \int_0^\beta d\tau_1\int_0^{\tau_1}d\tau_2\,\hat{\mathcal{H}}^{(2)}(\tau_1)\hat{\mathcal{H}}^{(2)}(\tau_2) + \int_0^\beta d\tau_1\int_0^{\tau_1}d\tau_2\int_0^{\tau_2}d\tau_3\cdots$$

$$= 1 + \sum_{l=1}^{\infty}(-1)^l\int_0^\beta d\tau_1\int_0^{\tau_1}d\tau_2\cdots\int_0^{\tau_{l-1}}d\tau_l\,\hat{\mathcal{H}}^{(2)}(\tau_1)\cdots\hat{\mathcal{H}}^{(2)}(\tau_l)$$



$l=2\ (\tau_1>\tau_2)$ $\quad$ $l=3\ (\tau_1>\tau_2>\tau_3)$

時間順序積 (Dyson記号)

$$P[\hat{X}(\tau)\hat{X}(\tau')] = \begin{cases}\hat{X}(\tau)\hat{X}(\tau') : (\tau>\tau') \\ \hat{X}(\tau')X(\tau) : (\tau'>\tau)\end{cases}$$

虚時間
大きい方が前

$$= 1 + \sum_{l=1}^{\infty}\frac{(-1)^l}{l!}\int_0^\beta d\tau_1\cdots\int_0^\beta d\tau_l\,P[\hat{\mathcal{H}}^{(2)}(\tau_1)\cdots\mathcal{H}^{(2)}(\tau_l)]$$

よって

$$\frac{Z_G}{Z_{G0}}=\langle U(\beta)\rangle_0=1+\sum_{\ell=1}^{\infty}\frac{(-1)^\ell}{\ell!}\int_0^\beta d\tau_1\cdots\int_0^\beta d\tau_\ell\langle P[\mathcal{H}^{(2)}(\tau_1)\cdots\mathcal{H}^{(2)}(\tau_\ell)]\rangle_0$$

$$=1+\sum_{\ell=1}^{\infty}\frac{(-1)^\ell}{\ell!}\int_0^\beta d\tau_1\cdots\int_0^\beta d\tau_\ell\left(\frac{1}{2}\right)^\ell\int dr_1\int dr_1'\cdots\int dr_\ell dr_\ell'\sum_{\sigma_1\sigma_1'\cdots\sigma_\ell\sigma_\ell'}\frac{1}{|r_1-r_1'|}\cdots\frac{1}{|r_\ell-r_\ell'|}$$

$$\times\langle P[\psi^\dagger_{\sigma_1}(r_1,\tau_1)\psi^\dagger_{\sigma_1'}(r_1',\tau_1)\psi_{\sigma_1'}(r_1',\tau_1)\psi_{\sigma_1}(r_1,\tau_1)$$

$$\cdots\psi^\dagger_{\sigma_\ell}(r_\ell,\tau_\ell)\psi^\dagger_{\sigma_\ell'}(r_\ell',\tau_\ell)\psi_{\sigma_\ell'}(r_\ell',\tau_\ell)\psi_{\sigma_\ell}(r_\ell,\tau_\ell)\rangle_0$$

$$e^{\tau\mathcal{H}_0}\hat{A}\hat{B}e^{-\tau\mathcal{H}_0}$$

$$=e^{\tau\mathcal{H}_0}\hat{A}e^{-\tau\mathcal{H}_0}e^{\tau\mathcal{H}_0}\hat{B}e^{-\tau\mathcal{H}_0}$$

$$=\hat{A}(\tau)\hat{B}(\tau)$$ を使った。

※ $$\mathcal{H}^{(2)}(\tau)=\frac{1}{2}\sum_{\sigma\sigma'}\int d^3r\int d^3r'\frac{\psi^\dagger_\sigma(r,\tau)\psi^\dagger_{\sigma'}(r',\tau)\psi_{\sigma'}(r',\tau)\psi_\sigma(r,\tau)}{|r-r'|}$$

・相互作用表示の具体的な表式

$$\frac{\partial}{\partial\tau}\psi_\sigma(r,\tau)=\mathcal{H}_0\psi_\sigma(r,\tau)-\psi_\sigma(r,\tau)\mathcal{H}_0$$

$$=e^{\tau\mathcal{H}_0}[\mathcal{H}_0,\psi_\sigma(r)]e^{-\tau\mathcal{H}_0}=-\left\{-\frac{\nabla^2}{2}+v(r)-\mu\right\}\psi_\sigma(r,\tau)$$

$$\left[\sum_{\sigma'}\int d^3r'\psi^\dagger_{\sigma'}(r')\left\{-\frac{\nabla_{r'}^2}{2}+v(r')-\mu\right\}\psi_{\sigma'}(r'),\psi_\sigma(r)\right]$$

$$-\left\{-\frac{\nabla^2}{2}+v(r)\right\}\psi_\sigma(r)$$

$$\psi_\sigma(r,0)=\psi_\sigma(r)$$

$$\psi_\sigma(r,\tau)=\exp\left[-\tau\left\{-\frac{\nabla^2}{2}+v(r)-\mu\right\}\right]\psi_\sigma(r)$$

以下まとめて
$h(r)$と書く

$$\hat{\psi}_\sigma^\dagger(r,\tau) = \exp\left[\tau\left\{-\frac{\nabla^2}{2}+v(r)-\mu\right\}\right]\psi_\sigma^\dagger(r)$$

※ $\{\psi_\sigma(r,\tau)\}^\dagger$: 虚時間なので。 $\{\psi(r,\tau)\}^\dagger = \psi^\dagger(r,-\tau)$

$$\{\psi_\sigma(r,\tau), \psi_{\sigma'}^\dagger(r',\tau')\} = \exp[-\tau h(r)]\exp[\tau' h(r')]$$

$$\times\{\psi_\sigma(r), \psi_{\sigma'}^\dagger(r')\} \rightarrow \delta_{\sigma\sigma'}\delta(r-r')$$

$$= \exp\left[(\tau'-\tau)h(r)\right]\delta_{\sigma\sigma'}\delta(r-r')$$

9.2 Bloch-de Dominicis の定理

(ブロッホ、ドミニシス)

※絶対零度(基底状態)ではWickの定理と呼ばれ、その有限温度版

$\langle \hat{A}_1\hat{A}_2\hat{A}_3\cdots\hat{A}_{2n}\rangle_0$ を計算。 A_i は $\psi_\sigma(r,\tau)$、$\psi_\sigma^\dagger(r,\tau)$

$\{\hat{A}_i, \hat{A}_j\} = a_{ij}$ であるとする ← この場合は成り立つ

演算子では無く数

$$\langle \hat{A}_1\hat{A}_2\cdots\hat{A}_{2n}\rangle_0 = a_{12}\langle\hat{A}_3\cdots\hat{A}_{2n}\rangle_0 - \langle\hat{A}_2\hat{A}_1\hat{A}_3\cdots\hat{A}_{2n}\rangle_0$$

$$= a_{12}\langle\hat{A}_3\cdots\hat{A}_{2n}\rangle_0 - a_{13}\langle\hat{A}_2\hat{A}_4\cdots\hat{A}_{2n}\rangle_0 + \langle\hat{A}_2\hat{A}_3\hat{A}_1\hat{A}_4\cdots\hat{A}_{2n}\rangle_0$$

$$= a_{12}\langle\hat{A}_3\cdots\hat{A}_{2n}\rangle_0 - a_{13}\langle\hat{A}_2\hat{A}_4\cdots\hat{A}_{2n}\rangle_0 + \cdots$$

$$+ a_{1,2n}\langle\hat{A}_2\hat{A}_3\cdots\hat{A}_{2n-1}\rangle_0 - \langle\hat{A}_2\hat{A}_3\cdots A_{2n}A_1\rangle_0$$

元の項×数に出来るか?

$$\langle A_2\cdots A_{2n}A_1\rangle_0 = \frac{1}{Z_{G0}}\mathrm{tr}\left[e^{-\beta\mathcal{H}_0}\hat{A}_2\cdots\hat{A}_{2n}\hat{A}_1\right]$$

トレースの順回不変

$$= \frac{1}{Z_{G0}}\mathrm{tr}\left[\hat{A}_1 e^{-\beta\mathcal{H}_0}\hat{A}_2\cdots\hat{A}_{2n}\right]$$

$$\psi(r,\tau)e^{-\beta\mathcal{H}_0} = e^{\tau\mathcal{H}_0}\psi(r)e^{-(\tau+\beta)\mathcal{H}_0}$$

$$= e^{-\beta\mathcal{H}_0}e^{(\tau+\beta)\mathcal{H}_0}\psi(r)e^{-(\tau+\beta)\mathcal{H}_0} = e^{-\beta\mathcal{H}_0}e^{-(\tau+\beta)h(r)}\psi(r)$$

$$= e^{-\beta\mathcal{H}_0}e^{-\beta h(r)}\psi(r,\tau)$$

$$\psi^\dagger(r,\tau)e^{-\beta\mathcal{H}_0} = e^{-\beta\mathcal{H}_0}\psi^\dagger(r,\tau+\beta) = e^{-\beta\mathcal{H}_0}e^{\beta h(r)}\psi^\dagger(r,\tau)$$

$$= \frac{1}{Z_{G0}}e^{\pm\beta h(r_1)}\left[e^{-\beta\mathcal{H}_0}A_1A_2\cdots A_{2n}\right] = e^{\pm\beta h(r_1)}\langle A_1\cdots A_{2n}\rangle_0$$

よって

$$(1+e^{\pm\beta h(r_1)})\langle A_1\cdots A_{2n}\rangle_0 = a_{12}\langle A_3\cdots A_{2n}\rangle_0 - a_{13}\langle A_2A_4\cdots A_{2n}\rangle_0$$
$$+ a_{1.2n}\langle A_2\cdots A_{2n-1}\rangle_0$$

$$\langle A_1\cdots A_{2n}\rangle_0 = \frac{a_{12}}{1+e^{\pm\beta h(r_1)}}\langle A_3\cdots A_{2n}\rangle_0 - \frac{a}{1+e^{\pm\beta h(r_1)}}\langle a_2\cdots A_{2n}\rangle_0$$

$$\cdots + \frac{a_{1.2n}}{1+e^{\pm\beta h(r_1)}}\langle A_2\cdots A_{2n-1}\rangle_0$$

特に $n=1$ のとき

$$\langle A_1A_2\rangle_0 = \frac{a_{12}}{1+e^{\pm\beta h(r_1)}}$$

・具体例

$$\langle\psi_\sigma(r,\tau)\psi^\dagger_{\sigma'}(r',\tau')\rangle_0 = \frac{e^{(\tau'-\tau)h(r)}\delta(r-r')\delta_{\sigma\sigma'}}{1+e^{-\beta h(r)}}$$

$$\langle\psi^\dagger_\sigma(r,\tau)\psi_{\sigma'}(r',\tau')\rangle_0 = \frac{e^{(\tau-\tau')h(r)}\delta(r-r')\delta_{\sigma\sigma'}}{1+e^{\beta h(r)}}$$

$$\langle A_1\cdots A_{2n}\rangle_0 = \langle A_1A_2\rangle\langle A_3\cdots A_{2n}\rangle - \langle A_1A_3\rangle\langle A_2\cdots A_{2n}\rangle$$
$$\cdots + \langle A_1A_{2n}\rangle\langle A_2\cdots A_{2n-1}\rangle$$

これを 〜 〜 〜 …等に繰り返し用いると、

$$
\begin{aligned}
&= \langle A_1 A_2\rangle\langle A_3 A_4\rangle \cdots \langle A_{2n-1} A_{2n}\rangle \\
&\quad - \langle A_1 A_3\rangle\langle A_2 A_4\rangle \cdots \langle A_{2n-1} A_{2n}\rangle \\
&\quad + \langle A_1 A_4\rangle\langle A_2 A_3\rangle \cdots \\
&\quad \vdots
\end{aligned}
$$

→ コントラクション

<u>ルール</u>
① 全ての可能なペアのとり方。ただし
② $\langle A_i A_j\rangle$ としたとき元の順序では $i<j$
③ 入れ換えが奇数回の時は -1 が付く

9.3 平均場近似 (Hartree-Fock近似)

ハートリー・フォック

相互作用項の期待値

$$
\langle \mathcal{H}^{(2)}\rangle_0 = \frac{1}{2}\sum_{\sigma\sigma'}\int d^3r\int d^3r' \frac{1}{|r-r'|}\langle \psi^\dagger_\sigma(r)\psi^\dagger_{\sigma'}(r')\psi_{\sigma'}(r')\psi_\sigma(r)\rangle_0
$$

$$
= \frac{1}{2}\sum_{\sigma\sigma'}\int d^3r\int d^3r' \frac{1}{|r-r'|}\Big(\langle \psi^\dagger_\sigma(r)\psi_\sigma(r)\rangle_0\langle \psi^\dagger_{\sigma'}(r')\psi_{\sigma'}(r')\rangle_0 - \langle \psi^\dagger_\sigma(r)\psi_{\sigma'}(r')\rangle_0\langle \psi^\dagger_{\sigma'}(r')\psi_\sigma(r)\rangle_0\Big)
$$

これを期待値として持つ様な一体の<u>有効ハミルトニアン</u>

$$
\begin{aligned}
\bar{\mathcal{H}}^{(2)} = \frac{1}{2}\sum_{\sigma\sigma'}\int d^3r\int d^3r' \frac{1}{|r-r'|}\Big\{ &\psi^\dagger_\sigma(r)\psi_\sigma(r)\langle \psi^\dagger_{\sigma'}(r')\psi_{\sigma'}(r')\rangle_0 \\
&\langle \psi^\dagger_\sigma(r)\psi_\sigma(r)\rangle_0\psi^\dagger_{\sigma'}(r')\psi_{\sigma'}(r') - \psi^\dagger_\sigma(r)\psi_{\sigma'}(r')\langle \psi^\dagger_{\sigma'}(r')\psi_\sigma(r)\rangle_0 \\
&- \langle \psi^\dagger_\sigma(r)\psi_{\sigma'}(r')\rangle_0\psi^\dagger_{\sigma'}(r')\psi_\sigma(r)\Big\}
\end{aligned}
$$

$$
= \sum_\sigma \int d^3r\, \psi^\dagger_\sigma(r)\Big\{\sum_{\sigma'}\int d^3r' \frac{1}{|r-r'|}\langle \psi^\dagger_{\sigma'}(r')\psi_{\sigma'}(r')\rangle_0\Big\}\psi_\sigma(r)
$$

$$
- \sum_{\sigma\sigma'}\int d^3r\, \psi^\dagger_\sigma(r)\int d^3r' \frac{\langle \psi^\dagger_{\sigma'}(r')\psi_\sigma(r)\rangle}{|r-r'|}\psi_{\sigma'}(r')
$$

$$\mathcal{H}^{(1)}+\overline{\mathcal{H}^{(2)}}=\sum_{\sigma\sigma'}\int d^3r\int d^3r'\,\hat{\psi}^{\dagger}_{\sigma}(r)\Big[\delta_{\sigma\sigma'}\delta(r-r')h(r')$$

$$+\frac{\langle\psi^{\dagger}_{\sigma'}(r')\psi_{\sigma'}(r')\rangle_0}{|r'-r|}-\frac{\langle\psi^{\dagger}_{\sigma'}(r')\psi_{\sigma}(r)\rangle_0}{|r-r'|}\Big]\hat{\psi}_{\sigma'}(r')$$

ここで

$$\left(-\frac{\nabla^2}{2}+v(r)-\mu+\sum_{\sigma}\int d^3r'\frac{\langle\psi^{\dagger}_{\sigma'}(r')\psi_{\sigma'}(r')\rangle}{|r-r'|}\right)\varphi_{j\sigma}(r)$$

$$-\sum_{\sigma}\int d^3r'\frac{\langle\psi^{\dagger}_{\sigma'}(r')\psi_{\sigma}(r)\rangle_0}{|r-r'|}\varphi_{j\sigma}(r')=\varepsilon_{j\sigma}\varphi_{j\sigma}(r)$$

となる $\varphi_j(r)$ で $\psi(r)$ を展開すれば

$$\mathcal{H}^{(1)}+\overline{\mathcal{H}^{(2)}}=\sum_{\sigma j}\varepsilon_{j\sigma}c^{\dagger}_{j\sigma}c_{j\sigma}$$

$$\sum_{\sigma'}\langle\psi^{\dagger}_{\sigma'}(r')\psi_{\sigma'}(r')\rangle_0=\sum_{j\sigma}f\left(\frac{\varepsilon_{j\sigma}-\mu}{T}\right)|\varphi_{j\sigma}(r')|^2$$

9.4 Feynman ダイヤグラム
ファインマン

$$\frac{Z_G}{Z_{G0}}=1+\sum_{l=1}^{\infty}\frac{(-1)^l}{l!}\int_0^{\beta}d\tau_1\cdots\int_0^{\beta}d\tau_l\left(\frac{1}{2}\right)^l\int dr_1\int dr_1'\cdots\int dr_l dr_l'\sum_{\sigma_1\sigma_1'\cdots\sigma_l\sigma_l'}\frac{1}{|r_1-r_1'|}\cdots\frac{1}{|r_l-r_l'|}$$

$$\times\langle P[\psi^{\dagger}_{\sigma_1}(r_1,\tau_1)\psi^{\dagger}_{\sigma_1'}(r_1',\tau_1)\psi_{\sigma_1'}(r_1',\tau_1)\psi_{\sigma_1}(r_1,\tau_1)$$

$$\cdots\psi^{\dagger}_{\sigma_l}(r_l,\tau_l)\psi^{\dagger}_{\sigma_l'}(r_l',\tau_l)\psi_{\sigma_l'}(r_l',\tau_l)\psi_{\sigma_l}(r_l,\tau_l)\rangle_0$$

略記 $r,\sigma\to r$ $\quad\psi_\sigma(r,\tau)\longrightarrow\psi(r,\tau)$ $\quad\sum_\sigma\int d^3r\to\sum_r$

$$\frac{1}{2}\frac{1}{|r-r'|}\to v(r,r')$$

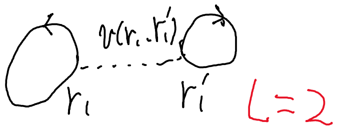
$$=1+\sum_{l=1}^{\infty}\frac{(-1)^l}{l!}\int_0^{\beta}d\tau_1\cdots\int_0^{\beta}d\tau_l\sum_{r_1\cdots r_l}v(r_1,r_1')\cdots v(r_l,r_l')$$

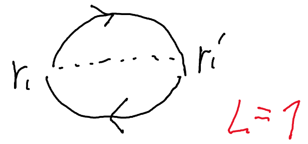
$$\times\langle P\,\psi^\dagger(r_1,\tau_1)\psi^\dagger(r_1',\tau_1)\psi(r_1',\tau_1)\psi(r_1,\tau_1)\cdots\psi(r_\ell,\tau_\ell)\rangle_0$$

↳ Bloch - de Dominicis $\sum_P(-1)^P P\langle\cdots\rangle\langle\cdots\rangle\langle\cdots\rangle\cdots\langle\cdots\rangle$

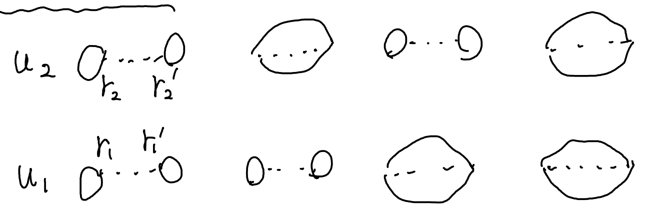
$\ell=1$の項　　　全て同(虚)時刻

$$v(r_1,r_1')\left\{P\langle\psi^\dagger(\underset{\tau_1}{r_1})\psi(\underset{\tau_1}{r_1})\rangle_0\langle\psi^\dagger(r_1')\psi(r_1')\rangle_0-P\langle\psi^\dagger(\underset{\tau_1}{r_1})\psi(\underset{\tau_1}{r_1'})\rangle_0\langle\psi^\dagger(\underset{\tau_1}{r_1'})\psi(\underset{\tau_1}{r_1})\rangle_0\right\}$$

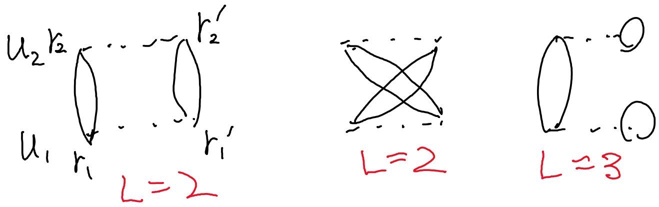




$\ell=2$の項



つながらない(非連結)ファインマンダイヤグラム



・・・ つながった(連結)ファインマンダイアグラム

exp(連結項)　　　Taylor展開

$$=1+(\text{連結項})+\underbrace{\frac{1}{2}(\text{連結項2個})+\frac{1}{6}(\text{連結項3個})\cdots\cdots}_{\text{非連結項}}$$

$$\frac{Z_G}{Z_{G0}}=e^{-\beta(F_G-F_{G0})}$$ より

$$-\beta(F_G-F_{G0})=(\text{連結項})$$

$$=\sum^{\text{連結}}\frac{(-1)^\ell}{\ell!}\sum_{r_1r_2\cdots}v(r_1,r_1')\cdots\sum_P(-1)^P\langle\cdots\rangle\langle\cdots\rangle\cdots\cdots$$

9.4 ファインマン則

$\leftarrow$ 入れ換え回数

Bloch-de Dominicisの定理の$(-1)^P$をどう計算するか

(リングの数) × (個々のコントラクションの時間順序)

証明は略

$$g_0(r,\tau,r',\tau') \equiv -\langle T\psi(r,\tau)\psi^\dagger(r',\tau')\rangle_0$$

$$\equiv \begin{cases} -\langle\psi(r,\tau)\psi^\dagger(r',\tau')\rangle_0 & (\tau>\tau') \\ \langle\psi^\dagger(r',\tau')\psi(r,\tau)\rangle_0 & (\tau'>\tau) \end{cases}$$

非相互作用系の松原グリーン関数

$$-\beta(F_G-F_{G0}) = \sum_{l=1}^{\infty}\frac{(-1)^l}{l!}\sum_{\text{連結}}(-1)^{\overbrace{L}^{\text{リングの数}}}\sum_{r_1 r_1' \cdots} v(r_1,r_1')v(\cdots)\cdots$$

$$\times\int_0^\beta d\tau_1\cdots\int_0^\beta d\tau_l\, g_0(\cdots)\cdots g_0(\cdots)$$

9.5 松原 Green 関数

$$g(r,\tau,r',\tau') = \begin{cases} -\dfrac{\delta(r-r')}{1+e^{-\beta h(r)}}e^{(\tau'-\tau)h(r)} & (\tau>\tau') \\ \dfrac{\delta(r-r')}{1+e^{\beta h(r)}}e^{(\tau'-\tau)h(r)} & (\tau'>\tau) \end{cases}$$

$\tau-\tau'$の関数

$$g_0(r,r';\underbrace{\tau-\tau'}_{-\beta\leqq\tau-\tau'\leqq\beta})$$

$0\leqq\tau,\tau'\leqq\beta$

$$g_0(r,r';\tau+\beta) = -g_0(r,r';\tau)$$

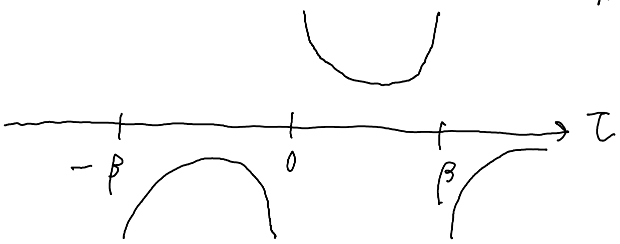
この範囲外に拡張

$$g_0(r,r';\tau+\underbrace{2\beta}_{\text{周期}})=g_0(r,r';\tau)$$

⇓ フーリエ級数展開

$$g_0(r,r',\tau)=\frac{1}{\beta}\sum_m \tilde{g}_0(r,r';i\omega_m)e^{-i\omega_m\tau} \longrightarrow \omega_m=\frac{2\pi}{2\beta}m$$

$m=-\infty\cdots-2,-1,0,1,2,\cdots\infty$



$$\tilde{g}_0(r,r';i\omega_m)=\frac{1}{2}\int_{-\beta}^{\beta}d\tau\, g_0(r,r',\tau)e^{i\omega_m\tau}$$

反周期 β

$$=\frac{1}{2}\underbrace{(1-e^{-i\pi m})}\int_0^{\beta}d\tau\, g_0(r,r';\tau)e^{i\omega_m\tau}$$

mが偶数の時 $\tilde{g}_0(r,r';i\omega_m)=0$

$$\sum_m F(\underset{\uparrow \atop \frac{2\pi m}{2\beta}}{\omega_m}) \longrightarrow \sum_m F(\underset{\uparrow \atop \frac{(2m+1)\pi}{\beta}}{\omega_m})$$

$$\frac{(2m+1)\pi}{\beta}=\pi T(2m+1)$$

Odd
Fermionic
} 松原振動数

$m=-\infty,\cdots-2,-1,0,1,2,\cdots\infty$

$$\tilde{g}_0(r,r';i\omega)=\frac{\delta(r-r')}{i\omega-h(r)}$$

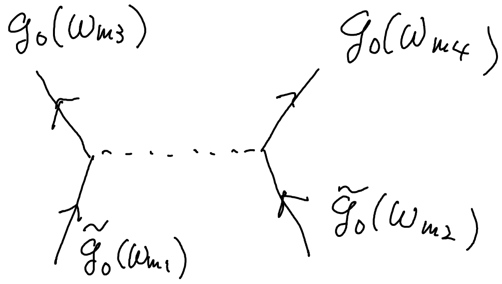
$\downarrow$ $h(r)\varphi_j=\varepsilon_j\varphi_j(r)$

$$=\sum_j\frac{\varphi_j(r)\varphi_j^*(r)}{i\omega-\varepsilon_j}$$

<u>振動数（エネルギー）保存</u>

$$\int_0^{\beta}d\tau\, e^{i(\omega_{m_1}+\omega_{m_2}-\omega_{m_3}-\omega_{m_4})\tau}$$

$$=\beta\,\delta_{m_1+m_2,\,m_3+m_4}$$



リングの数

$$-\beta(F_G-F_{G0})=\sum_{\ell=1}^{\infty}\frac{(-1)^\ell}{\ell!}\sum_{連結}(-1)^L\sum_{r_1r_1'\cdots}v(r_1,r_1')v(\cdots)\cdots$$

$$\times\frac{1}{\beta^\ell}\sum_{\omega_1\omega_1'\omega_2\cdots}\tilde{g}_0(\cdots)\cdots\tilde{g}_0(\cdots)$$

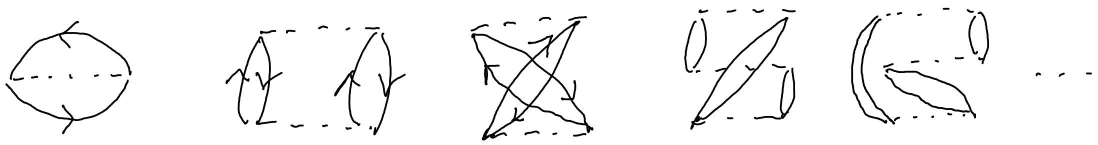
振動数保存の拘束

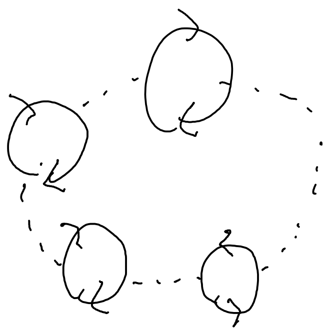
9.6 リング近似

もしくはバブル近似、乱雑位相近似(RPA)

Random Phase Approximation

$\ell=1$　$\ell=2$　$\ell=3$





こういうトポロジーのダイヤグラムだけ無限次まで

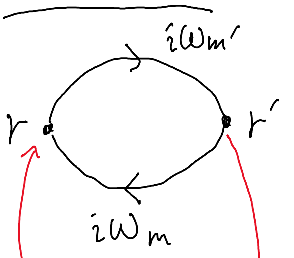
左右の組合

ℓ 次では等価なダイヤグラムが $2^{\ell-1}(\ell-1)!$ 個

時間の組合

バブル

リング1個



$$-\frac{1}{\beta}\sum_{m m'} g_0(r', r, i\omega_{m'})\, g_0(r, r', i\omega_m)$$

$$\to -\frac{1}{\beta}\sum_{m} g_0(r', r, i\omega_m + i\nu)\, g_0(r, r', i\omega_m)$$

$$\nu_{m'-m} = \omega_{m'} - \omega_m = \frac{2\pi(m'-m)}{\beta}$$

$$\omega_{m'} = \omega_m + \nu_{m'-m}$$

$$= -\frac{1}{\beta}\sum_{jj'}\sum_{m} \frac{\varphi_j(r')\varphi_j^*(r)\varphi_{j'}(r)\varphi_{j'}^*(r')}{(i\omega_m + i\nu_{m'} - \varepsilon_j)(i\omega_m - \varepsilon_{j'})}$$

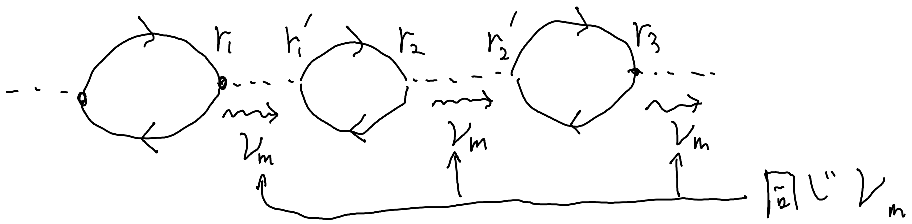
フェルミ分布

$$\frac{1}{\beta}\sum_{m} \frac{1}{(i\omega_m + i\nu_{m'} - \varepsilon_j)(i\omega_m - \varepsilon_{j'})} = \frac{f(\beta\varepsilon_j) - f(\beta\varepsilon_{j'})}{\varepsilon_j - \varepsilon_{j'} - i\nu_{m'}}$$

$$\Pi_0(r, r', i\nu_m) = -\sum_{jj'} \frac{f(\beta\varepsilon_j) - f(\beta\varepsilon_{j'})}{\varepsilon_j - \varepsilon_{j'} - i\nu_m}\varphi_j(r')\varphi_j^*(r)\varphi_{j'}(r)\varphi_{j'}^*(r')$$

独立電子分極関数 (5.7節)

これがつながっている



$$-\beta(F_{G,RPA} - F_{G0}) = \sum_{\ell=1}^{\infty} \frac{(-1)^\ell}{\cancel{\ell!}\;\ell}\, 2^{\ell-1}\cancel{(\ell-1)!}$$

$$\sum_{m}\sum_{r_1 r_1' \cdots r_\ell'} v(r_1, r_1')\,\Pi_0(r_1', r_2, i\nu_m)\, v(r_2, r_2')\,\Pi_0(r_2', r_3, i\nu_m)\cdots\Pi(r_\ell', r_1, i\nu_m)$$

Taylar級数 $\ln(1+x) = x - \frac{x^2}{2} + \frac{x^3}{3} - \frac{x^4}{4} + \cdots$

$$= \frac{1}{2}\sum_{r\, m}\ln\left[1 + \sum_{r'} v(r, r')\,\Pi_0(r', r, i\nu_m)\right]$$