# RPA 近似による計算の流れ

① 既約感受率$\chi_0(\vec{q}, i\omega_m)$ を計算。

$$\chi_0(\vec{q}, i\omega_m) = -\frac{\mathrm{k_B T}}{\mathrm{N}}\sum_{\vec{\mathrm{k}},n} \mathrm{G_0}\left(\vec{\mathrm{q}} + \vec{k}, i\omega_m + i\epsilon_n\right)\mathrm{G_0}\left(\vec{k}, i\epsilon_n\right)$$

$$= \frac{1}{\mathrm{N}}\sum_{\vec{\mathrm{k}}} \frac{\mathrm{f}(\xi(\vec{\mathrm{q}} + \vec{k})) - \mathrm{f}(\xi(\vec{k}))}{\mathrm{i}\omega_\mathrm{m} - \ (\xi\left(\vec{\mathrm{q}} + \vec{k}\right) - \xi(\vec{k}))}$$

（各値の計算）

$$\mathrm{G_0}\left(\vec{k}, i\epsilon_n\right) = \frac{1}{\mathrm{i}\epsilon_\mathrm{n} - \xi(\vec{\mathrm{k}})}$$

$$\epsilon_n = (2n+1)\pi k_B T$$

$$\omega_m = 2m\pi k_B T$$

$$\mathrm{f(E)} = \frac{1}{\exp\left(\frac{\mathrm{E} - \mu}{\mathrm{k_B T}}\right) + 1}$$

$$\xi\left(\vec{\mathrm{k}}\right) = \mathrm{E_0} + 2\mathrm{t}\{\cos(\mathrm{k_x}) + \cos\,(\mathrm{k_y})\}$$

② スピン動的感受率$\chi_s(\vec{q}, i\omega_m)$、電荷動的感受率$\chi_c(\vec{q}, i\omega_m)$を計算

$$\chi_s(\vec{q}, i\omega_m) = \frac{\chi_0(\vec{q}, i\omega_m)}{1 - U\chi_0(\vec{q}, i\omega_m)}$$

$$\chi_c(\vec{q}, i\omega_m) = \frac{\chi_0(\vec{q}, i\omega_m)}{1 + U\chi_0(\vec{q}, i\omega_m)}$$

③ 反平行スピン間有効相互作用$\Gamma_{\sigma,-\sigma}\left(\vec{\mathrm{k}}, \vec{\mathrm{q}}, \mathrm{i}\epsilon_\mathrm{n}, \mathrm{i}\epsilon_\mathrm{m}\right)$の計算

$$\Gamma_{\sigma,-\sigma}\left(\vec{\mathrm{k}}, \vec{\mathrm{q}}, \mathrm{i}\epsilon_\mathrm{n}, \mathrm{i}\epsilon_\mathrm{m}\right)$$

$$= \mathrm{U} - \frac{1}{2}\mathrm{U}^2\chi_\mathrm{c}\left(\vec{\mathrm{k}} - \vec{\mathrm{q}}, \mathrm{i}\epsilon_\mathrm{n} - \mathrm{i}\epsilon_\mathrm{m}\right) + \frac{1}{2}\mathrm{U}^2\chi_\mathrm{s}\left(\vec{\mathrm{k}} - \vec{\mathrm{q}}, \mathrm{i}\epsilon_\mathrm{n} - \mathrm{i}\epsilon_\mathrm{m}\right)$$

$$+ \mathrm{U}^2\chi_\mathrm{s}\left(\vec{\mathrm{k}} + \vec{\mathrm{q}}, \mathrm{i}\epsilon_\mathrm{n} + \mathrm{i}\epsilon_\mathrm{m}\right)$$

④ 平行スピン間有効相互作用$\Gamma_{\sigma,\sigma}\left(\vec{\mathrm{k}}, \vec{\mathrm{q}}, \mathrm{i}\epsilon_\mathrm{n}, \mathrm{i}\epsilon_\mathrm{m}\right) = \Gamma_{\sigma,\sigma}\left(\vec{\mathrm{k}} - \vec{\mathrm{q}}, \mathrm{i}\epsilon_\mathrm{n} - \mathrm{i}\epsilon_\mathrm{m}\right)$を計算

$$\Gamma_{\sigma,\sigma}\left(\vec{\mathrm{k}}, \vec{\mathrm{q}}, \mathrm{i}\epsilon_\mathrm{n}, \mathrm{i}\epsilon_\mathrm{m}\right) = \Gamma_{\sigma,\sigma}\left(\vec{\mathrm{k}} - \vec{\mathrm{q}}, \mathrm{i}\epsilon_\mathrm{n} - \mathrm{i}\epsilon_\mathrm{m}\right)$$

$$= -\frac{1}{2}\mathrm{U}^2\chi_\mathrm{c}\left(\vec{\mathrm{k}} - \vec{\mathrm{q}}, \mathrm{i}\epsilon_\mathrm{n} - \mathrm{i}\epsilon_\mathrm{m}\right) - \frac{3}{2}\mathrm{U}^2\chi_\mathrm{s}\left(\vec{\mathrm{k}} - \vec{\mathrm{q}}, \mathrm{i}\epsilon_\mathrm{n} - \mathrm{i}\epsilon_\mathrm{m}\right)$$

⑤ 次のダイソン方程式をといて、繰りこまれたグリーン関数$G(\vec{k}, i\epsilon_n)$を計算。

$$\left[G(\vec{k}, i\epsilon_n)\right]^{-1} = \left[G_0(\vec{k}, i\epsilon_n)\right]^{-1} - \Sigma(\vec{k}, i\epsilon_n)$$

$$\Sigma(\vec{k}, i\epsilon_n) = -\frac{k_B T}{N}\sum_{\vec{q},m}[G(\vec{q}, i\epsilon_m)\Gamma_{\sigma,\sigma}(\vec{k}-\vec{q}, i\epsilon_n - i\epsilon_m) - U^2 G_0(\vec{q}, i\epsilon_m)\chi_0(\vec{k}-\vec{q}, i\epsilon_n - i\epsilon_m)]$$

⑥ 次のギャップ方程式を解いて、$\Delta(\vec{k}, i\epsilon_n)$を計算。

$$\Delta(\vec{k}, i\epsilon_n) = -\frac{k_B T}{N}\sum_{\vec{q},m} G(\vec{q}, i\epsilon_m)G(-\vec{q}, -i\epsilon_m)\,\Gamma_{\sigma,-\sigma}(\vec{k}, \vec{q}, i\epsilon_n, i\epsilon_m)\Delta(\vec{q}, i\epsilon_m)$$