BCS 理论

任杰

BCS 有效作用量

电-声相互作用

自由声子的哈密顿量为:

$$\hat{H}_{ph} = \sum_{\boldsymbol{q},j} \omega_{\boldsymbol{q}} \hat{a}_{\boldsymbol{q},j}^{\dagger} a_{\boldsymbol{q},j} + \text{const.}$$
(1)

其中 ω_q 是声子能量。声子是晶格振动的准粒子,与电子相互作用的微观机制是在电中性背景下由于晶格离开平 衡位置产生局部电荷,从而对电子产生作用,即

$$\hat{V}_{el-ph} \simeq \gamma \int d^d r \hat{\rho}_e(\mathbf{r}) \hat{\rho}_{ind}(\mathbf{r}). \tag{2}$$

其中 γ 是耦合常数, $\hat{\rho}_r$ 是电子密度算符, $\hat{\rho}_{ind}$ 是晶格畸变产生的电荷,其大小正比于晶格振动坐标u的散度:

$$\rho_{ind} \simeq \nabla \cdot \boldsymbol{u}. \tag{3}$$

量子化下的晶格简正坐标为:

$$u = \sum_{\mathbf{q}} u_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}} = e_j \frac{1}{\sqrt{2m\omega_{\mathbf{q}}}} (a_{\mathbf{q},j} + a_{-\mathbf{q},j}^{\dagger}) e^{i\mathbf{q}\cdot\mathbf{r}}.$$
 (4)

求散度得到:

$$\nabla \cdot \boldsymbol{u} = \sum_{\boldsymbol{q},j} \frac{iq_j}{\sqrt{2m\omega_q}} (a_{\boldsymbol{q},j} + a_{-\boldsymbol{q},j}^{\dagger}) e^{i\boldsymbol{q}\cdot\boldsymbol{r}}.$$
 (5)

电-声相互作用为:

$$\hat{V}_{el-ph} = \gamma \sum_{\mathbf{q},j} \left[\int d^d r \hat{\rho}_e(\mathbf{r}) e^{i\mathbf{q}\cdot\mathbf{r}} \right] \frac{iq_j}{\sqrt{2m\omega_q}} \left(\hat{a}_{\mathbf{a},j} + \hat{a}_{\mathbf{q},j}^{\dagger} \right)
= \gamma \sum_{\mathbf{q},j} \frac{iq_j}{\sqrt{2m\omega_q}} \hat{\rho}_{e,\mathbf{q}} \left(\hat{a}_{\mathbf{a},j} + \hat{a}_{\mathbf{q},j}^{\dagger} \right).$$
(6)

其中电子密度算符傅立叶变换具体为:

$$\hat{\rho}_{e,q} = \int d^d r \ \hat{c}^{\dagger}(\boldsymbol{r}) \hat{c}(\boldsymbol{r}) e^{i\boldsymbol{q}\cdot\boldsymbol{r}} = \frac{1}{L^d} \int d^d r \sum_{\boldsymbol{k}_1,\boldsymbol{k}_2} \hat{c}^{\dagger}_{\boldsymbol{k}_1} \hat{c}_{\boldsymbol{k}_2} e^{i(\boldsymbol{q}+\boldsymbol{k}_2-\boldsymbol{k}_1)\cdot\boldsymbol{r}} = \sum_{\boldsymbol{k}} \hat{c}^{\dagger}_{\boldsymbol{k}+\boldsymbol{q}} \hat{c}_{\boldsymbol{k}}.$$
(7)

电子-电子有效作用

考虑电-声相互作用后,电子-声子系统总配分函数为在路径积分下写为:

$$Z = \int D[\psi, \bar{\psi}] \int D[\phi, \bar{\phi}] \exp\left\{-S_{el}[\psi, \bar{\psi}] - S_{ph}[\phi, \bar{\phi}] - S_{el-ph}[\psi, \bar{\psi}, \phi, \bar{\phi}]\right\}. \tag{8}$$

其中 Sph, Sel-ph 分别为自由声子和电-声耦合作用量:

$$S_{ph}[\phi, \bar{\phi}] = \sum_{q,j} \bar{\phi}_{q,j} (-i\omega_n + \omega_q) \phi_{q,j},$$

$$S_{el-ph}[\psi, \bar{\psi}, \phi, \bar{\phi}] = \gamma \sum_{q,j} \frac{iq_j}{\sqrt{2m\omega_q}} \rho_q(\phi_{q,j} + \bar{\phi}_{-q,j}),$$
(9)

其中 $\rho_q = \sum_k \bar{\psi}_{k+q} \psi_k$. 要得到电子直接通过电-声耦合产生的有效相互作用,需要将声子场积掉。注意自由声子和电-声耦合部分的作用量是二次型:

$$S_{ph} + S_{el-ph} = \sum_{q,j} \left[\bar{\phi}_{q,j} (-i\omega_n + \omega_q) \phi_{q,j} + \gamma \frac{iq_j}{\sqrt{2m\omega_q}} \rho_q (\phi_{q,j} + \bar{\phi}_{-q,j}) \right]. \tag{10}$$

将其配平方后,得到:

$$S_{ph} + S_{el-ph} = \sum_{q,j} \left[\bar{\Phi}_{q,j} (-i\omega_n + \omega_q) \Phi_{q,j} + \frac{i\gamma^2 q_j^2}{2m\omega_q(\omega_n + i\omega_q)} \right]. \tag{11}$$

其中

$$\Phi_{q,j} = \phi_{q,j} + \frac{\gamma q_j}{\sqrt{2m\omega_q}(\omega_n + i\omega_q)},
\bar{\Phi}_{q,j} = \bar{\phi}_{q,j} - \frac{\gamma q_j}{\sqrt{2m\omega_q}(\omega_n + i\omega_q)},$$
(12)

二次项积分得到一个常数因子,可吸收至积分测度中,实际作用量贡献为:

$$S'_{ph} \simeq \sum_{q,j} \frac{i\gamma^2 q_j^2}{2m\omega_q(\omega_n + i\omega_q)} = \frac{\gamma^2}{2m} \sum_q \frac{q^2}{\omega_n^2 + \omega_q^2}.$$
 (13)

上式第二个等号对 $(\omega_n, -\omega_n)$ 求了平均。最终,有效作用量为:

$$S_{eff}[\psi, \bar{\psi}] = S_{el}[\psi, \bar{\psi}] - \frac{\gamma^2}{2m} \sum_{q} \frac{q^2}{\omega_n^2 + \omega_q^2} \rho_q \rho_{-q}.$$
 (14)

将虚时变为实时,即做替换 $i\omega_n \to \omega$,相互作用势为:

$$V(\mathbf{q},\omega) = \frac{\gamma^2 q^2}{2m(\omega^2 - \omega_q^2)}.$$
 (15)

当 $\omega < \omega_q$ 时,有效相互作用为吸引势。

有效作用量

费米面附近宽度为德拜频率 ω_D 的能壳内,电子为净吸引作用。当电-声耦合常数足够大,能壳内电子总相互作用是吸引的。BSC 模型近似将电子直接吸引势看作常数,其有效哈密顿量为:

$$\hat{H}_{BCS} = \int d^d r c_{\sigma}^{\dagger}(\mathbf{r}) \left(-\frac{\nabla^2}{2m} - \mu \right) c_{\sigma}(\mathbf{r}) - g \int d^d r c_{\uparrow}^{\dagger}(\mathbf{r}) c_{\downarrow}^{\dagger}(\mathbf{r}) c_{\downarrow}(\mathbf{r}) c_{\uparrow}(\mathbf{r}), \tag{16}$$

其中 g 为有效耦合常数。此哈密顿量对应的欧几里德作用量为:

$$S[\psi, \bar{\psi}] = \int_0^\beta d\tau \int d^d r \left[\bar{\psi}_\sigma \left(\partial_\tau - \frac{\nabla^2}{2m} - \mu \right) \psi_\sigma - g \bar{\psi}_\uparrow \bar{\psi}_\downarrow \psi_\uparrow \right]. \tag{17}$$

辅助场路径积分

辅助场作用量

现在,利用高斯积分公式,有恒等式:

$$\exp\left\{g\int_{0}^{\beta} d\tau \int d^{d}r \ \bar{\psi}_{\uparrow}\bar{\psi}_{\downarrow}\psi_{\downarrow}\psi_{\uparrow}\right\}$$

$$= \int D[\Delta, \bar{\Delta}] \exp\left\{-\int_{0}^{\beta} d\tau \int d^{d}r \left[\frac{1}{g}|\Delta|^{2} - \bar{\Delta}\psi_{\downarrow}\psi_{\uparrow} - \Delta\bar{\psi}_{\uparrow}\bar{\psi}_{\downarrow}\right]\right\}, \tag{18}$$

用其替换作用量中的相互作用项,得到配分函数为:

$$Z = \int D[\psi, \bar{\psi}] \int D[\Delta, \bar{\Delta}] \exp\left\{-\int_0^\beta d\tau \int d^d r \left[\frac{1}{g}|\Delta|^2 - \bar{\Psi}\hat{\mathcal{G}}^{-1}\Psi\right]\right\}. \tag{19}$$

其中引入了 Nambu spinor 算符:

$$\Psi = (\psi_{\uparrow}, \ \bar{\psi}_{\downarrow})^T, \ \bar{\Psi} = \Psi^{\dagger} \tag{20}$$

此时格林函数 $\hat{\mathcal{G}}^{-1}$ 在自旋空间是一个 2×2 矩阵, 其矩阵形式为:

$$\hat{\mathcal{G}}^{-1} = \begin{pmatrix} \hat{G}_p^{-1} & \Delta \\ \bar{\Delta} & \hat{G}_h^{-1} \end{pmatrix}, \tag{21}$$

其中粒子格林函数部分为:

$$\hat{G}_p^{-1} = -\partial_\tau + \frac{\nabla^2}{2m} + \mu. \tag{22}$$

而空穴格林函数部分为:

$$\hat{G}_h^{-1} = -\partial_\tau - \frac{\nabla^2}{2m} - \mu. \tag{23}$$

以上符号的差异来源于粒子-空穴共轭:对于 Grassmann 二次型,粒子-空穴共轭相当于交换 $\psi,\bar{\psi}$ 位置,净效果为添上一负号;对于带有偏导数的项,利用分部积分:

$$\bar{\psi}\partial\psi = -(\partial\psi)\bar{\psi} \simeq \psi\partial\bar{\psi}. \tag{24}$$

现在,作用量中的费米场部分变为高斯形,因此可以积掉费米子自由度:

$$\int D[\psi, \bar{\psi}] \exp\left(-\bar{\Psi}\hat{\mathcal{G}}^{-1}\Psi\right) = \det\hat{\mathcal{G}}^{-1} = \exp\left(\operatorname{Tr}\ln\hat{\mathcal{G}}^{-1}\right). \tag{25}$$

注意此处取迹运算 Tr 包括自旋自由度和时空自由度 (用 tr 代表仅在自旋空间求迹)。最终,配分函数转换为关于辅助场 $\Delta,\bar{\Delta}$ 的路径积分:

$$Z = \int D[\Delta, \bar{\Delta}] e^{-S[\Delta, \bar{\Delta}]}, \tag{26}$$

其中关于辅助场 Δ , $\bar{\Delta}$ 的作用量为:

$$S[\Delta, \bar{\Delta}] = \frac{1}{g} \int_0^\beta d\tau \int d^d r |\Delta|^2 - \text{Tr} \ln \hat{\mathcal{G}}^{-1}.$$
 (27)

鞍点近似

对辅助场作用量取极值:

$$0 = \frac{\delta S}{\delta \bar{\Delta}(\mathbf{r}, \tau)}$$

$$= \frac{1}{g} \Delta(\mathbf{r}, \tau) - \operatorname{Tr} \left[\hat{\mathcal{G}}(\mathbf{r}, \tau) \cdot \frac{\delta \hat{\mathcal{G}}^{-1}}{\delta \bar{\Delta}(\mathbf{r}, \tau)} \right]$$

$$= \frac{1}{g} \Delta(\mathbf{r}, \tau) - \operatorname{Tr} \left[\begin{pmatrix} -\partial_{\tau} + \frac{\nabla^{2}}{2m} + \mu & \Delta(\mathbf{r}, \tau) \\ \bar{\Delta}(\mathbf{r}, \tau) & -\partial_{\tau} - \frac{\nabla^{2}}{2m} - \mu \end{pmatrix}^{-1} \cdot \begin{pmatrix} 0 & 0 \\ \delta^{(d)}(\mathbf{r} - \mathbf{r}') \delta(\tau - \tau') & 0 \end{pmatrix} \right]. \quad (28)$$

注意以上求迹运算包括自旋空间求迹和场构型空间内求迹。在实空间下不容易对场构型求迹,可在动量空间完成,动量空间的一组基底为:

$$\psi_p = \sqrt{\frac{T}{L^d}} e^{i\mathbf{p}\cdot\mathbf{r} - i\omega_n\tau} \tag{29}$$

在这组基底下, 算符 \hat{F} 矩阵元可通过在基底上的作用得到:

$$(\hat{F})_{p',p} = \int d\tau \int d^d r \; \bar{\psi}_{p'} \hat{F} \psi_p = \frac{T}{L^d} \int d\tau \int d^d r \left(e^{-i\mathbf{p'}\cdot\mathbf{r} + i\omega_{n'}\tau} \hat{F} e^{i\mathbf{p}\cdot\mathbf{r} - i\omega_n\tau} \right). \tag{30}$$

比如:

$$(\partial_{\tau})_{p',p} = -i\delta_{pp'}\omega_n, \tag{31}$$

$$(\nabla)_{p',p} = i\delta_{pp'} \mathbf{p}, \tag{32}$$

$$(f(\mathbf{r},\tau))_{p',p} = \delta_{pp'}f_p. \tag{33}$$

由此作用,得到格林函数动量空间矩阵元为:

$$(\hat{\mathcal{G}})_{p',p} = \begin{pmatrix} \delta_{pp'}(i\omega_n - \xi_{\mathbf{p}}) & \Delta_{p'-p} \\ \bar{\Delta}_{p-p'} & \delta_{pp'}(i\omega_n + \xi_{\mathbf{p}}) \end{pmatrix}^{-1}$$
(34)

其中 $\xi_p = \frac{p^2}{2m} - \mu$, Δ_p 是 $\Delta(r, \tau)$ 的频率分量。而变分导数动量空间矩阵元为:

$$\left(\frac{\delta \hat{\mathcal{G}}^{-1}}{\delta \bar{\Delta}(\mathbf{r},\tau)}\right)_{p',p} = \frac{T}{L^d} \begin{pmatrix} 0 & 0\\ e^{-i(\mathbf{p}'-\mathbf{p})\cdot\mathbf{r}+i(\omega_{n'}-\omega_n)\tau} & 0 \end{pmatrix}.$$
(35)

这样,我们可以写出上述求迹表达式。这里假设极值解 $\Delta = \Delta_0 = \mathrm{const}$,极值解变为:

$$\frac{1}{g}\Delta_0 = \frac{T}{L^d} \sum_{\boldsymbol{p}} \begin{pmatrix} i\omega_n - \xi_{\boldsymbol{p}} & \Delta_0 \\ \bar{\Delta}_0 & i\omega_n + \xi_{\boldsymbol{p}} \end{pmatrix}_{12}^{-1} = \frac{T}{L^d} \sum_{\boldsymbol{p},n} \frac{\Delta_0}{\omega_n^2 + \xi_{\boldsymbol{p}}^2 + |\Delta_0|^2}.$$
 (36)

由此得到方程

$$\frac{1}{g} = \frac{T}{L^d} \sum_{\boldsymbol{p},n} \frac{1}{\omega_n^2 + \lambda_{\boldsymbol{p}}^2}.$$
 (37)

其中令 $\lambda_{q} = (\xi_{p}^{2} + |\Delta_{0}|^{2})^{1/2}$. 对频率求和:

$$T\sum_{n} \frac{1}{\omega_n^2 + \lambda_p^2} = \sum_{z_* = \pm \lambda_p} n_F(z_*) \operatorname{Res} \left[\frac{1}{z^2 - \lambda_p^2} \right]_{z = z_*} = \frac{1 - 2n_F(\lambda_p)}{2\lambda_p}.$$
(38)

动量空间求和中,只需考虑费米面附近 ω_D 的电子:

$$\frac{1}{g} = \frac{1}{L^d} \sum_{\mathbf{p}} \frac{1 - n_F(\lambda_{\mathbf{p}})}{2\lambda_{\mathbf{p}}} = \int_{-\omega_D}^{\omega_D} d\xi \ \nu(\xi) \frac{1 - n_F(\lambda(\xi))}{2\lambda(\xi)},\tag{39}$$

其中 ν 是态密度。由于 $1-2n_F(\xi)=\tanh(\xi/2T)$,得到能隙方程:

$$\frac{1}{g\nu} = \int_0^{\omega_D} d\xi \frac{\tanh(\xi/2T)}{\lambda(\xi)}.$$
 (40)

Ginzburg-Landau 理论

在相边界附近, Δ 可看作微扰, 可以将 BCS 有效作用量

$$S_{BCS}[\Psi, \bar{\Psi}] = \frac{1}{g} \int d\tau \int d^d r |\Delta|^2 - \text{Tr} \ln \hat{\mathcal{G}}^{-1}. \tag{41}$$

展开成 Δ 的级数。为此需要考虑 $\operatorname{Tr} \ln \hat{\mathcal{G}}^{-1}$ 关于 Δ 的级数展开。定义:

$$\hat{\mathcal{G}}_{0}^{-1} \equiv \begin{pmatrix} \hat{G}_{p}^{-1} & 0 \\ 0 & \hat{G}_{h}^{-1} \end{pmatrix},
\hat{\Delta} \equiv \begin{pmatrix} 0 & \Delta \\ \bar{\Delta} & 0 \end{pmatrix}.$$
(42)

由此可以做变换:

$$\operatorname{Tr} \ln \hat{\mathcal{G}}^{-1} = \operatorname{Tr} \ln \left[\hat{\mathcal{G}}_0^{-1} (1 + \hat{\mathcal{G}}_0^{-1} \hat{\Delta}) \right] = \operatorname{Tr} \ln \hat{\mathcal{G}}_0^{-1} + \operatorname{Tr} \ln [1 + \hat{\mathcal{G}}_0^{-1}]. \tag{43}$$

右边第二项可以展开为:

$$\ln[1 + \hat{\mathcal{G}}_0^{-1}\hat{\Delta}] = -\sum_{n} \frac{1}{2n} (\hat{\mathcal{G}}_0^{-1}\hat{\Delta})^{2n}.$$
 (44)

注意展开式没有奇数次项,因为奇数次 $\hat{\mathcal{G}}_0^{-1}\hat{\Delta}$ 乘积是无迹矩阵。

二阶近似

首先将表达式展开到二阶项 (n=1), 其结果为:

$$-\frac{1}{2}\operatorname{Tr}(\hat{\mathcal{G}}_0^{-1}\hat{\Delta})^2 = -\operatorname{Tr}[\hat{G}_p\bar{\Delta}\hat{G}_h\Delta]$$
(45)

同样, 求迹操作在频率空间完成。首先考虑傅立叶变换:

$$(\hat{\mathcal{G}}_0)_{p',p} \longrightarrow \delta_{pp'} \begin{pmatrix} G_p & 0 \\ 0 & -G_{-p} \end{pmatrix},$$
 (46)

$$(\hat{\Delta})_{p',p} \longrightarrow \begin{pmatrix} 0 & \Delta_{p'-p} \\ \bar{\Delta}_{p-p'} & 0 \end{pmatrix}.$$
 (47)

其中

$$G_p = \frac{1}{i\omega_n - \xi_n}. (48)$$

因此,展开到二阶项的作用量为:

$$S^{(2)} = \sum_{q} \Gamma_q^{-1} |\Delta(q)|^2, \ \Gamma_q^{-1} = \frac{1}{g} - \frac{T}{L^d} \sum_{p} G_p G_{q-p}.$$
 (49)

现在考虑求和式 $\sum_{p} G_{p}G_{q-p}$. 首先对频率求和:

$$T \sum_{m} \frac{1}{i\omega_{m} - \xi_{\mathbf{p}}} \frac{1}{i\omega_{n} - i\omega_{m} - \xi_{\mathbf{q} - \mathbf{p}}} = \sum_{z=z_{*}} n_{F}(z_{*}) \operatorname{Res} \left[\frac{1}{z - \xi_{\mathbf{p}}} \frac{1}{i\omega_{n} - z - \xi_{\mathbf{q} - \mathbf{p}}} \right]_{z-z_{*}}$$
$$= \frac{1 - n_{F}(\xi_{\mathbf{p}}) - n_{F}(\xi_{\mathbf{q} - \mathbf{p}})}{i\omega_{n} - \xi_{\mathbf{p}} - \xi_{\mathbf{q} - \mathbf{p}}}.$$
(50)

注意上式中 $q=({\pmb q},\omega_n)$ 是声子 4 动量。相变发生在 $\Gamma_q^{-1}=0$ 处。此时我们考虑时空均匀的解,即 q=(0,0). 由于 $\xi_{\pmb p}=\xi_{-\pmb p}$:

$$\frac{T}{L^d} \sum_{p} G_p G_{-p} = \int_{-\omega_D}^{\omega_D} d\xi \nu(\xi) \frac{1 - 2n_F(\xi)}{2\xi}.$$
 (51)

进一步化简上式之前,注意积分式正负频率对称,只需考虑正频部分。另外,由于分母 ξ 存在,零温下该积分是发散的。有限温度时,在 $0<\xi< T$ 区间的积分被费米分布函数控制。实际贡献主要在 $T<\xi<\omega_D$ 区间,在此小区间态密度可近似为相同,因此得到:

$$\frac{T}{L^d} \sum_{p} G_p G_{-p} \simeq \nu \int_{T}^{\omega_D} \frac{d\xi}{\xi} = \nu \ln \left(\frac{\omega_D}{T}\right). \tag{52}$$

由此确定相变点为:

$$T_c \simeq \omega_D \exp\left(-\frac{1}{g\nu}\right).$$
 (53)

四阶近似

当 $T < T_c$ 时,二次型的作用量变得不稳定,这时为得到对体系有效的描述,需要引入更高阶的微扰。二阶作用量的不稳定性源于时空均匀部分,而不是时空导数部分,因此对更高阶的微扰项,我们也只考虑时空均匀的部分,即:

$$S^{(4)} = \frac{1}{4} \operatorname{Tr}(\hat{\mathcal{G}}^{-1}\hat{\Delta})^4 \simeq \frac{1}{2n} \sum_{p} (G_p G_{-p})^2 |\Delta|^4.$$
 (54)

上式可近似为:

$$S^{(4)} \simeq \frac{\nu|\Delta|^4}{4} \sum_n \int_{-\omega_D}^{\omega_D} \frac{d\xi}{(\omega_n^2 + \xi^2)^2} \propto \nu|\Delta|^4 \sum_n \frac{1}{\omega_n^3} \propto \nu T \left(\frac{|\Delta|}{T}\right)^4. \tag{55}$$

Ginzburg-Landau 经典作用量为:

$$S_{GL}[\Delta, \bar{\Delta}] = \beta \int d^d r \left[\frac{r}{2} |\Delta|^2 + \frac{c}{2} |\partial \Delta|^2 + u|\Delta|^4 \right]. \tag{56}$$

从 Ginzburg-Landau 作用量看出, 当 r < 0 时, 辅助场 Δ 具有的 U(1) 对称性发生自发破缺。

规范对称性自发破缺

规范不变作用量

费米场具有 U(1) 规范对称性:

$$\psi \rightarrow e^{i\theta}\psi,$$
(57)

$$\bar{\psi} \rightarrow e^{-i\theta}\bar{\psi}.$$
 (58)

相应地,为了保证作用量是规范不变的,将对 ψ 作用的时空导数算符替换为协变导数算符:

$$\partial_{\tau} \rightarrow \partial_{\tau} + ie\phi,$$
 (59)

$$\nabla \rightarrow \nabla - ie\mathbf{A}.$$
 (60)

其中电磁势在规范变换下:

$$\phi \rightarrow \phi - \frac{1}{e}\partial_{\tau}\theta,$$
 (61)

$$\mathbf{A} \rightarrow \mathbf{A} + \frac{1}{e} \nabla \theta.$$
 (62)

类似的,对共轭场 $\bar{\psi}$ 作用的时空导数算符在规范变换下:

$$\partial_{\tau} \rightarrow \partial_{\tau} - ie\phi,$$
 (63)

$$\nabla \rightarrow \nabla + ie\mathbf{A}.$$
 (64)

因此, 考虑外电磁场情况下, 辅助场 Δ 的有效作用量变为:

$$S[\Delta, \bar{\Delta}] = \frac{1}{a} \int d\tau \int d^d r |\Delta|^2 - \operatorname{Tr} \ln \hat{\mathcal{G}}^{-1}.$$
 (65)

其中规范不变的格林函数为:

$$\hat{\mathcal{G}}^{-1} = \begin{pmatrix} -(\partial_{\tau} + i\phi) + \frac{1}{2m}(\nabla - i\mathbf{A})^{2} + \mu & \Delta \\ \bar{\Delta} & -(\partial_{\tau} - i\phi) - \frac{1}{2m}(\nabla + i\mathbf{A})^{2} - \mu \end{pmatrix}.$$
(66)

规范场微扰展开

对 Ginzburg-Landau 作用量, 当 $T < T_c$ 时, r(T) < 0, 此时经典作用量在

$$|\Delta| = \Delta_0 = \sqrt{\frac{-r}{4u}} \tag{67}$$

取得极值。极值场选取有一个整体相位不确定性:

$$\Delta = \Delta_0 e^{2i\theta}. (68)$$

此相位也对应费米场的 U(1) 定域规范对称性。此作用量的经典基态对应一个确定的相位 θ ,此时规范对称性发生自发破缺。

我们从对称性破缺的基态开始,建立剩余自由度: 规范场 (ϕ, \mathbf{A}) 和相位 θ 的低能场论 (此时辅助场 Δ 绝对值固定,只剩一个相位自由度)。首先,我们引入一个规范变换:

$$\hat{U}(\mathbf{r},\tau) = \begin{pmatrix} e^{-i\theta(\mathbf{r},\tau)} & 0\\ 0 & e^{i\theta(\mathbf{r},\tau)} \end{pmatrix}$$
(69)

此规范变换将 $\Delta_0 e^{2i\theta}$ 的相位消去:

$$\hat{\mathcal{G}}^{-1} \to \hat{U}^{-1}\hat{\mathcal{G}}^{-1}\hat{U} = \begin{pmatrix} -(\partial_{\tau} + i\tilde{\phi}) + \frac{1}{2m}(\nabla - i\tilde{A})^2 + \mu & \Delta_0 \\ \Delta_0 & -(\partial_{\tau} - i\tilde{\phi}) - \frac{1}{2m}(\nabla + i\tilde{A})^2 - \mu \end{pmatrix}.$$
(70)

其中 $\tilde{\phi}$, \tilde{A} 是规范场相应的规范变换:

$$\tilde{\phi} = \phi + \partial_{\tau}\theta, \ \tilde{\mathbf{A}} = \mathbf{A} - \nabla\theta. \tag{71}$$

将格林函数中规范场部分显式写出来:

$$\hat{\mathcal{G}}^{-1} = \hat{\mathcal{G}}_0^{-1} - \hat{\mathcal{X}}_1 - \hat{\mathcal{X}}_2. \tag{72}$$

其中

$$\hat{\mathcal{G}}_0^{-1} = -\sigma_0 \partial_\tau + \sigma_1 \Delta_0 + \sigma_3 \left(\frac{\nabla^2}{2m} + \mu \right), \tag{73}$$

$$\hat{\mathcal{X}}_1 = \sigma_3 \tilde{\phi} + \frac{i}{2m} \sigma_0 (\nabla \tilde{\mathbf{A}} + \tilde{\mathbf{A}} \nabla), \tag{74}$$

$$\hat{\mathcal{X}}_2 = \sigma_3 \frac{1}{2m} \tilde{A}^2. \tag{75}$$

精确至二阶的展开式为:

$$-\operatorname{Tr}\ln\left(\hat{\mathcal{G}}_{0}^{-1} - \hat{\mathcal{X}}_{1} - \hat{\mathcal{X}}_{2}\right) = -\operatorname{Tr}\ln\hat{\mathcal{G}}_{0}^{-1} - \operatorname{Tr}\ln\left(1 - \hat{\mathcal{G}}_{0}\hat{\mathcal{X}}_{1} - \hat{\mathcal{G}}_{0}\hat{\mathcal{X}}_{2}\right)$$

$$= -\operatorname{Tr}\ln\hat{\mathcal{G}}_{0}^{-1} + \operatorname{Tr}\left(\hat{\mathcal{G}}_{0}\hat{\mathcal{X}}_{1}\right) + \operatorname{Tr}\left(\hat{\mathcal{G}}_{0}\hat{\mathcal{X}}_{2} + \frac{1}{2}\hat{\mathcal{G}}_{0}\hat{\mathcal{X}}_{1}\hat{\mathcal{G}}_{0}\hat{\mathcal{X}}_{1}\right). \tag{76}$$

首先考虑一阶微扰 $S^{(1)}=\mathrm{Tr}\left(\hat{\mathcal{G}}_0^{-1}\hat{\mathcal{X}}_1\right)$. 为了方便求迹,首先在动量空间写出前三个算符的傅立叶变换:

$$(\hat{\mathcal{G}}_0^{-1})_{p',p} = \delta_{pp'}(i\sigma_0\omega_n + \sigma_1\Delta_0 - \sigma_3\xi_{\boldsymbol{p}}), \tag{77}$$

$$(\hat{\mathcal{X}}_1)_{p',p} = i\sigma_3 \tilde{\phi}_{p'-p} - \delta_{pp'} \sigma_0 \frac{(\mathbf{p'} + \mathbf{p}) \cdot \tilde{\mathbf{A}}_{p'-p}}{2m}, \tag{78}$$

$$(\hat{\mathcal{X}}_2)_{p',p} = \frac{1}{2m} \sigma_3(\tilde{\mathbf{A}}^2)_{p'-p}. \tag{79}$$

求迹转换为动量求和:

$$S^{(1)}[A] = \sum_{p} \operatorname{tr} \left[\hat{\mathcal{G}}_{0,p} \left(i \sigma_3 \tilde{\phi}_0 - \frac{1}{m} \sigma_0 \mathbf{p} \cdot \tilde{\mathbf{A}}_0 \right) \right]. \tag{80}$$

注意上式已经对时空求迹。由于第二项含有p的奇数次项,因此为零,因此作用量变为:

$$S^{(1)}[A] = i\tilde{\phi}_0 \sum_{p} \text{tr}\left(\hat{\mathcal{G}}_{0,p}\sigma_3\right) = i\tilde{\phi}_0 \sum_{p} \left[\left(\hat{\mathcal{G}}_{0,p}\right)_{1,1} - \left(\hat{\mathcal{G}}_{0,p}\right)_{2,2} \right]. \tag{81}$$

频率求和之后:

$$\sum_{\mathbf{p}} \sum_{n} \left(\hat{\mathcal{G}}_{0,p} \right)_{1,1} = -\sum_{\mathbf{p}} \sum_{n} \left(\hat{\mathcal{G}}_{0,p} \right)_{2,2} = \frac{1}{T} \sum_{\mathbf{p}} n_F(\xi_{\mathbf{p}}) = \frac{N_e}{T}.$$
 (82)

因此:

$$S^{(1)}[A] = iN_e\beta\tilde{\phi}_0 = iN_e\beta\int\frac{d\tau}{\beta}\int\frac{d^dr}{L^d}\phi(\mathbf{r},\tau) = in_e\int d\tau d^dr\phi(\mathbf{r},\tau). \tag{83}$$

其中 $n \equiv N_e/L^d$, 此贡献来源于静电场于电子耦合。现在考虑二阶微扰,首先考虑第一部分贡献:

$$S^{(2,1)} = \operatorname{Tr}\left(\hat{\mathcal{G}}_0\hat{\mathcal{X}}_2\right). \tag{84}$$

求迹为:

$$S^{(2,1)} = \frac{(\tilde{\mathbf{A}}^2)_0}{2m} \sum_{p} \operatorname{tr}\left(\hat{\mathcal{G}}_{0,p}\sigma_3\right) = \frac{n_e}{2m} L^d \beta(\tilde{\mathbf{A}}^2)_0 = \frac{n_e}{2m} \int d\tau d^d r \tilde{\mathbf{A}}^2(\mathbf{r},\tau). \tag{85}$$

现在考虑第二部分贡献:

$$S^{(2,2)} = \frac{1}{2} \operatorname{tr} \left(\hat{\mathcal{G}}_0 \hat{\mathcal{X}}_1 \hat{\mathcal{G}}_0 \hat{\mathcal{X}}_1 \right). \tag{86}$$

注意包含 p 奇数次项的部分求迹为零,因此作用量分为两部分, $S^{(2,2)}=S_A^{(2,2)}+S_B^{(2,2)}$:

$$S_A^{(2,2)} = \sum_{p,q} \operatorname{tr} \left(-\hat{\mathcal{G}}_{0,p} \sigma_3 \tilde{\phi}_q \hat{\mathcal{G}}_{0,p+q} \sigma_3 \tilde{\phi}_{-p} \right), \tag{87}$$

$$S_B^{(2,2)} = \sum_{p,q} \operatorname{tr} \left(\hat{\mathcal{G}}_{0,p} \frac{\sigma_0(2p+q) \cdot \tilde{\mathbf{A}}_q}{2m} \hat{\mathcal{G}}_{0,p+q} \frac{\sigma_0(2p+q) \cdot \tilde{\mathbf{A}}_{-q}}{2m} \right). \tag{88}$$

在微扰意义下,规范场时空导数较小,即 $q \ll p$,因此做近似:

$$S_A^{(2,2)} \approx -\sum_{p,q} \operatorname{tr} \left(\hat{\mathcal{G}}_{0,p} \sigma_3 \tilde{\phi}_q \hat{\mathcal{G}}_{0,p} \sigma_3 \tilde{\phi}_{-p} \right), \tag{89}$$

$$S_B^{(2,2)} \approx \frac{1}{m^2} \sum_{p,q} \operatorname{tr} \left(\hat{\mathcal{G}}_{0,p} \sigma_0 \boldsymbol{p} \cdot \tilde{\boldsymbol{A}}_q \hat{\mathcal{G}}_{0,p} \sigma_0 \boldsymbol{p} \cdot \tilde{\boldsymbol{A}}_{-q} \right). \tag{90}$$

利用等式:

$$\hat{\mathcal{G}}_{0,p} = \frac{-i\sigma_0\omega_n - \sigma_3\xi_{\mathbf{p}} + \sigma_1\Delta_0}{\omega_n^2 + \lambda_{\mathbf{p}}^2},\tag{91}$$

得到 A 项:

$$S_A^{(2,2)} = \sum_{p,q} \frac{\tilde{\phi}_q \tilde{\phi}_{-q} (\omega_n^2 - \lambda_p^2 + 2\Delta_0^2)}{(\omega_n^2 + \lambda_p^2)^2}$$
(92)

对 B 项, 利用恒等式:

$$\sum_{\mathbf{p}} (\mathbf{p} \cdot \tilde{\mathbf{A}}_q) (\mathbf{p} \cdot \tilde{\mathbf{A}}_{-q}) F(\mathbf{p}^2) = \frac{\tilde{\mathbf{A}}_q \cdot \tilde{\mathbf{A}}_{-q}}{d} \sum_{\mathbf{p}} \mathbf{p}^2 F(\mathbf{p}^2).$$
(93)

其中 $F(p^2)$ 是任意旋转不变函数,因此:

$$S_B^{(2,2)} = \sum_{p,q} \frac{-\omega_n^2 + \lambda_p^2}{(\omega_n^2 + \lambda_p^2)^2} \frac{p^2 \tilde{A}_q \cdot \tilde{A}_{-q}}{dm^2}.$$
 (94)

现在变换回实空间:

$$S^{(2)}[A] = \int d\tau d^d r \left[c_1 (\phi + \partial_\tau \theta)^2 + c_2 (\boldsymbol{A} - \nabla \theta)^2 \right]. \tag{95}$$

其中:

$$c_1 = \frac{T}{L^d} \sum_{p} \frac{\omega_n^2 - \lambda_p^2 + 2\Delta_0^2}{(\omega_n^2 + \lambda_p^2)^2}, \tag{96}$$

$$c_2 = \frac{n_e}{2m} + \frac{1}{dm^2} \frac{T}{L^d} \sum_{p} \frac{p^2(-\omega_n^2 + \lambda_p^2)}{(\omega_n^2 + \lambda_p^2)}.$$
 (97)

首先考虑 c₁ 求和式。频率求和为:

$$T \sum_{n} \frac{\omega_{n}^{2} - \lambda_{p}^{2} + 2\Delta_{0}^{2}}{(\omega_{n}^{2} + \lambda_{p}^{2})^{2}}$$

$$= \sum_{z_{*}=\pm\lambda_{p}} \operatorname{Res} \left[\frac{n_{F}(z)(-z^{2} - \lambda_{p}^{2} + 2\Delta_{0}^{2})}{(z + \lambda_{p})^{2}(z - \lambda_{p})^{2}} \right]_{z=z_{*}}$$

$$= \left[\frac{n_{F}(z)(-z^{2} - \lambda_{p}^{2} + 2\Delta_{0}^{2})}{(z + \lambda_{p})^{2}} \right]_{z=\lambda_{p}}' + \left[\frac{n_{F}(z)(-z^{2} - \lambda_{p}^{2} + 2\Delta_{0}^{2})}{(z - \lambda_{p})^{2}} \right]_{z=-\lambda_{p}}'$$

$$= \frac{1}{2\lambda_{p}} \left[-n'_{F}(\lambda_{p})\xi_{p}^{2} - n_{F}(\lambda_{p}) \left(\frac{\Delta_{0}}{\lambda_{p}} \right)^{2} + n'_{F}(-\lambda_{p})\xi_{p}^{2} + n_{F}(-\lambda_{p}) \left(\frac{\Delta_{0}}{\lambda_{p}} \right)^{2} \right]. \tag{98}$$

由于我们现在考虑的是 $T < T_c$ 情形, $T/\Delta \to 0$,此时频率求和的贡献几乎全部来源于含有费米分布 $n_F(-\lambda_p)$ 的项,即:

$$c_1 \simeq \frac{1}{L^d} \sum_{\mathbf{p}} \frac{\Delta_0^2}{2\lambda_{\mathbf{p}}^3} = \frac{\nu}{2} \int d\xi \frac{\Delta_0^2}{(\xi^2 + \Delta_0^2)^{3/2}} = \nu.$$
 (99)

因此, 我们得到了作用量的系数 c_1 等于费米面附近的态密度 ν . 下面考虑 c_2 的求和式。频率求和为:

$$T \sum_{n} \frac{-\omega_n^2 + \lambda_{\mathbf{p}}^2}{(\omega_n^2 + \lambda_{\mathbf{p}}^2)^2} = \sum_{z_* = \pm \lambda_{\mathbf{p}}} \text{Res} \left[\frac{n_F(z)(z^2 + \lambda_{\mathbf{p}}^2)}{(z + \lambda_{\mathbf{p}})^2 (z - \lambda_{\mathbf{p}})^2} \right]_{z = z_*}$$

$$= \left[\frac{n_F(z)(z^2 + \lambda_p^2)}{(z + \lambda_p)^2}\right]'_{z=\lambda_p} + \left[\frac{n_F(z)(z^2 + \lambda_p^2)}{(z - \lambda_p)^2}\right]'_{z=-\lambda_p}$$

$$= n'_F(\lambda_p)$$

$$= -\beta n_F(\lambda_p)(1 - n_F(\lambda_p)). \tag{100}$$

费米面附近 $p^2 \approx 2m\mu$, 由此得到:

$$c_2 = \frac{n_e}{2m} - \frac{\nu\mu}{dm} \int d\xi \, \beta n_F(\lambda) (1 - n_F(\lambda)). \tag{101}$$

定义超导电子密度:

$$n_s = n_e - \frac{2\nu\mu}{d} \int d\xi \, \beta n_F(\lambda) (1 - n_F(\lambda)). \tag{102}$$

在低温 $T \ll \Delta_0$ 时, $\lambda > \Delta_0 \gg T$, 因此 $n_F(\lambda) \approx 0$, 此时 $n_s \approx n_e$. 相反, 在高温 $T \gg \delta_0$ 时:

$$\int d\xi \beta n_F(\lambda) (1 - n_F(\lambda)) \approx \int_0^\infty d\xi \beta n_F(\lambda) (1 - n_F(\lambda))$$

$$= -\int_0^\infty d\xi \partial_\xi n_F(\xi) = 1. \tag{103}$$

此时

$$n_s \simeq \frac{n_e}{2m} - \frac{\nu\mu}{dm} = 0. \tag{104}$$

第二个等式来自于电子密度与态密度关系:

$$\nu = \frac{\partial n_e}{\partial \xi}$$

$$= \frac{\partial (V_d p^d)}{\partial p} \left(\frac{\partial (p^2/2m)}{\partial p}\right)^{-1}$$

$$= \frac{dV_d p^{d-1}}{p/m} = \frac{dn_e}{2\mu}.$$
(105)

Meissner 效应

现在我们已经得到破缺对称性后的低能理论作用量:

$$S[A, \theta] = S_{E-M} + \int d\tau d^d r \left[\nu (\partial_\tau \theta + \phi)^2 + \frac{n_s}{2m} (\nabla \theta - \mathbf{A})^2 \right]$$
 (106)

其中

$$S_{E-M} = \int d\tau d^d r \frac{1}{4} F_{\mu\nu} F^{\mu\nu}$$
 (107)

是电磁场作用量。现在考虑只有静磁场的情况,即要求:

$$\phi = 0, \ \partial_{\tau} \mathbf{A} = 0. \tag{108}$$

此时,作用量可分为:

$$S[\mathbf{A}, \theta] = S_{cl}[\mathbf{A}, \theta] + \nu \int d\tau \int d^d r (\partial_\tau \theta)^2.$$
 (109)

其中 Scl 是经典作用量 (场量在虚时间上无涨落):

$$S_{cl}[\mathbf{A}, \theta] = \frac{\beta}{2} \int d^d r \left[\frac{n_s}{m} (\nabla \theta - \mathbf{A})^2 + (\nabla \times \mathbf{A})^2 \right].$$
 (110)

此时,作用量中的量子量子涨落完全来源于第二项

$$\nu \int d\tau \int d^d r (\partial_\tau \theta)^2 = \nu \sum_{\mathbf{q},n} \omega_n \theta_{\mathbf{q},n} \theta_{-\mathbf{q},-n}. \tag{111}$$

这项的大小与温度密切相关,当我们考虑较高温度 (但仍有 $T < T_c$) 时,n > 0 的松原频率贡献的作用量可能远大于 S_{cl} ,此时我们就可以忽略这些"高能"的自由度,而只考虑经典部分作用量。下面考虑这个经典作用量给出的有效理论。首先,将作用量写在动量空间中:

$$S_{cl}[\boldsymbol{A}, \boldsymbol{\theta}] = \frac{\beta}{2} \sum_{\boldsymbol{q}} \left[\frac{n_s}{m} (i\boldsymbol{q}\boldsymbol{\theta}_{\boldsymbol{q}} - \boldsymbol{A}_{\boldsymbol{q}}) \cdot (-i\boldsymbol{q}\boldsymbol{\theta}_{-\boldsymbol{q}} - \boldsymbol{A}_{-\boldsymbol{q}}) + (\boldsymbol{q} \times \boldsymbol{A}_{\boldsymbol{q}}) \cdot (\boldsymbol{q} \times \boldsymbol{A}_{-\boldsymbol{q}}) \right]$$

$$= \frac{\beta}{2} \sum_{\boldsymbol{q}} \left[\frac{n_s}{m} (\boldsymbol{\theta}_{\boldsymbol{q}} \boldsymbol{q}^2 \boldsymbol{\theta}_{-\boldsymbol{q}} - 2i\boldsymbol{\theta}_{\boldsymbol{q}} \boldsymbol{q} \cdot \boldsymbol{A}_{-\boldsymbol{q}} + \boldsymbol{A}_{\boldsymbol{q}} \cdot \boldsymbol{A}_{-\boldsymbol{q}}) + (\boldsymbol{q} \times \boldsymbol{A}_{\boldsymbol{q}}) \cdot (\boldsymbol{q} \times \boldsymbol{A}_{-\boldsymbol{q}}) \right]$$
(112)

为得到规范场的有效理论,我们积掉 θ_q ,得到有效作用量:

$$S_{eff}[\mathbf{A}] = \frac{\beta}{2} \sum_{\mathbf{q}} \left[\frac{n_s}{m} \left(\mathbf{A}_{\mathbf{q}} \cdot \mathbf{A}_{-\mathbf{q}} - \frac{(\mathbf{q} \cdot \mathbf{A}_{\mathbf{q}}) \cdot (\mathbf{q} \cdot \mathbf{A}_{-\mathbf{q}})}{\mathbf{q}^2} \right) + (\mathbf{q} \times \mathbf{A}_{\mathbf{q}}) \cdot (\mathbf{q} \times \mathbf{A}_{-\mathbf{q}}) \right]$$
(113)

将矢势分解成横向和纵向分量:

$$\mathbf{A}_{q} = \mathbf{A}_{q}^{\perp} + \mathbf{A}_{q}^{\parallel},
\mathbf{A}_{q}^{\perp} = \mathbf{A}_{q} - \frac{q(q \cdot \mathbf{A}_{q})}{q^{2}},
\mathbf{A}_{q}^{\parallel} = \frac{q(q \cdot \mathbf{A}_{q})}{a^{2}}.$$
(114)

注意到

$$\boldsymbol{A}_{\boldsymbol{q}}^{\perp} \cdot \boldsymbol{A}_{-\boldsymbol{q}}^{\perp} = \boldsymbol{A}_{\boldsymbol{q}} \cdot \boldsymbol{A}_{-\boldsymbol{q}} - \frac{(\boldsymbol{q} \cdot \boldsymbol{A}_{\boldsymbol{q}}) \cdot (\boldsymbol{q} \cdot \boldsymbol{A}_{-\boldsymbol{q}})}{\boldsymbol{q}^2}. \tag{115}$$

同时由于 $\mathbf{q} \times \mathbf{A}_{\mathbf{q}}^{\parallel} = 0$:

$$(\mathbf{q} \times \mathbf{A}_{\mathbf{q}}) \cdot (\mathbf{q} \times \mathbf{A}_{-\mathbf{q}}) = (\mathbf{q} \times \mathbf{A}_{\mathbf{q}}^{\perp}) \cdot (\mathbf{q} \times \mathbf{A}_{-\mathbf{q}}^{\perp})$$
$$= \mathbf{q}^{2} \mathbf{A}_{\mathbf{q}}^{\perp} \cdot \mathbf{A}_{-\mathbf{q}}^{\perp}$$
(116)

第二个等号利用了恒等式:

$$(u_1 \times u_2) \cdot (v_1 \times v_2) = (u_1 \cdot v_1)(u_2 \cdot v_2) - (u_1 \cdot v_2)(u_2 \cdot v_1). \tag{117}$$

由此得到作用量:

$$S_{eff}[\mathbf{A}] = \frac{\beta}{2} \sum_{\mathbf{q}} \left(\frac{n_s}{m} + \mathbf{q}^2 \right) \mathbf{A}_{\mathbf{q}}^{\perp} \cdot \mathbf{A}_{-\mathbf{q}}^{\perp}. \tag{118}$$

此时规范场 A_q^\perp 的有效作用量含有一个质量项,这导致超导体内部的抗磁性。我们考虑这个经典作用量给出的运动方程:

$$\left(\frac{n_s}{m} - \nabla^2\right) \mathbf{A}(\mathbf{r}) = 0. \tag{119}$$

对方程两边作用 ∇×:

$$\left(\frac{n_s}{m} - \nabla^2\right) \mathbf{B}(\mathbf{r}) = 0. \tag{120}$$

此运动方程给出一个指数衰减的解: $\boldsymbol{B}(x)\sim \exp(-x/\lambda)$,其中 $\lambda=\sqrt{m/n_s}$.