凝聚态场论-Basis

李梓瑞

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1 Classical Field

在介绍量子场论之前, 我们先回顾一下经典场论的内容. 取度规为 $(+---)$

$$H = \int d^3x \mathcal{H}, \quad L = \int d^3x \mathcal{L} \tag{1}$$

其中 $\mathcal{H}, \mathcal{L}$ 分别是对应的密度. 由拉格朗日量和哈密顿量的关系可知

$$\mathcal{L}[\phi, \dot{\phi}] = \pi[\phi, \dot{\phi}]\dot{\phi} - \mathcal{H}[\phi, \pi[\phi, \dot{\phi}]], \quad \pi = \frac{\partial \mathcal{L}[\phi, \dot{\phi}]}{\partial \dot{\phi}} \tag{2}$$

where

$$\mathcal{H} = \mathcal{K} + \mathcal{V}, \quad \mathcal{L} = \mathcal{K} - \mathcal{V} \tag{3}$$

动能项比如

$$\frac{1}{2}\phi\partial^2\phi, \quad \bar{\psi}\not{\partial}\psi, \quad \frac{1}{4}F_{\mu\nu}^2, \quad \frac{1}{2}m^2\phi^2 \ldots \tag{4}$$

相互作用项比如

$$\lambda\phi^3, \quad g\bar{\psi}\not{A}\psi, \quad g^2 A_\mu^2 A_\nu^2 \ldots \tag{5}$$

变分得到欧拉-拉格朗日方程

$$\frac{\partial \mathcal{L}}{\partial \phi} - \partial_\mu \frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi)} = 0 \tag{6}$$

对于连续对称性有诺特定理, 对应的诺特流 (满足运动方程)

$$J_\mu = \sum_n \frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi_n)} \frac{\delta \phi_n}{\delta \alpha}, \quad \partial_\mu J_\mu = 0 \tag{7}$$

其中荷

$$Q = \int d^3 x J_0 \tag{8}$$

进一步定义能动张量 (对应平移不变性)

$$\mathcal{T}_{\mu\nu} = \sum_n \frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi_n)} \partial_\nu \phi_n - g_{\mu\nu}\mathcal{L}, \quad \partial_\mu \mathcal{T}_{\mu\nu} = 0 \tag{9}$$

其中能量密度

$$\mathcal{E} = \mathcal{T}_{00} = \sum_n \frac{\partial \mathcal{L}}{\partial \dot{\phi}} \dot{\phi}_n - \mathcal{L} \tag{10}$$

2 Q.M. and Stat.Phy.

不同于普通量子力学和相对论量子场论的操作, 我们这里直接做路径积分量子化. 考虑 ($\hbar = c = 1$)

$$H = \frac{p^2}{2m} + V(q), \quad U(q_f, q_i, \epsilon) = \langle q_f | e^{-iH\epsilon} | q_i \rangle \simeq \langle q_f | e^{-i\epsilon \frac{p^2}{2m}} e^{-i\epsilon V} | q_i \rangle \tag{11}$$

插入动量的完备性关系式计算

$$U(q_f, q_i, \epsilon) = \left(\frac{m}{2\pi i \epsilon}\right)^{1/2} \exp\left\{ i\epsilon \left[\frac{m}{2} \frac{(q_f - q_i)^2}{\epsilon^2} - V(q_i) \right] \right\} = \left(\frac{m}{2\pi i \epsilon}\right)^{1/2} e^{iS(q_f, q_i, \epsilon) + \mathcal{O}(\epsilon^2)} \tag{12}$$

对于有限时间的演化

$$\begin{aligned} U(q_f, q_i, t = t_f - t_i) &= \langle q_f | e^{-iH\epsilon} \cdots e^{-iH\epsilon} | q_i \rangle && (13) \\ &= \int \prod_{k=1}^{N-1} dq_k \prod_{k=1}^{N} U(q_k, q_{k-1}, \epsilon) && (14) \\ &= \lim_{N\to\infty} \left(\frac{mN}{2\pi i t}\right)^{N/2} \int \prod_{k=1}^{N-1} dq_k e^{iS[q]} && (15) \end{aligned}$$

where

$$S[q]=\sum_{k=1}^{N}S(q_k,q_{k-1};\epsilon)=\epsilon\sum_{k=1}^{N}\left[\frac{m}{2}\frac{(q_k-q_{k-1})^2}{\epsilon^2}-V(q_{k-1})\right] \tag{16}$$

在连续化极限下, 可以形式地写出

$$U(q_f,q_i,t=t_f-t_i)=\int_{q(t_i)=q_i}^{q(t_f)=q_f}\mathcal{D}[q]e^{\frac{i}{\hbar}S[q]} \tag{17}$$

where

$$\mathcal{D}[q]=\lim_{N\to\infty}\left(\frac{mN}{2\pi i\hbar t}\right)^{N/2}\prod_{k=1}^{N-1}dq_k,\quad S[q]=\int_{t_i}^{t_f}dtL(q,\dot{q}) \tag{18}$$

在海森堡表象下 $q(t)=e^{iHt}qe^{-iHt}$, 矩阵元

$$\langle q_f,t_f|q(t)|q_i,t_i\rangle=\langle q_f|e^{-iH(t_f-t)}qe^{-iH(t-t_i)}|q_i\rangle=\int_{q(t_i)=q_i}^{q(t_f)=q_f}\mathcal{D}[q]q(t)e^{iS[q]} \tag{19}$$

同样对于两算符关联

$$\langle q_f,t_f|Tq(t)q(t')|q_i,t_i\rangle=\int_{q(t_i)=q_i}^{q(t_f)=q_f}\mathcal{D}[q]q(t)q(t')e^{iS[q]} \tag{20}$$

时序算符定义为

$$Tq(t)q(t')=\Theta(t-t')q(t)q(t')+\Theta(t'-t)q(t')q(t) \tag{21}$$

接下来我们考虑配分函数, 在 qft 中这是指对场的所有构型加权求和

$$Z=\mathrm{Tr}e^{-\beta H}=\int dq\,\langle q|e^{-\beta H}|q\rangle \tag{22}$$

定义 Wick 转动 $t\to -i\tau$, 于是演化算符变为

$$U(q_f,q_i;-i\tau)=\lim_{N\to\infty}\left(\frac{mN}{2\pi\tau}\right)^{N/2}\int\prod_{k=1}^{N-1}dq_k\exp\left\{-\epsilon\sum_{k=1}^{N}\left[\frac{m}{2}\frac{(q_k-q_{k-1})^2}{\epsilon^2}+V(q_{k-1})\right]\right\} \tag{23}$$

$$=\int_{q(0)=q_i}^{q(\tau)=q_f}\mathcal{D}[q]e^{-S_E[q]} \tag{24}$$

where

$$S_E[q] = \int_0^\tau d\tau' \left[\frac{m}{2}\dot{q} + V(q)\right] \tag{25}$$

这称为 Euclidean 空间的作用量或虚时作用量, 相应的原来的作用量称为实时作用量. 于是配分函数可以写成

$$Z = \int dq U(q, q, -i\beta) = \int_{q(\beta)=q(0)} \mathcal{D}[q] e^{-S_E[q]} \tag{26}$$

进一步可以算出单点平均和两点平均

$$\langle q(\tau)\rangle = \frac{1}{Z}\mathrm{Tr}[e^{-\beta H} q(\tau)] = \frac{1}{Z}\int_{q(\beta)=q(0)} \mathcal{D}[q] q(\tau) e^{-S_E[q]} \tag{27}$$

$$\langle T_\tau q(\tau) q(\tau')\rangle = \frac{1}{Z}\int_{q(\beta)=q(0)} \mathcal{D}[q] q(\tau) q(\tau') e^{-S_E[q]} \tag{28}$$

考虑耦合上磁场, 这里 q 和 A 都是三维矢量

$$H = \frac{1}{2m}[p - eA(q)]^2, \quad S(q_k, q_{k-1}; \epsilon) = \frac{m}{2}\frac{q_k^2 - q_{k-1}^2}{\epsilon^2} + e(q_k - q_{k-1}) \cdot A(q) \tag{29}$$

做规范变换 $A \to A + \nabla\Lambda$

$$U(q_f, q_i; t = t_f - t_i) \to e^{i\epsilon\Lambda(q_f)} U(q_f, q_i; t = t_f - t_i) e^{-i\epsilon\Lambda(q_i)} \tag{30}$$

$$\psi(q) \to e^{-i\epsilon\Lambda(q)}\psi(q) \tag{31}$$

对于演化算符有 midpoint rule

$$U(q_k, q_{k-1}; \epsilon) = \left(\frac{m}{2\pi i\epsilon}\right)^{3/2} \exp\left\{ i\epsilon \left[\frac{m}{2}\frac{(q_k - q_{k-1})^2}{\epsilon^2} + \frac{e}{2}\frac{q_k - q_{k-1}}{\epsilon} \cdot (A(q_k) + A(q_{k-1}))\right]\right\} \tag{32}$$

凝聚态体系中都是多粒子系统, 为此我们需要拓展单粒子的路径积分形式

$$Z = \frac{1}{N!}\sum_{P\in S_N} \epsilon_P \int dq_1 \cdots dq_N (q_1 \cdots q_N | e^{-\beta H} | q_{P(1)} \cdots q_{P(N)}) \tag{33}$$

$$= \frac{1}{N!}\sum_{P\in S_N} \epsilon_P \int_{q_i(\beta) = q_{P(i)}(0)} \mathcal{D}[q] e^{-S_E[q]} \tag{34}$$

其中 $|q_1\cdots q_N\,)=|q_1\rangle\cdots|q_N\rangle$, 求和表示取轮换,$\epsilon_P$ 区分 boson 和 fermion, 前者是 1 而后者是 $(-1)^P$ (对于偶数次轮换为 1, 对于奇数次轮换为-1).

$$\int dq_1\cdots dq_N|q_1\cdots q_N\,)\,(\,q_1\cdots q_N|=1 \tag{35}$$

$$S_E[q]=\int_0^\beta d\tau\left[\frac{m}{2}\sum_{i=1}^N\dot{q}_i^2+\sum_{i,j=1\,(i<j)}^N v(q_i-q_j)\right] \tag{36}$$

下面补充一点统计中的泛函积分, 考虑振动弦

$$\mathcal{L}(\partial_x\phi,\dot{\phi})=\frac{1}{2}\rho\dot{\phi}^2-\frac{1}{2}\kappa(\partial_x\phi)^2 \tag{37}$$

于是

$$\Pi(x,t)=\rho\dot{\phi}(x,t),\quad H=\int_0^L dx\left[\frac{\Pi^2}{2\rho}+\frac{1}{2}\kappa(\partial_x\phi)^2\right] \tag{38}$$

做正则量子化, 设场算符和动量算符满足对易关系

$$[\phi(x),\Pi(x')]=i\delta(x-x') \tag{39}$$

引入傅里叶变换后动量空间的算符

$$\phi(k)=\frac{1}{\sqrt{L}}\int_0^L dx e^{-ikx}\phi(x)=\phi^\dagger(-k) \tag{40}$$

$$\Pi(k)=\frac{1}{\sqrt{L}}\int_0^L dx e^{-ikx}\Pi(x)=\Pi^\dagger(-k) \tag{41}$$

$$[\phi(k),\phi(k')]=[\Pi(k),\Pi(k')]=0,\quad [\phi(k),\Pi^\dagger(k')]=i\delta_{k,k'} \tag{42}$$

重写原来的哈密顿量

$$H=\sum_k\left[\frac{1}{2\rho}\Pi^\dagger(k)\Pi(k)+\frac{1}{2}\rho\omega_k^2\phi^\dagger(k)\phi(k)\right]=\sum_k\omega_k\left(a_k^\dagger a_k+\frac{1}{2}\right) \tag{43}$$

where $\omega_k=c|k|$, $c=\sqrt{\kappa/\rho}$, $k=p(2\pi/L)\,(p\in\mathbb{Z})$,

$$a(k)=\sqrt{\frac{\rho\omega_k}{2}}\left[\phi(k)+\frac{i}{\rho\omega_k}\Pi(k)\right],\quad a^\dagger(k)=\sqrt{\frac{\rho\omega_k}{2}}\left[\phi^\dagger(k)-\frac{i}{\rho\omega_k}\Pi^\dagger(k)\right] \tag{44}$$

and

$$[a(k), a(k')] = [a^\dagger(k), a^\dagger(k')] = 0, \quad [a(k), a^\dagger(k')] = \delta_{k,k'} \tag{45}$$

类似于量子力学中的谐振子模型, 可以直接写出

$$|n_k\rangle = \frac{1}{\sqrt{n_k!}}(a_k^\dagger)^{n_k} |0\rangle, \quad a_k |0\rangle = 0, \quad \langle 0|0\rangle = 1 \tag{46}$$

$$a_k |n_k\rangle = \sqrt{n_k} |n_k - 1\rangle, \quad a_k^\dagger |n_k\rangle = \sqrt{n_k + 1} |n_k + 1\rangle \tag{47}$$

对于多粒子系统

$$|n_{k_1} \cdots n_{k_i} \cdots\rangle = |n_{k_1}\rangle \otimes \cdots \otimes |n_{k_i}\rangle \otimes \cdots = \prod_i \frac{(a_k^\dagger)^{n_k}}{\sqrt{n_k!}} |\text{vac}\rangle \tag{48}$$

$$H |n_{k_1} \cdots n_{k_i} \cdots\rangle = \left[\sum_j \left(n_{k_j} + \frac{1}{2}\right) \omega_{k_j}\right] |n_{k_1} \cdots n_{k_i} \cdots\rangle \tag{49}$$

这里实际上是把整个希尔伯特空间依照粒子数划分子空间, 这种结构称为 Fock space. 将粒子视为空间中场的能量激发 (振动弦形式) 是 qft 的基础.

对于场的位置算符和动量算符 ϕ 和 Π, 可以自然地定义他们的本征态 $\hat{\phi}(x) |\phi\rangle = \phi(x)$, $\hat{\Pi}(x) |\Pi\rangle = \Pi(x) |\Pi\rangle$, 且他们组成一组完备基

$$\mathcal{N} \lim_{a\to} \int \prod_{l=0}^{L/a} d\phi(la) |\phi\rangle \langle\phi| = 1 \tag{50}$$

$$\mathcal{N}' \lim_{a\to} \int \prod_{l=0}^{L/a} d\Pi(la) |\Pi\rangle \langle\Pi| = 1 \tag{51}$$

其中 $\mathcal{N}$, $\mathcal{N}'$ 只是不重要的系数, 后面的计算中略去.

$$Z = \sum_n \langle n|e^{-\beta H}|n\rangle = \int d\phi \sum_n \langle n|e^{-\beta H}|\phi\rangle \langle\phi|n\rangle = \int d\phi \langle\phi|e^{-\beta H}|\phi\rangle \tag{52}$$

类似于我们之前的操作, 将其分割成一小段 $\epsilon = \beta/N$ 分别积分, 利用 $\langle\phi_k|\Pi_k\rangle = \exp\left(i \int dx \Pi_k \phi_k\right)$, 经过一些不太复杂的计算可以得到

$$Z = \int_{\phi(x,\beta)=\phi(x,0)} = \mathcal{D}[\phi] e^{-S_E[\phi]} \tag{53}$$

where

$$S_E[\phi] = \frac{1}{2}\int_0^\beta d\tau \int_0^L dx \left[\rho\dot{\phi}^2 + \kappa(\partial_x\phi)^2\right] \tag{54}$$

$$\mathcal{D}[\phi] = \lim_{N\to\infty}\lim_{a\to}\prod_{k=1}^{N}\prod_{l=0}^{L/a} d\phi(la, k\beta/N) \tag{55}$$

将场分解为傅里叶级数, 注意这里不是算符

$$\phi(x,\tau) = \frac{1}{\sqrt{\beta}}\sum_{\omega_n} e^{-i\omega_n\tau}\phi(x,i\omega_n), \quad \phi(x,i\omega_n) = \frac{1}{\sqrt{\beta}}\int_0^\beta d\tau e^{i\omega_n\tau}\phi(x,\tau) \tag{56}$$

其中 $\omega_n = \frac{2\pi}{\beta}n$ 称为 Matsubara (imaginary) frequency. 变换后可以对角化作用量

$$S_E[\phi] = \frac{\rho}{2}\sum_{k,\omega_n}\phi(-k,-i\omega_n)(\omega_n^2+\omega_k^2)\phi(k,i\omega_n) \tag{57}$$

因为 $\phi(x,\tau)$ 是实数,$\phi(-k,-i\omega_n) = \phi^*(k,i\omega_n)$. 值得一提,d+1 维的经典系统等价于 d 维量子系统, 这是因为虚时的存在.

可以定义关联函数 (格林函数)

$$G(k,\tau) = \langle\phi(k,\tau)\phi(-k,0)\rangle = \frac{1}{Z}\int\mathcal{D}[\phi]\phi(k,\tau)\phi(-k,0)e^{-S_E[\phi]} \tag{58}$$

或

$$G(k,\tau) = \langle T_\tau\phi(k,\tau)\phi(-k,0)\rangle, \quad G(k,i\omega_n) = \langle\phi(k,i\omega_n)\phi(-k,-i\omega_n)\rangle \tag{59}$$

where

$$\phi(k,\tau) = e^{\tau H}\phi(k)e^{-\tau H} \tag{60}$$

此外, 我们也可以做解析延拓 $i\omega_n \to \omega + i\eta$, 定义推迟 (retarded) 格林函数和谱函数

$$G^R(k,\omega) = G(k,\omega - i\eta), \quad A(k,\omega) = \Im[G^R(k,\omega)] \tag{61}$$

with $\eta \to 0^+$. 例如, 对于二次型作用量 $S_E[\phi] = \frac{\rho}{2}\sum_{k,\omega_n}\phi(-k,-i\omega_n)(\omega_n^2 + \omega_k^2)\phi(k,i\omega_n)$, 精确计算得

$$G(k,i\omega_n) = \frac{1}{\rho}\frac{1}{\omega_n^2+\omega_k^2}, \quad G^R(k,\omega) = -\frac{1}{\rho}\frac{1}{(\omega+i\eta)^2-\omega_k^2} \tag{62}$$

$$A(k,\omega) = \frac{\pi}{2\rho\omega_k}\left[\delta(\omega-\omega_k)-\delta(\omega+\omega_k)\right] \tag{63}$$

之后在线性响应理论中我们可以从谱函数中提取激发态的信息.

在这一小节中, 我们勾勒出了多体系统泛函积分的大体框架, 接下来几节会详细的讨论理论细节.

3 Second Quantization

二次量子化可以视为一种初步的简单的量子场论. 在二次量子化的视角中, 通过产生湮灭算符来描述粒子或准粒子的算符, 其希尔伯特空间 (Fock space) 正如之前说的, 以粒子数划分子空间, 以粒子数为标志构造的基就是 Fock space 的完备基.

$$\mathcal{H} = \bigotimes_{n=0}^{n=\infty}\mathcal{H}_n \tag{64}$$

如图,n 粒子态 (以费米子为例, 注意泡利不相容)

$$(\alpha_1'\cdots|\alpha_1) = \delta_{\alpha_1',\alpha}\cdots, \quad \{\alpha_1'\cdots|\alpha_1\cdots\} = \begin{cases}(-1)^P, \text{ (fermions)} \\ n_{\alpha_1}!\cdots, \text{ (bosons)}\end{cases} \tag{65}$$

$$(\, r_1\cdots r_n\,|\alpha_1\cdots\alpha_n\rangle = \begin{cases}\frac{1}{\sqrt{n!}}\det(\varphi_{\alpha_i}(r_j)), \text{ (fermions)} \\ \frac{1}{\left(n!\prod_{i=1}^{p} n_{\alpha_i}!\right)^{1/2}}\mathrm{per}(\varphi_{\alpha_i}(r_j)), \text{ (bosons)}\end{cases} \tag{66}$$

对于费米子上述定义需要考虑符号, 而玻色子只需要都乘起来就好了.

Many-body states	$\lvert\alpha_1\cdots\alpha_n) = \lvert\alpha_1\rangle\otimes\cdots\otimes\lvert\alpha_n\rangle$ $\lvert\alpha_1\cdots\alpha_n\} = \frac{1}{\sqrt{n!}}\sum_P \zeta^P\lvert\alpha_{P(1)}\cdots\alpha_{P(n)})$ $\lvert\alpha_1\cdots\alpha_n\rangle = \frac{1}{(\prod_{i=1}^p n_{\alpha_i}!)^{1/2}}\lvert\alpha_1\cdots\alpha_n\}$
Closure relation	$\sum_{n=0}^{\infty}\frac{1}{n!}\sum_{\alpha_1\cdots\alpha_n}\lvert\alpha_1\cdots\alpha_n\}\{\alpha_1\cdots\alpha_n\rvert = 1$
Creation and annihilation operators	$\hat\psi^\dagger_\alpha\lvert\alpha_1\cdots\alpha_n\} = \lvert\alpha\alpha_1\cdots\alpha_n\}$ $\hat\psi_\alpha\lvert\alpha_1\cdots\alpha_n\} = \sum_{i=1}^n \zeta^{i-1}\delta_{\alpha,\alpha_i}\lvert\alpha_1\cdots\hat\alpha_i\cdots\alpha_n\}$ $\hat\psi^\dagger_\alpha\lvert\alpha_1\cdots\alpha_n\rangle = \sqrt{n_\alpha+1}\lvert\alpha\alpha_1\cdots\alpha_n\rangle$ $\hat\psi_\alpha\lvert\alpha_1\cdots\alpha_n\rangle = \frac{1}{\sqrt{n_\alpha}}\sum_{i=1}^n \zeta^{i-1}\delta_{\alpha,\alpha_i}\lvert\alpha_1\cdots\hat\alpha_i\cdots\alpha_n\rangle$
(Anti)commutation relations	$[\hat\psi_\alpha,\hat\psi_{\alpha'}]_{-\zeta} = [\hat\psi^\dagger_\alpha,\hat\psi^\dagger_{\alpha'}]_{-\zeta} = 0$ $[\hat\psi_\alpha,\hat\psi^\dagger_{\alpha'}]_{-\zeta} = \delta_{\alpha,\alpha'}$
Field operators	$\hat\psi_\sigma(\mathbf{r}) = \sum_\alpha\langle\mathbf{r},\sigma\lvert\alpha\rangle\hat\psi_\alpha$ $\hat\psi^\dagger_\sigma(\mathbf{r}) = \sum_\alpha\langle\alpha\lvert\mathbf{r},\sigma\rangle\hat\psi^\dagger_\alpha$ $[\hat\psi_\sigma(\mathbf{r}),\hat\psi_{\sigma'}(\mathbf{r}')]_{-\zeta} = [\hat\psi^\dagger_\sigma(\mathbf{r}),\hat\psi^\dagger_{\sigma'}(\mathbf{r}')]_{-\zeta} = 0$ $[\hat\psi_\sigma(\mathbf{r}),\hat\psi^\dagger_{\sigma'}(\mathbf{r}')]_{-\zeta} = \delta_{\sigma,\sigma'}\delta(\mathbf{r}-\mathbf{r}')$
One-body operator	$\hat V^{(1)} = \sum_{\alpha,\alpha'}\langle\alpha\lvert\hat V\rvert\alpha'\rangle\hat\psi^\dagger_\alpha\hat\psi_{\alpha'}$ $= \int d^d r d^d r'\sum_{\sigma,\sigma'}\langle\mathbf{r},\sigma\lvert\hat V\rvert\mathbf{r}',\sigma'\rangle\hat\psi^\dagger_\sigma(\mathbf{r})\hat\psi_{\sigma'}(\mathbf{r}')$
Two-body operator	$\hat V^{(2)} = \frac{1}{2}\sum_{\alpha_1\cdots\alpha_2'}(\alpha_1\alpha_2\lvert\hat V\rvert\alpha_1'\alpha_2')\hat\psi^\dagger_{\alpha_1}\hat\psi^\dagger_{\alpha_2}\hat\psi_{\alpha_2'}\hat\psi_{\alpha_1'}$

紧接着可以定义产生湮灭算符, 如图, 有

$$\lvert\alpha_1\cdots\alpha_n\rangle = \frac{1}{(\prod_{i=1}^p n_{\alpha_i}!)^{1/2}}\psi^\dagger_{\alpha_1}\cdots\psi^\dagger_{\alpha_n}\lvert\mathrm{vac}\rangle \tag{67}$$

玻色子也相同

$$|n_{\alpha_1}\cdots n_{\alpha_p}\rangle = \frac{1}{(\prod_{i=1}^{p} n_{\alpha_i}!)^{1/2}}(\psi^\dagger_{\alpha_1})^{n_{\alpha_1}}\cdots(\psi^\dagger_{\alpha_n})^{n_{\alpha_p}}|\mathrm{vac}\rangle \tag{68}$$

定义粒子数算符 $n_\alpha = \psi^\dagger_\alpha\psi_\alpha$

$$\hat{n}_\alpha |n_{\alpha_1}\cdots n_{\alpha_p}\rangle = \sum_{i=1}^{p}\delta_{\alpha,\alpha_i} n_\alpha |n_{\alpha_1}\cdots n_{\alpha_p}\rangle \tag{69}$$

由于玻色子和费米子的交换对称和反对称性, 产生湮灭算符的关系式也不同, 他们分别满足对易关系式和反对易关系式

$$[\psi^\dagger_\alpha, \psi^\dagger_{\alpha'}]_{-\zeta} = [\psi_\alpha, \psi_{\alpha'}]_{-\zeta} = 0, \quad [\psi_\alpha, \psi^\dagger_{\alpha'}]_{-\zeta} = \delta_{\alpha,\alpha'} \tag{70}$$

这里使用了统一的写法,$[\cdot,\cdot]_-$ 表示对易式,$[\cdot,\cdot]_+$ 表示反对易式. 若做变换 $|\tilde{\alpha}\rangle = \sum_\alpha \langle\alpha|\tilde{\alpha}\rangle |\alpha\rangle$, 则对易关系变为

$$[\psi^\dagger_{\tilde{\alpha}}, \psi^\dagger_{\tilde{\alpha}'}]_{-\zeta} = [\psi_{\tilde{\alpha}}, \psi_{\tilde{\alpha}'}]_{-\zeta} = 0, \quad [\psi_{\tilde{\alpha}}, \psi^\dagger_{\tilde{\alpha}'}]_{-\zeta} = \langle\tilde{\alpha}|\tilde{\alpha}'\rangle \tag{71}$$

算符也做对应的幺正变换. 接下来定义场算符

$$\psi_\sigma(r) = \sum_\alpha \langle r,\sigma|\alpha\rangle \psi_\alpha = \frac{1}{\sqrt{\mathcal{V}}}\sum_k e^{ik\cdot r}\psi_\sigma(k) \tag{72}$$

$$\psi^\dagger_\sigma(r) = \sum_\alpha \langle \alpha|r,\sigma\rangle \psi^\dagger_\alpha = \frac{1}{\sqrt{\mathcal{V}}}\sum_k e^{-ik\cdot r}\psi^\dagger_\sigma(k) \tag{73}$$

$$[\psi^\dagger_\sigma(r), \psi^\dagger_{\sigma'}(r')]_{-\zeta} = [\psi_\sigma(r), \psi_{\sigma'}(r')]_{-\zeta} = 0, \quad [\psi_\sigma(r), \psi^\dagger_{\sigma'}(r')]_{-\zeta} = \delta_{\sigma,\sigma'}\delta(r-r') \tag{74}$$

二次量子化的算符形式经过简单的推导也可以得到

$$V^{(1)} = \sum_{\alpha,\alpha'}\langle\alpha|V|\alpha'\rangle \psi^\dagger_\alpha\psi_{\alpha'} = \int d^d r d^d r' \sum_{\sigma,\sigma'}\langle r,\sigma|V|r',\sigma'\rangle \psi^\dagger_\sigma(r)\psi_{\sigma'}(r') \tag{75}$$

$$V^{(2)} = \frac{1}{2}\sum_{\alpha_1\cdots\alpha_2'}(\alpha_1\alpha_2|V|\alpha_1'\alpha_2')\psi^\dagger_{\alpha_1}\psi^\dagger_{\alpha_2}\psi_{\alpha_2'}\psi_{\alpha'} \tag{76}$$

$$= \frac{1}{2}\int d^d r_1\cdots d^d r_2' \sum_{\sigma_1\cdots\sigma_2'}(r_1\sigma_1, r_2\sigma_2|V|r_1'\sigma_1', r_2'\sigma_2')\psi^\dagger_{\sigma_1}(r_1)\psi^\dagger_{\sigma_2}(r_2)\psi_{\sigma_2'}(r_2')\psi_{\sigma_1'}(r_1') \tag{77}$$

or

$$V^{(2)} = \frac{1}{4} \sum_{\alpha_1 \cdots \alpha_2'} \{\alpha_1\alpha_2|V|\alpha_1'\alpha_2'\} \psi^\dagger_{\alpha_1}\psi^\dagger_{\alpha_2}\psi_{\alpha_2'}\psi_{\alpha'} \tag{78}$$

with

$$\{\alpha_1\alpha_2|V|\alpha_1'\alpha_2'\} = (1+\zeta)(\alpha_1\alpha_2|V|\alpha_1'\alpha_2') \tag{79}$$

一般地,n 体算符可以表达为

$$V^{(n)} = \frac{1}{n!} \sum_{\alpha_i,\alpha_i'} (\alpha_1 \cdots \alpha_n|V|\alpha_1' \cdots \alpha_n') \psi^\dagger_{\alpha_1} \cdots \psi^\dagger_{\alpha_n} \psi_{\alpha_n'} \cdots \psi_{\alpha_1'} \tag{80}$$

$$= \frac{1}{(n!)^2} \sum_{\alpha_i,\alpha_i'} \{\alpha_1 \cdots \alpha_n|V|\alpha_1' \cdots \alpha_n'\} \psi^\dagger_{\alpha_1} \cdots \psi^\dagger_{\alpha_n} \psi_{\alpha_n'} \cdots \psi_{\alpha_1'} \tag{81}$$

这里直接给出 4 个常用的例子

$$T = \sum_{k,\sigma} \frac{k^2}{2m} \psi^\dagger_\sigma(k)\psi_\sigma(k) = \frac{1}{2m} \int d^d r \sum_\sigma \nabla\psi^\dagger_\sigma(r) \cdot \nabla\psi_\sigma(r) \tag{82}$$

$$j(r) = \frac{1}{2m} \sum_i [p_i \delta(r - r_i) + \delta(r - r_i) p_i] = -\frac{i}{2m} \sum_\sigma \left[\psi^\dagger_\sigma(r)\nabla\psi_\sigma(r) - h.c.\right] \tag{83}$$

$$H_0(\text{non-interacting particles}) = \sum_\alpha \xi_\alpha \psi^\dagger_\alpha \psi_\alpha, \quad \xi_\alpha = \epsilon_\alpha - \mu \tag{84}$$

$$V^{(2)} = \sum_{i<j} v(r_i - r_j) = \frac{1}{2\mathcal{V}} \sum_{k,k',q,\sigma,\sigma'} v(q) \psi^\dagger_\sigma(k+q)\psi^\dagger_{\sigma'}(k'-q)\psi_{\sigma'}(k')\psi_\sigma(k) \tag{85}$$

我们在上一节引入了格林函数. 推迟格林函数表示为

$$G^R(r, r'; t) = -i\Theta(t) \langle r|e^{-iHt}|r'\rangle = -i\Theta(t) \sum_n e^{-i\epsilon_n t} \varphi_n(r)\varphi_n^*(r') \tag{86}$$

$$G^R(r, r'; \omega) = \int_\infty^\infty dt e^{i(\omega+i\eta)t} G^R(r, r'; t) = \sum_n \frac{\varphi_n(r)\varphi_n^*(r')}{\omega + i\eta - \epsilon_n} \tag{87}$$

with $\eta \to 0^+ s$. 其中推迟代表了正常的因果, 即过去可以影响未来, 但未来不能影响过去. 因此其实也可以想到定义对应的超前 (advanced) 格林函数 $G^A = i\Theta(-t) \cdots$. 傅里叶变换 e 指数上额外的小虚部保证了整个积分的收

敛, 而这个数学操作却能给出系统关键的谱信息. 当然格林函数也可以选择更像二次量子化的等价的形式, 其满足 $G^R(r,t^+;r',t)=-i\delta(r-r')$

$$G^R(r,r';t)=-i\Theta(t)\left\langle 0\right|[\psi(r,t),\psi^\dagger(r',0)]_{-\zeta}\left|0\right\rangle \tag{88}$$

where

$$\psi(r,t)=e^{iHt}\psi(r)e^{-iHt},\quad \psi^\dagger(r,t)=e^{iHt}\psi^\dagger(r)e^{-iHt} \tag{89}$$

如果考虑巨正则系综, 只需要在哈密顿量中加入一项 $-\mu N$. 另外如果拓展到有限温系统, 只需要换成 trace

$$G^R(\alpha,\alpha';t)=-i\Theta(t)\frac{1}{Z}\mathrm{Tr}\left\{e^{-\beta H}[\psi_\alpha(t),\psi^\dagger_{\alpha'}]_{-\zeta}\right\} \tag{90}$$

where $\alpha\equiv(r,\sigma)$. 例如, 还是对于自由粒子 $H_0=\sum_\alpha\xi_\alpha\psi^\dagger_\alpha\psi_\alpha\,(\xi_\alpha=\epsilon_\alpha-\mu)$

$$G^R_0(\alpha,t)=-i\Theta(t)e^{-i\xi_\alpha t},\quad G^R_0(\alpha,\omega)=\frac{1}{\omega+i\eta-\xi_\alpha} \tag{91}$$

介绍另外一个更重要的格林函数, Matsubara Green function

$$G(\alpha,\alpha';\tau)=-\left\langle T_\tau\psi_\alpha(\tau)\psi^\dagger_{\alpha'}\right\rangle,\quad T_\tau\equiv\Theta(\tau)+\zeta\Theta(-\tau) \tag{92}$$

需要注意的是 $\psi^\dagger_\alpha(\tau)\neq[\psi_\alpha(\tau)]^\dagger$. 当正虚时时, 格林函数表示产生了一个粒子并传播 τ 后湮灭; 当负虚时时, 格林函数表示粒子湮灭而对应的空穴 (hole) 传播. 推迟 G 可以由 Matsubara G 通过解析延拓获得

$$G^R_0(\alpha,\omega)=G_0(\alpha,i\omega_n\to\omega+i\eta) \tag{93}$$

Matsubara 格林函数通常定义在 $[-\beta,\beta]$ 上, 其具有周期

$$G(\alpha,\alpha';\tau)=\zeta G(\alpha,\alpha';\tau+\beta),\quad -\beta<\tau<0 \tag{94}$$

$$G(\alpha,\alpha';\tau)=\zeta G(\alpha,\alpha';\tau-\beta),\quad 0<\tau<\beta \tag{95}$$

对于周期函数, 自然想到对其做傅里叶分解

$$G(\alpha,\alpha';\tau)=\frac{1}{\beta}\sum_{\omega_n}e^{-i\omega_n\tau}G(\alpha,\alpha';i\omega_n) \tag{96}$$

$$G(\alpha,\alpha';i\omega)=\int_0^\beta d\tau e^{i\omega_n\tau}G(\alpha,\alpha';\tau) \tag{97}$$

where Matsubara frequencies

$$\omega_n = \begin{cases} \frac{2\pi}{\beta} n, & (bosons) \\ \frac{2\pi}{\beta}(n+\frac{1}{2}), & (fermions) \end{cases} \tag{98}$$

还是考虑我们的自由粒子,Matsubara 格林函数

$$G_0(\alpha, \tau) = -e^{-\xi_\alpha \tau} \left[\Theta(\tau)(1+\zeta n_\alpha) + \zeta\Theta(-\tau)\zeta n_\alpha\right] \tag{99}$$

$$G_0(\alpha, i\omega_n) = \frac{1}{i\omega_n - \xi_\alpha} \tag{100}$$

其中粒子数算符引出的粒子分布 n_α 自然就和统计物理中的 F-D 分布、B-E 分布联系起来, 从这里可以直接看出来粒子种类对系统性质的影响, 系统所有的信息基本都 encode 在格林函数中了.

简单介绍一下高阶的格林函数

$$G^{(2n)}(\alpha_1\tau_1, \ldots, \alpha_n\tau_n; \alpha'_n\tau'_n, \ldots, \alpha'_1\tau'_1) = (-1)^n \left\langle T_\tau \psi_{\alpha_1}(\tau_1)\cdots\psi_{\alpha_n}(\tau_n)\psi^\dagger_{\alpha'_n}(\tau'_n)\cdots\psi^\dagger_{\alpha'_1}(\tau'_1)\right\rangle \tag{101}$$

where

$$T_\tau A_{\alpha_1}(\tau_1)\cdots A_{\alpha_n}(\tau_n) = \zeta^P A_{\alpha_{P(1)}}(\tau_{P(1)})\cdots A_{\alpha_{P(n)}}(\tau_{P(n)}) \tag{102}$$

和我们之前介绍的时序算符一致, 相当于按虚时从大到小重排.

实时格林函数

$$G^{(2n)}(\alpha_1 t_1, \ldots, \alpha_n t_n; \alpha'_n t'_n, \ldots, \alpha'_1 t'_1) = (-i)^n \left\langle T_\tau \psi_{\alpha_1}(t_1)\cdots\psi_{\alpha_n}(t_n)\psi^\dagger_{\alpha'_n}(t'_n)\cdots\psi^\dagger_{\alpha'_1}(t'_1)\right\rangle \tag{103}$$

4 Coherent States

本节介绍多体系统中的相干态 (coherent states), 这部分更直观的展示了玻色子和费米子的不同. 对于任意一个态, 我们期望

$$\hat{\psi}_\alpha |\psi\rangle = \psi_\alpha |\psi\rangle, \quad \left[\hat{\psi}_\alpha, \hat{\psi}_\beta\right]_{-\zeta} = 0 \Rightarrow \left[\psi_\alpha, \psi_\beta\right]_{-\zeta} = 0 \tag{104}$$

对于玻色子这自然对应着本征值的阿贝尔性 (c-number), 然而对于费米子这隐藏着一个相当奇怪的性质

$$\psi_\alpha\psi_\beta = -\psi_\beta\psi_\alpha \tag{105}$$

这种数学对象称为 Grassmann number.

我们先回过头来看玻色子, 定义 boson coherent states

$$|\psi\rangle = \exp\left(\sum_\alpha \psi_\alpha \hat{\psi}_\alpha^\dagger\right)|\text{vac}\rangle = \sum_{n_{\alpha_1},\cdots=0}^{\infty} \frac{\left(\psi_{\alpha_1}^{n_{\alpha_1}}\cdots\right)}{\left(n_{\alpha_1}!\cdots\right)^{1/2}}|n_{\alpha_1}\cdots\rangle \tag{106}$$

满足性质

$$\hat{\psi}_\alpha^\dagger|\psi\rangle = \frac{\partial}{\partial\psi_\alpha}|\psi\rangle, \quad \langle\psi|\psi'\rangle = \exp\left(\sum_\alpha \psi_\alpha^*\psi_\alpha'\right) \tag{107}$$

$$\int\prod_\alpha \frac{d\psi_\alpha^* d\psi_\alpha}{2i\pi} e^{-\sum_\alpha|\psi_\alpha|^2}|\psi\rangle\langle\psi| = 1, \quad \frac{d\psi_\alpha^* d\psi_\alpha}{2i\pi} = \frac{1}{\pi}d\Re(\psi_\alpha)d\Im(\psi_\alpha) \tag{108}$$

考虑 normal ordered 的算符 $A(\hat{\psi}_\alpha^\dagger, \hat{\psi}_\alpha)$

$$\langle\psi|A(\hat{\psi}_\alpha^\dagger, \hat{\psi}_\alpha)|\psi'\rangle = e^{\sum_\alpha \psi_\alpha^*\psi_\alpha'} A(\psi_\alpha^\dagger, \psi_\alpha) \tag{109}$$

考虑粒子数

$$|\langle n_{\alpha_1}\cdots|\psi\rangle|^2 = \prod_\alpha \frac{|\psi_\alpha|^{2n_\alpha}}{n_\alpha!} \tag{110}$$

$$N = \langle\hat{N}\rangle = \sum_\alpha|\psi_\alpha|^2, \quad \sigma^2 = N \tag{111}$$

相干态在多体系统中代表了满足不确定性原理下的最小位置和动量的不确定度, 有时也会表现出准经典的行为.

接下来考虑费米子和 Grassmann number. 对于 Grassmann variables $\{\psi_1,\ldots,\psi_n\}$, 有性质、定义:

$$[\psi_i,\psi_j]_+ = 0, \quad \frac{\partial}{\partial\psi_i}\psi_j = \delta_{ij}, \quad [\partial_{\psi_i},\partial_{\psi_j}]_+ = 0 \tag{112}$$

对于 Grassmann 函数, 有微分和积分法则

$$\frac{\partial}{\partial \psi_i} f(g) = \frac{\partial g}{\partial \psi_i} \frac{\partial f}{\partial g} \tag{113}$$

$$\int d\psi_i f(\psi_1, \ldots, \psi_n) = \frac{\partial}{\partial \psi_i} f(\psi_1, \ldots, \psi_n) \tag{114}$$

定义的积分和微分是等价的, 因此

$$\int d\psi_i \frac{\partial}{\partial \psi_i} f(\psi_1, \ldots, \psi_n) = \frac{\partial}{\partial \psi_i} \int d\psi_i f(\psi_1, \ldots, \psi_n) = 0 \tag{115}$$

定义 Grassmann variables 的复共轭和 c-number 的操作类似. 按照我们定义的 Grassmann variables 的性质, 可以写出 fermion coherent states

$$|\psi\rangle = \exp\left(-\sum_\alpha \psi_\alpha \hat{\psi}_\alpha^\dagger\right)|\text{vac}\rangle = \prod_\alpha (1 - \psi_\alpha \hat{\psi}_\alpha^\dagger)|\text{vac}\rangle \tag{116}$$

满足性质

$$\hat{\psi}_\alpha |\psi\rangle = \psi_\alpha |\psi\rangle, \quad \hat{\psi}_\alpha^\dagger |\psi\rangle = -\frac{\partial}{\partial \psi_\alpha}|\psi\rangle, \quad \langle\psi|\psi'\rangle = \exp\left(\sum_\alpha \psi_\alpha^* \psi_\alpha'\right) \tag{117}$$

$$\int \prod_\alpha d\psi_\alpha^* d\psi_\alpha e^{-\sum_\alpha \psi_\alpha^* \psi_\alpha} |\psi\rangle\langle\psi| = 1, \quad \langle\psi|A(\hat{\psi}_\alpha^\dagger, \hat{\psi}_\alpha)|\psi'\rangle = e^{\sum_\alpha \psi_\alpha^* \psi_\alpha'} A(\psi_\alpha^\dagger, \psi_\alpha) \tag{118}$$

总结如下

Definition	$\|\psi\rangle = e^{\zeta \sum_\alpha \psi_\alpha \hat{\psi}_\alpha^\dagger}\|\text{vac}\rangle$ $\langle\psi\| = \langle\text{vac}\|e^{\sum_\alpha \psi_\alpha^* \hat{\psi}_\alpha}$
	$\hat{\psi}_\alpha\|\psi\rangle = \psi_\alpha\|\psi\rangle, \qquad \langle\psi\|\hat{\psi}_\alpha^\dagger = \langle\psi\|\psi_\alpha^*$
Overlap	$\langle\psi\|\psi'\rangle = e^{\sum_\alpha \psi_\alpha^* \psi_\alpha'}$
Closure relation	$\int \prod_\alpha \frac{d\psi_\alpha^* d\psi_\alpha}{\mathcal{N}} e^{-\sum_\alpha \|\psi_\alpha\|^2}\|\psi\rangle\langle\psi\| = 1$
Trace	$\text{Tr}(\hat{A}) = \int \prod_\alpha \frac{d\psi_\alpha^* d\psi_\alpha}{\mathcal{N}} e^{-\sum_\alpha \|\psi_\alpha\|^2}\langle\zeta\psi\|\hat{A}\|\psi\rangle$
Normal-ordered operator	$\langle\psi\|A(\hat{\psi}_\alpha^\dagger, \hat{\psi}_\alpha)\|\psi'\rangle = e^{\sum_\alpha \psi_\alpha^* \psi_\alpha'} A(\psi_\alpha^*, \psi_\alpha')$

然而需要注意 fermion coherent states 不是物理态 (physical states), 其不在 Fock space 中 (因为希尔伯特空间内的态都可以在多项式时间内制备). 其粒子数不是一个可观测的实数 $N = \sum_\alpha \psi_\alpha^* \psi_\alpha$.

5 Green Functions

6 Functional Integral

7 Perturbation Theory

8 Perturbation Theory in the Operator Formalism

9 Generating Functionals

10 Saddle-Point Approximation and Loop Expansion

11 Perturbation Theory at Zero Temperature

12 QED

13 Symmetries

14 Ward Identities