Quantum Field Theory
- based on A. Zee's textbook -

万思扬

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Contents

convention, notation, and units

- 笔记中的**度规号差**约定为 $(-,+,+,+)$.
- 使用 Planck units, 此时 $G, \hbar, c, k_B = 1$, 因此,

name/dimension	expression/value
Planck length (L)	$l_P = \sqrt{\frac{\hbar G}{c^3}} = 1.616 \times 10^{-35}\,\mathrm{m}$
Planck time (T)	$t_P = \frac{l_P}{c} = 5.391 \times 10^{-44}\,\mathrm{s}$
Planck mass (M)	$m_P = \sqrt{\frac{\hbar c}{G}} = 2.176 \times 10^{-8}\,\mathrm{kg} \simeq 10^{19}\,\mathrm{GeV}$
Planck temperature (Θ)	$T_P = \sqrt{\frac{\hbar c^5}{G k_B^2}} = 1.417 \times 10^{32}\,\mathrm{K}$

- 时空维度用 $d = D + 1$ 表示.

Part I

motivation and foundation

Chapter 1

free field theory

1.1 partition function

- 考虑如下标量场,

$$\mathcal{L} = -\frac{1}{2}(\partial\phi)^2 - V(\phi) \tag{1.1.1}$$

A. Zee 说: 在作用量里, 时间的导数项必须是正的, 包括标量场的 $(\partial_0\phi)^2$ 和电磁场的 $(\partial_0 A_i)^2$.

- 含有 source function 的路径积分为,

$$Z(J) = \int D\phi \, e^{i \int d^d x \left(-\frac{1}{2}(\partial\phi)^2 - V(\phi) + J(x)\phi(x)\right)} \tag{1.1.2}$$

- 当 $V(\phi) = \frac{1}{2}m^2\phi^2$ 时, 称作 free or Gaussian theory.

- 计算 free theory 的 partition function, 得到,

$$Z(J) = \mathcal{C}e^{-\frac{i}{2}\int d^d x d^d y \, J(x) D(x-y) J(y)} \tag{1.1.3}$$

另外, 用 $W(J)$ 表示指数上的部分 (去除掉虚数 i).

> **proof:**
>
> 注意 $\partial^\mu\phi\partial_\mu\phi = \partial^\mu(\phi\partial_\mu\phi) - \phi\partial^2\phi$, 忽略全微分项, 那么,
>
> $$Z(J) = \int D\phi \, e^{i \int d^d x \frac{1}{2}(\phi(\partial^2 - m^2)\phi + J(x)\phi(x))} \tag{1.1.4}$$
>
> 代入 (B.1.1), 可知,
>
> $$Z(J) = \mathcal{C}e^{-\frac{i}{2}\int d^d x d^d y \, J(x) D(x-y) J(y)} \tag{1.1.5}$$
>
> 其中 $D(x-y)$ 满足,
>
> $$\begin{cases} (\partial^2 - m^2)D(x-y) = \delta^{(d)}(x-y) \\ (-p^2 - m^2)\tilde{D}(p,q) = (2\pi)^d \delta^{(d)}(p-q) \end{cases} \implies D(x-y) = \int \frac{d^d k}{(2\pi)^d} \frac{e^{ik\cdot(x-y)}}{-k^2 - m^2} \tag{1.1.6}$$

1.2 free propagator

- 为了使 (1.1.4) 中的积分在 ϕ 较大时收敛, 作替换 $m^2 \mapsto m^2 - i\epsilon$, 这样被积函数中会出现一项 $e^{-\epsilon \int d^d x \phi^2}$.
- 注意 (1.1.6) 中的积分会遇到奇点, 必须加入正无穷小量 ϵ 避免发散,

$$D(x) = \int \frac{d^d k}{(2\pi)^d} \frac{e^{ik\cdot x}}{-k^2 - m^2 + i\epsilon} = -i \int \frac{d^D k}{(2\pi)^D 2\omega_k} \left(e^{i(-\omega_k t + \vec{k}\cdot\vec{x})}\theta(t) + e^{i(\omega_k t + \vec{k}\cdot\vec{x})}\theta(-t)\right) \tag{1.2.1}$$

> **calculation:**
>
> 对 k^0 积分, 注意有两个奇点 $k^0 = \pm(\omega_k - i\epsilon)$, 当 $t > 0$ 时, contour 处于下半平面, ...

- $D(x)$ 的取值与 x 的类时, 类空性质关系密切.
  - 类时区域,
  $$D(t,0) = -i \int \frac{d^D k}{(2\pi)^D 2\omega_k} \left(e^{-i\omega_k t}\theta(t) + e^{i\omega_k t}\theta(-t) \right) \tag{1.2.2}$$
  - 类空区域,
  $$D(0,\vec{x}) = -i \int \frac{d^D k}{(2\pi)^D 2\omega_k} e^{i\vec{k}\cdot\vec{x}} \sim e^{-m|\vec{x}|} \tag{1.2.3}$$

Chapter 2

from field to particle to force

2.1 from field to particle

- 考虑 (1.1.3) 中的 $W(J)$,

$$W(J) = -\frac{1}{2} \int d^d x d^d y\, J(y) D(x - y) J(y) \tag{2.1.1}$$

$$= -\frac{1}{2} \int \frac{d^d k}{(2\pi)^d} \tilde{J}(-k) \frac{1}{-k^2 - m^2 + i\epsilon} \tilde{J}(k) \tag{2.1.2}$$

其中, 如果 $J(x)$ 是实函数, 那么 $\tilde{J}(-k) = \tilde{J}^*(k)$.

- 考虑 $J(x) = J_1(x) + J_2(x)$, 那么 $W(J)$ 共有 4 项, 其中一个交叉项如下,

$$W_{12}(J) = -\frac{1}{2} \int \frac{d^d k}{(2\pi)^d} \tilde{J}_1(-k) \frac{1}{-k^2 - m^2 + i\epsilon} \tilde{J}_2(k) \tag{2.1.3}$$

可见 $W(J)$ 取值较大的条件是:

1. $\tilde{J}_1(k), \tilde{J}_2(k)$ 有较大重叠,
2. 重叠位置的 k 是 on shell (即 $k^2 = -m^2$).

- 可以看出来, 这里有一个粒子从 1 传递到 2 (?).

2.2 from particle to force

- 考虑 $J(x) = \delta^{(D)}(\vec{x} - \vec{x}_1) + \delta^{(D)}(\vec{x} - \vec{x}_1) \Longrightarrow \tilde{J}_a(k) = 2\pi e^{-i\vec{k} \cdot \vec{x}_a} \delta(k^0)$, 那么,

$$W_{12}(J) + W_{21}(J) = \delta(0) \int \frac{d^D k}{(2\pi)^{D-1}} \frac{1}{|\vec{k}|^2 + m^2 - i\epsilon} \cos(\vec{k} \cdot (\vec{x}_1 - \vec{x}_2))$$

$$\overset{D=3}{=} 2\pi \delta(0) \frac{1}{4\pi r} e^{-mr} \tag{2.2.1}$$

($-i\epsilon$ 显然可以舍去), 注意到 $\langle 0|e^{-iHT}|0\rangle = e^{-iET}$, 而时间间隔 $T = \int dx^0 = 2\pi\delta(0)$, 所以,

$$E = -\frac{W(J)}{T} \overset{D=3}{=} -\frac{1}{4\pi r} e^{-mr} \tag{2.2.2}$$

> **calculation:**
>
> 计算 (2.2.1) 中的积分, 令 $\vec{x}_1 - \vec{x}_2 = \vec{r}$,
>
> $$I_D = \int \frac{d^D k}{(2\pi)^D} \frac{1}{|\vec{k}|^2 + m^2} \overset{\mapsto e^{i\vec{k} \cdot \vec{r}}}{\cos(\vec{k} \cdot \vec{r})}$$

$$= \frac{1}{(2\pi)^D} \int (k\sin\theta_1)^{D-2} d\Omega_{D-2} \int k d\theta_1 dk \frac{1}{k^2+m^2} e^{ikr\cos\theta_1}$$

$$= \frac{S_{D-2}}{(2\pi)^D} \int k^{D-1} \sin^{D-2}\theta_1 d\theta_1 dk \frac{1}{k^2+m^2} e^{ikr\cos\theta_1} \tag{2.2.3}$$

取 $D = 3$, 那么,

$$I_{D=3} = \frac{1}{(2\pi)^2} \int k^2 \sin\theta_1 d\theta_1 dk \frac{1}{k^2+m^2} e^{ik\cos\theta_1}$$

$$= \frac{1}{2\pi^2 r} \int_0^\infty \sin(kr) \frac{kdk}{k^2+m^2} = \frac{-i}{4\pi^2 r} \int_{-\infty}^\infty e^{ikr} \frac{kdk}{k^2+m^2}$$

$$= \frac{-i}{4\pi^2 r} 2\pi i \underbrace{\text{Res}(f, im)}_{=\frac{1}{2}e^{-mr}} = \frac{1}{4\pi r} e^{-mr} \tag{2.2.4}$$

Chapter 3

Coulomb and Newton: repulsive and attraction

3.1 massive spin-1 particle & QED

- 构造有质量的光子的 Lagrangian density,

$$\mathcal{L} = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} - \frac{1}{2}m^2 A_\mu A^\mu \tag{3.1.1}$$

其中 $F_{\mu\nu} = 2\partial_{[\mu}A_{\nu]}$.

- 做路径积分,

$$Z(J) = \int DA\, e^{i\int d^d x(\mathcal{L}+J_\mu A^\mu)} = \mathcal{C}e^{-\frac{i}{2}\int d^d x d^d y\, J_\mu D^{\mu\nu}(x-y)J_\nu(y)} \tag{3.1.2}$$

---

calculation:

massive photon 的作用量为,

$$
\begin{aligned}
S(A) &= \int d^d x\, \frac{1}{2}\Big(-(\partial_\mu A_\nu)(\partial^\mu A^\nu) + (\partial_\mu A_\nu)(\partial^\nu A^\mu) - m^2 A_\mu A^\mu \Big) \\
&= \int d^d x\, \frac{1}{2}\Big(A_\nu \partial^2 A^\nu - A_\nu \partial^\nu \partial_\mu A^\mu - m^2 A_\mu A^\mu \Big) + \text{total differential} \\
&= \int d^d x\, \frac{1}{2} A_\mu \Big(-\partial^\mu \partial^\nu + \eta^{\mu\nu}(\partial^2 - m^2) \Big) A_\nu + \text{total differential}
\end{aligned} \tag{3.1.3}
$$

那么, 需要有,

$$(-\partial^\mu \partial^\rho + \eta^{\mu\rho}(\partial^2 - m^2))D_{\rho\nu}(x-y) = \delta^\mu_\nu \delta^{(d)}(x-y)$$

$$\Longrightarrow \tilde{D}_{\mu\nu}(k) = \frac{k_\mu k_\nu/m^2 + \eta_{\mu\nu}}{-k^2 - m^2} \tag{3.1.4}$$

考虑到积分需要收敛, 作替换 $m^2 \mapsto m^2 - i\epsilon$, (为什么 A_μ 类空 (?)).

- 因此,

$$W(J) = -\frac{1}{2}\int d^d x d^d y\, J_\mu(x)D^{\mu\nu}(x-y)J_\nu(y) \tag{3.1.5}$$

$$= -\frac{1}{2}\int \frac{d^d k}{(2\pi)^d} \tilde{J}_\mu(-k)\frac{k^\mu k^\nu/m^2 + \eta^{\mu\nu}}{-k^2 - m^2 + i\epsilon}\tilde{J}_\nu(k) \tag{3.1.6}$$

注意到 current conservation, 有 $\partial_\mu J^\mu = 0 \iff k^\mu \tilde{J}_\mu(k) = 0$, 所以,

$$W(J) = -\frac{1}{2}\int \frac{d^d k}{(2\pi)^d}\tilde{J}^\mu(-k)\frac{1}{-k^2 - m^2 + i\epsilon}\tilde{J}_\mu(k) \tag{3.1.7}$$

观察电荷分量, 可见同性相斥, 异性相吸.

3.1.1 spin & polarization vector

- spin-1 particle 可以有 3 个极化方向, 即空间的 x, y, z 方向, 在粒子静止系下, 极化矢量 $(\epsilon^i)_\mu = \delta^i_\mu, i = 1, 2, 3$, 而 $k_\mu = (-m, 0, 0, 0)$, 所以,

$$k^\mu (\epsilon^i)_\mu = 0 \tag{3.1.8}$$

  - 注意, 一个粒子的极化方向用 e^i (这不是矢量) 表示, 极化矢量为 $\sum_{i=1}^{3} e^i (\epsilon^i)_\mu$.

- 在粒子静止系下, 考虑,

$$\sum_{i=1}^{3} (\epsilon^i)_\mu (\epsilon^i)_\nu = \begin{pmatrix} 0 & 0 \\ 0 & \delta_{ij} \end{pmatrix} = \frac{k_\mu k_\nu}{m^2} + \eta_{\mu\nu} := -G_{\mu\nu} \tag{3.1.9}$$

  可见,

$$\tilde{D}_{\mu\nu}(k) = \frac{\sum_{i=1}^{3} (\epsilon^i)_\mu (\epsilon^i)_\nu}{-k^2 - m^2 + i\epsilon} \tag{3.1.10}$$

3.2 massive spin-2 particle & gravity

- Lagrangian for spin-2 particle = linearized Einstein Lagrangian.

- 受 subsection 3.1.1 启发, 对于 spin-2 particle, 其极化矢量有 5 个方向, 满足,

$$\begin{cases} k^\mu (\epsilon^a)_{(\mu\nu)} = 0 \\ \eta^{\mu\nu} (\epsilon^a)_{(\mu\nu)} = 0 \end{cases} \tag{3.2.1}$$

  其中下指标 μ, ν 对称, $a = 1, \cdots, 5$, (可以验证 $(\epsilon^a)_{\mu\nu}$ 确实有 5 个独立分量).

  - 对 $(\epsilon^a)_{\mu\nu}$ 的归一化条件可以定义为 $\sum_{a=1}^{5} (\epsilon^a)_{12} (\epsilon^a)_{12} = 1$.
  - 与 subsection 3.1.1 中提示一样, 粒子的极化方向用 e^a 表示.

- 那么,

$$\sum_{a=1}^{5} (\epsilon^a)_{\mu\nu} (\epsilon^a)_{\rho\sigma} = (G_{\mu\rho} G_{\nu\sigma} + G_{\mu\sigma} G_{\nu\rho}) - \frac{2}{3} G_{\mu\nu} G_{\rho\sigma} \tag{3.2.2}$$

> **calculation:**
>
> 首先用 k_μ 和 $\eta_{\mu\nu}$ 构造最一般的关于 $\mu \leftrightarrow \nu, \rho \leftrightarrow \sigma, \mu\nu \leftrightarrow \rho\sigma$ 对称的 4 阶张量, (下式中把 $\frac{k_\mu}{m}$ 略写作 k_μ),
>
> $$A k_\mu k_\nu k_\rho k_\sigma + B(k_\mu k_\nu \eta_{\rho\sigma} + k_\rho k_\sigma \eta_{\mu\nu}) + C(k_\mu k_\rho \eta_{\nu\sigma} + k_\mu k_\sigma \eta_{\nu\rho} + k_\nu k_\rho \eta_{\mu\sigma} + k_\nu k_\sigma \eta_{\mu\rho})$$
> $$+ D \eta_{\mu\nu} \eta_{\rho\sigma} + E(\eta_{\mu\rho} \eta_{\nu\sigma} + \eta_{\mu\sigma} \eta_{\nu\rho}) \tag{3.2.3}$$
>
> 代入 (3.2.1) 得,
>
> $$\begin{cases} 0 = -A + B + 2C = -B + D = -C + E \\ 0 = -A + 4B + 4C = -B + 4D + 2E \end{cases} \implies \frac{B = D, C = E}{A} = -\frac{1}{2}, \frac{3}{4} \tag{3.2.4}$$
>
> 因此, 这个 4 阶张量最终确定为,
>
> $$\frac{3}{4} A \Big((G_{\mu\rho} G_{\nu\sigma} + G_{\mu\sigma} G_{\nu\rho}) - \frac{2}{3} G_{\mu\nu} G_{\rho\sigma} \Big) \tag{3.2.5}$$

- 所以,

$$\tilde{D}_{\mu\nu\rho\sigma}(k) = \frac{(G_{\mu\rho} G_{\nu\sigma} + G_{\mu\sigma} G_{\nu\rho}) - \frac{2}{3} G_{\mu\nu} G_{\rho\sigma}}{-k^2 - m^2 + i\epsilon} \tag{3.2.6}$$

- 计算路径积分中的 $W(T)$,

$$W(T) = -\frac{1}{2} \int \frac{d^4 k}{(2\pi)^4} \tilde{T}_{\mu\nu}(-k) \frac{(G^{\mu\rho} G^{\nu\sigma} + G^{\mu\sigma} G^{\nu\rho}) - \frac{2}{3} G^{\mu\nu} G^{\rho\sigma}}{-k^2 - m^2 + i\epsilon} \tilde{T}_{\rho\sigma}(k) \tag{3.2.7}$$

注意到 $\partial_\mu T^{\mu\nu}(x) = 0 \iff k_\mu \tilde{T}^{\mu\nu}(k) = 0$, 并考虑到 T 是对称张量, 所以,

$$W(T) = -\frac{1}{2} \int \frac{d^4 k}{(2\pi)^4} \tilde{T}_{\mu\nu}(-k) \frac{2\eta^{\mu\rho}\eta^{\nu\sigma} - \frac{2}{3}\eta^{\mu\nu}\eta^{\rho\sigma}}{-k^2 - m^2 + i\epsilon} \tilde{T}_{\rho\sigma}(k) \tag{3.2.8}$$

考虑能量项, 可见质量互相吸引.

3.3 remarks

- 由于 seesaw mechanism (见 appendix C), 引入扰动一般会降低基态能量, 因此大多数相互作用表现为吸引, 而 spin-1 表现为同性相斥是因为 $\eta^{00} = -1$.

- 本 chapter 中的计算都是 $m \neq 0$ 的粒子, 与真实世界有差异.

Appendices

Appendix A

Dirac delta function & Fourier transformation

A.1   Delta function

- 可以认为以下是定义式,

$$\delta(x) = \int \frac{dk}{2\pi} e^{ikx} \iff \tilde{\delta}(k) = 1 = \int dx\, \delta(x) e^{-ikx} \tag{A.1.1}$$

- 第一个常用的公式,

$$\int_{-\infty}^{+\infty} \delta(f(x))g(x)dx = \sum_{\{i, f(x_i)=0\}} \frac{g(x_i)}{|f'(x_i)|} \tag{A.1.2}$$

- 第二个常用的公式 (Sokhotski-Plemelj theorem),

$$\lim_{\epsilon \to 0^+} \frac{1}{x + i\epsilon} = \mathcal{P}\frac{1}{x} - i\pi\delta(x) \tag{A.1.3}$$

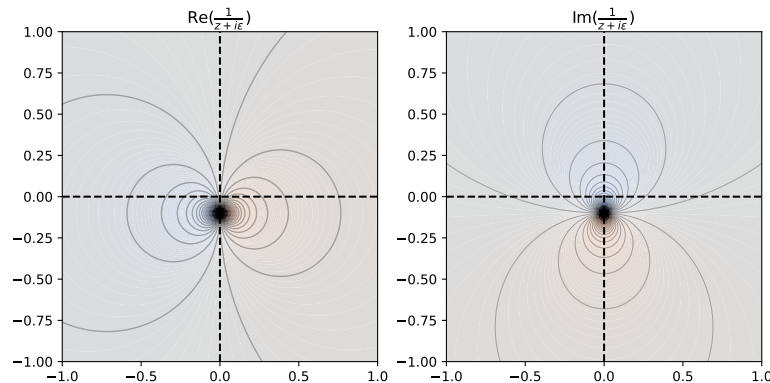其中 $\mathcal{P}$ 表示复函数的主值 (principal value).

> **proof:**
>
> 考虑,
>
> $$\frac{1}{x + i\epsilon} = \frac{x - i\epsilon}{x^2 + \epsilon^2} \tag{A.1.4}$$
>
> 且注意到,
>
> $$\int \frac{\epsilon}{x^2 + \epsilon^2} dx = 2\pi i \operatorname{Res}(f, i\epsilon) = \pi \tag{A.1.5}$$
>
> 所以...
>
> ---
>
> 取 $\epsilon = 0.1$ 时, 复变函数的实部, 虚部分别如下,
>
>

A.2　Fourier transformation

- d-dim. Fourier transformation 如下,

$$
\begin{cases}
\phi(x) = \displaystyle\int \frac{d^d k}{(2\pi)^d} e^{ik\cdot x} \tilde{\phi}(k) \\[2ex]
\tilde{\phi}(k) = \displaystyle\int d^d x\, e^{-ik\cdot x} \phi(x)
\end{cases}
\tag{A.2.1}
$$

- 因此,

$$
\partial_\mu \phi(x) \mapsto ik_\mu \tilde{\phi}(k)
\tag{A.2.2}
$$

Appendix B

Gaussian integrals

- 最基本的几个 Gaussian integral 如下,

$$\int dx\, e^{-\frac{1}{2}ax^2} = \sqrt{\frac{2\pi}{a}} \tag{B.0.1}$$

$$\langle x^{2n} \rangle = \frac{\int dx\, e^{-\frac{1}{2}ax^2} x^{2n}}{\int dx\, e^{-\frac{1}{2}ax^2}} = \frac{1}{a^n}(2n-1)!! \tag{B.0.2}$$

其中 $(2n-1)!! = 1 \cdot 3 \cdots (2n-3)(2n-1)$.

- 一个重要的变体如下,

$$\int dx\, e^{-\frac{a}{2}x^2 + Jx} = \sqrt{\frac{2\pi}{a}} e^{\frac{J^2}{2a}} \tag{B.0.3}$$

另外, 将 a, J 分别替换为 $-ia, iJ$ 也是重要的变体.

B.1 N-dim. generalization

- 考虑如下积分,

$$Z(A, J) = \int dx_1 \cdots dx_N\, e^{-\frac{1}{2}x^T \cdot A \cdot x + J^T \cdot x} = \sqrt{\frac{(2\pi)^N}{\det A}} e^{\frac{1}{2}J^T \cdot A^{-1} \cdot J} \tag{B.1.1}$$

其中 x, J 是 N-dim. 列向量, A 是 $N \times N$ 实对称矩阵.

> **calculation:**
>
> 根据 spectral theorem for normal matrices (对称矩阵是厄密矩阵在实数域上的对应), 可知存在 orthogonal transformation 使得,
>
> $$A = O^{-1} \cdot D \cdot O \tag{B.1.2}$$
>
> 其中 D 是一个 diagonal matrix. 令 $y = O \cdot x$, 那么,
>
> $$Z(A, J) = \int dy_1 \cdots dy_N\, e^{-\frac{1}{2}y^T \cdot D \cdot y + (OJ)^T \cdot y}$$
>
> $$= \prod_{i=1}^{N} \sqrt{\frac{2\pi}{D_{ii}}} e^{\frac{1}{2D_{ii}}(OJ)_i^2} = \sqrt{\frac{(2\pi)^N}{\det A}} e^{\frac{1}{2}J^T \cdot A^{-1} \cdot J} \tag{B.1.3}$$
>
> 其中, 注意到了 $\frac{1}{D_{ii}} = (O \cdot A^{-1} \cdot O^{-1})_{ii}$ 以及 $\operatorname{tr} D = \det A$.

- 一个重要的变体是 $A \mapsto -iA, J \mapsto iJ$.
- 考虑 (B.0.2) 的变体, (注意 A 是对称的),

$$\langle x_i x_j \rangle = \frac{1}{Z(A, 0)} \frac{\partial}{\partial J_i} \frac{\partial}{\partial J_j} Z(A, J) \Big|_{J=0} = A_{ij}^{-1} \tag{B.1.4}$$

$$\langle x_i x_j \cdots x_k x_l \rangle = \sum_{\text{Wick}} A_{i'j'}^{-1} \cdots A_{k'l'}^{-1} \tag{B.1.5}$$

其中 (B.1.5) 中有偶数个 x, 否则等于零.

$$\langle x_i x_j \cdots x_k x_l \rangle = \frac{1}{Z(A,0)} \frac{\partial}{\partial J_i} \frac{\partial}{\partial J_j} \cdots \frac{\partial}{\partial J_k} \frac{\partial}{\partial J_l} Z(A,J)\Big|_{J=0} = \cdots \tag{B.1.6}$$

例如,

$$\langle x_i x_j x_k x_l \rangle = A_{ij}^{-1} A_{kl}^{-1} + A_{ik}^{-1} A_{jl}^{-1} + A_{il}^{-1} A_{jk}^{-1} \tag{B.1.7}$$

其中, 可以用 Wick contraction 计算上式, 如下,

$$\langle \overbrace{x_i x_j x_k x_l} \rangle = A_{ik}^{-1} A_{jl}^{-1} \tag{B.1.8}$$

Appendix C

perturbation theory in QM

- this chapter is based on MIT OpenCourseWare Quantum Physics III Chapter 1: Perturbation Theory.

- 研究的 Hamiltonian 与 well studied Hamiltonian 有微小差异时, 使用 perturbation theory,

$$H(\lambda) = H^{(0)} + \lambda \delta H \tag{C.0.1}$$

其中 $\lambda \in [0,1]$.

- 考虑 $H^{(0)}$ 的本征态为,

$$H^{(0)} |k^{(0)}\rangle = E_k^{(0)} |k^{(0)}\rangle \quad \text{and} \quad \begin{cases} \langle k^{(0)}|l^{(0)}\rangle = \delta_{kl} \\ E_0^{(0)} \leq E_1^{(0)} \leq E_2^{(0)} \leq \cdots \end{cases} \tag{C.0.2}$$

C.1 non-degenerate perturbation theory

- 考虑 non-degenerate 能级 k, 有 $\cdots \leq E_{k-1}^{(0)} < E_k^{(0)} < E_{k+1}^{(0)} \leq \cdots$, 在 perturbation theory 适用的情况下,

$$\begin{cases} |k\rangle_\lambda = |k^{(0)}\rangle + \lambda |k^{(1)}\rangle + \lambda^2 |k^{(2)}\rangle + \cdots \\ E_k(\lambda) = E_k^{(0)} + \lambda E_k^{(1)} + \lambda^2 E_k^{(2)} + \cdots \end{cases} \tag{C.1.1}$$

– 注意, 我们可以选取修正项满足,
$$\langle k^{(0)}|k^{(n)}\rangle = 0, n = 1, 2, \cdots \tag{C.1.2}$$

> **proof:**
>
> 假设我们求解得到的修正项不满足 $\langle k^{(0)}|k^{(n)}\rangle = 0, n = 1, 2, \cdots$, 考虑,
>
> $$|k^{(n)}\rangle' = |k^{(n)}\rangle + a_n |k^{(0)}\rangle \quad \text{with} \quad \langle k^{(0)}|k^{(n)}\rangle' = 0 \tag{C.1.3}$$
>
> 那么, (注意到态矢量可以乘一个常数, $\frac{1}{1-a_1\lambda-a_2\lambda^2-\cdots} = 1 + a_1\lambda + (a_1^2 + a_2)\lambda^2 + \cdots$),
>
> $$|k\rangle_\lambda = (1 - a_1\lambda - a_2\lambda^2 - \cdots) |k^{(0)}\rangle + \lambda |k^{(1)}\rangle' + \lambda^2 |k^{(2)}\rangle' + \cdots$$
> $$|k\rangle'_\lambda = |k^{(0)}\rangle + \frac{1}{1-a_1\lambda-a_2\lambda^2-\cdots} \left(\lambda |k^{(1)}\rangle' + \lambda^2 |k^{(2)}\rangle' + \cdots \right)$$
> $$= |k^{(0)}\rangle + \lambda |k^{(1)}\rangle' + \lambda^2 (a_1 |k^{(1)}\rangle' + |k^{(2)}\rangle') + \cdots \tag{C.1.4}$$
>
> 可见修正项都与 $|k^{(0)}\rangle$ 正交.

– 注意, 不能要求 $_\lambda\langle k|k\rangle_\lambda = 1$, 否则 $|k^{(n)}\rangle$ 将与 λ 相关 (包括 $|k^{(0)}\rangle$),

$$\begin{aligned} _\lambda\langle k|k\rangle_\lambda = {} & \langle k^{(0)}|k^{(0)}\rangle \\ & + \lambda(\langle k^{(1)}|k^{(0)}\rangle + \langle k^{(0)}|k^{(1)}\rangle) \\ & + \lambda^2(\langle k^{(2)}|k^{(0)}\rangle + \langle k^{(1)}|k^{(1)}\rangle + \langle k^{(0)}|k^{(2)}\rangle) \end{aligned}$$

$$\vdots$$
$$+ \lambda^n (\langle k^{(n)}|k^{(0)}\rangle + \langle k^{(n-1)}|k^{(1)}\rangle + \cdots + \langle k^{(0)}|k^{(n)}\rangle) \tag{C.1.5}$$

- 将 (C.1.1) 代入 Schrodinger's eq., 得到,

$$
\begin{array}{ll}
\lambda^0 & (H^{(0)} - E_k^{(0)})\,|k^{(0)}\rangle = 0 \\[4pt]
\lambda^1 & (H^{(0)} - E_k^{(0)})\,|k^{(1)}\rangle = (E_k^{(1)} - \delta H)\,|k^{(0)}\rangle \\[4pt]
\lambda^2 & (H^{(0)} - E_k^{(0)})\,|k^{(2)}\rangle = (E_k^{(1)} - \delta H)\,|k^{(1)}\rangle + E_k^{(2)}\,|k^{(0)}\rangle \\[2pt]
\vdots & \qquad\qquad\qquad\qquad\qquad\vdots \\[2pt]
\lambda^n & (H^{(0)} - E_k^{(0)})\,|k^{(n)}\rangle = (E_k^{(1)} - \delta H)\,|k^{(n-1)}\rangle + E_k^{(2)}\,|k^{(n-2)}\rangle + \cdots + E_k^{(n)}\,|k^{(0)}\rangle
\end{array}
$$

> **calculation:**
>
> Schrodinger's eq. 为,
> $$(H^{(0)} + \lambda \delta H - E_k(\lambda))\,|k\rangle_\lambda = 0 \tag{C.1.6}$$
> 展开为,
> $$\Big((H^{(0)} - E_k^{(0)}) + \lambda(\delta H - E_k^{(1)}) - \lambda^2 E_k^{(2)} - \cdots \Big)(|k^{(0)}\rangle + \lambda\,|k^{(1)}\rangle + \lambda^2\,|k^{(2)}\rangle + \cdots) = 0 \tag{C.1.7}$$

- 现在来计算 $\langle l^{(0)}|k^{(n)}\rangle$, 有,

$$
\begin{cases}
(E_l^{(0)} - E_k^{(0)})\,\langle l^{(0)}|k^{(1)}\rangle = & E_k^{(1)}\delta_{lk} - \delta H_{lk} \\[4pt]
(E_l^{(0)} - E_k^{(0)})\,\langle l^{(0)}|k^{(2)}\rangle = & E_k^{(1)}\,\langle l^{(0)}|k^{(1)}\rangle - \langle l^{(0)}|\delta H|k^{(1)}\rangle + E_k^{(2)}\delta_{lk} \\[2pt]
\quad\vdots & \qquad\qquad\qquad\vdots \\[2pt]
(E_l^{(0)} - E_k^{(0)})\,\langle l^{(0)}|k^{(n)}\rangle = & E_k^{(1)}\,\langle l^{(0)}|k^{(n-1)}\rangle - \langle l^{(0)}|\delta H|k^{(n-1)}\rangle \\[2pt]
& + E_k^{(2)}\,\langle l^{(0)}|k^{(n-2)}\rangle + \cdots + E_k^{(n)}\delta_{lk}
\end{cases} \tag{C.1.8}
$$

其中 $\delta H_{lk} = \langle l^{(0)}|\delta H|k^{(0)}\rangle$, 对于满足 (C.1.2) 的解, 有,

$$E_k^{(n)} = \langle k^{(0)}|\delta H|k^{(n-1)}\rangle,\, n = 1, 2, \cdots \tag{C.1.9}$$

并且,

$$|k^{(1)}\rangle = -\sum_{l \neq k} \frac{\delta H_{lk}}{E_l^{(0)} - E_k^{(0)}}\,|l^{(0)}\rangle \implies E_k^{(2)} = -\sum_{l \neq k} \frac{|\delta H_{lk}|^2}{E_l^{(0)} - E_k^{(0)}} \tag{C.1.10}$$

> **calculation:**
>
> 将 (C.1.10) 代入 (C.1.8), 得到 $(l \neq k)$,
> $$(E_l^{(0)} - E_k^{(0)})\,\langle l^{(0)}|k^{(2)}\rangle = -E_k^{(1)} \frac{\delta H_{lk}}{E_l^{(0)} - E_k^{(0)}} + \sum_{m \neq k} \frac{\delta H_{lm}\delta H_{mk}}{E_m^{(0)} - E_k^{(0)}} \tag{C.1.11}$$
>
> 所以,
> $$
> \begin{cases}
> |k^{(2)}\rangle = \displaystyle\sum_{l \neq k} \Big(-\frac{\delta H_{00}\delta H_{lk}}{(E_l^{(0)} - E_k^{(0)})^2} + \sum_{m \neq k} \frac{\delta H_{lm}\delta H_{mk}}{E_m^{(0)} - E_k^{(0)}} \Big)\,|l^{(0)}\rangle \\[12pt]
> E_k^{(3)} = \displaystyle\sum_{l \neq k} \Big(-\frac{\delta H_{00}|\delta H_{lk}|^2}{(E_l^{(0)} - E_k^{(0)})^2} + \sum_{m \neq k} \frac{\delta H_{kl}\delta H_{lm}\delta H_{mk}}{E_m^{(0)} - E_k^{(0)}} \Big)
> \end{cases} \tag{C.1.12}
> $$
>
> ---
> 计算归一化系数,
> $$_\lambda\langle k|k\rangle_\lambda = 1 + \lambda^2 \sum_{l \neq k} \frac{|\delta H_{lk}|^2}{(E_l^{(0)} - E_k^{(0)})^2} + O(\lambda^3) \tag{C.1.13}$$

C.1.1   level repulsion or the seesaw mechanism

- 能量的展开式为,

$$E_k(\lambda) = E_k^{(0)} + \lambda \delta H_{kk} - \lambda^2 \sum_{l \neq k} \frac{|\delta H_{lk}|^2}{E_l^{(0)} - E_k^{(0)}} + O(\lambda^3) \tag{C.1.14}$$

二阶项的效果是使能级间距增大, 对于基态能级, 二阶项使其能量减小.

C.1.2   validity of the perturbation expansion

- 考虑两能级系统, 可以得出微扰展开收敛的条件, 即,

$$|\lambda V| < \frac{1}{2} \Delta E^{(0)} \tag{C.1.15}$$

因此, 对于能级简并的情况, $\Delta E^{(0)} = 0$, 情况会更复杂.

---

calculation:

对于两能级系统,

$$H(\lambda) = H^{(0)} + \lambda \hat{V} = \begin{pmatrix} E_1^{(0)} & \lambda V \\ \lambda V^* & E_2^{(0)} \end{pmatrix} \tag{C.1.16}$$
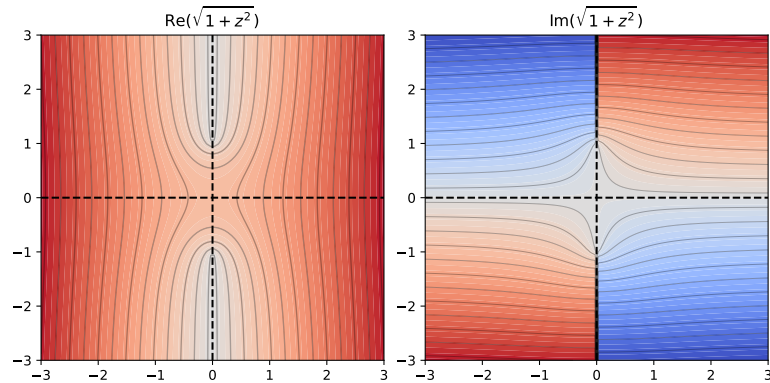
$H(\lambda)$ 的本征值可以直接计算,

$$E_{\pm}(\lambda) = \frac{1}{2}(E_1^{(0)} + E_2^{(0)}) \pm \frac{1}{2}(E_1^{(0)} - E_2^{(0)}) \sqrt{1 + \left(\frac{\lambda |V|}{\frac{1}{2}(E_1^{(0)} - E_2^{(0)})} \right)^2} \tag{C.1.17}$$

考虑 $\sqrt{1 + z^2}$ 的 Taylor 展开,

$$\sqrt{1 + z^2} = 1 + \frac{z^2}{2} - \frac{z^4}{8} + \cdots + (-1)^{n+1} \frac{(2n-3)!!}{2^n n!} z^{2n} + \cdots \tag{C.1.18}$$

注意到 $\sqrt{1 + z^2}$ 在 $z = \pm i$ 有 branch cut, 因此 $z = 0$ 附件的 Taylor expansion 只有在 $|z| < 1$ 内才收敛.

C.2   degenerate perturbation theory

- 暂时先跳过.