

Quantum Field Theory

- based on A. Zee's textbook -

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

- 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,

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

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,

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

- 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,

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

另外, 用 $W(J)$ 表示指数上的部分 (去掉虚数 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,

$$Z(J) = \int D\phi e^{i \int d^d x \frac{1}{2} (\phi (\partial^2 - m^2) \phi + J(x)\phi(x))} \quad (1.1.4)$$

代入 (B.1.1), 可知,

$$Z(J) = \mathcal{C} e^{-\frac{i}{2} \int d^d x d^d y J(x) D(x-y) J(y)} \quad (1.1.5)$$

其中 $D(x-y)$ 满足,

$$\begin{cases} (\partial^2 - m^2) D(x-y) = \delta^{(d)}(x-y) \\ (-p^2 - m^2) \tilde{D}(p, q) = (2\pi)^d \delta^{(d)}(p-q) \end{cases} \implies D(x-y) = \int \frac{d^d k}{(2\pi)^d} \frac{e^{ik \cdot (x-y)}}{-k^2 - m^2} \quad (1.1.6)$$

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,

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

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,

$$D(t, 0) = -i \int \frac{d^D k}{(2\pi)^D 2\omega_k} \left(e^{-i\omega_k t} \theta(t) + e^{i\omega_k t} \theta(-t) \right) \quad (1.2.2)$$

- 类空区域,

$$D(0, \vec{x}) = -i \int \frac{d^D k}{(2\pi)^D 2\omega_k} e^{i\vec{k} \cdot \vec{x}} \sim e^{-m|\vec{x}|} \quad (1.2.3)$$

Chapter 2

from field to particle to force

2.1 from field to particle

- 考虑 (1.1.3) 中的 $W(J)$,

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

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

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,

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

可见 $W(J)$ 取值较大的条件是:

- $\tilde{J}_1(k), \tilde{J}_2(k)$ 有较大重叠,
 - 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 $J(x) = \delta^{(D)}(\vec{x} - \vec{x}_1) + \delta^{(D)}(\vec{x} - \vec{x}_2) \implies \tilde{J}_a(k) = 2\pi e^{-i\vec{k} \cdot \vec{x}_a} \delta(k^0)$, 那么,

$$\begin{aligned} W_{12}(J) + W_{21}(J) &= \delta(0) \int \frac{d^D k}{(2\pi)^{D-1}} \frac{1}{|\vec{k}|^2 + m^2 - i\epsilon} \cos(\vec{k} \cdot (\vec{x}_1 - \vec{x}_2)) \\ &\stackrel{D=3}{=} 2\pi \delta(0) \frac{1}{4\pi r} e^{-mr} \end{aligned} \quad (2.2.1)$$

($-i\epsilon$ 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,

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

calculation:

计算 (2.2.1) 中的积分, 令 $\vec{x}_1 - \vec{x}_2 = \vec{r}$,

$$I_D = \int \frac{d^D k}{(2\pi)^D} \frac{1}{|\vec{k}|^2 + m^2} \overbrace{\cos(\vec{k} \cdot \vec{r})}^{\mapsto e^{i\vec{k} \cdot \vec{r}}}$$

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

取 $D = 3$, 那么,

$$\begin{aligned}
I_{D=3} &= \frac{1}{(2\pi)^2} \int k^2 \sin \theta_1 d\theta_1 dk \frac{1}{k^2 + m^2} e^{ik \cos \theta_1} \\
&= \frac{1}{2\pi^2 r} \int_0^\infty \sin(kr) \frac{k dk}{k^2 + m^2} = \frac{-i}{4\pi^2 r} \int_{-\infty}^\infty e^{ikr} \frac{k dk}{k^2 + m^2} \\
&= \frac{-i}{4\pi^2 r} 2\pi i \underbrace{\text{Res}(f, im)}_{=\frac{1}{2}e^{-mr}} = \frac{1}{4\pi r} e^{-mr}
\end{aligned} \tag{2.2.4}$$

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,

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

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

- 做路径积分,

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

calculation:

massive photon 的作用量为,

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

那么, 需要有,

$$\begin{aligned} (-\partial^\mu \partial^\rho + \eta^{\mu\rho}(\partial^2 - m^2)) D_{\rho\nu}(x-y) &= \delta_\nu^\mu \delta^{(d)}(x-y) \\ \implies \tilde{D}_{\mu\nu}(k) &= \frac{k_\mu k_\nu / m^2 + \eta_{\mu\nu}}{-k^2 - m^2} \end{aligned} \quad (3.1.4)$$

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,

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

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

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

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

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 $(\epsilon^i)_\mu = \delta_\mu^i, i = 1, 2, 3$, 而 $k_\mu = (-m, 0, 0, 0)$, 所以,

$$k^\mu (\epsilon^i)_\mu = 0 \quad (3.1.8)$$

– 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,

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

可见,

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

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,

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

其中下指标 μ, ν 对称, $a = 1, \dots, 5$, (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,

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

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),

$$A k_\mu k_\nu k_\rho k_\sigma + B(k_\mu k_\nu \eta_{\rho\sigma} + k_\rho k_\sigma \eta_{\mu\nu}) + C(k_\mu k_\rho \eta_{\nu\sigma} + k_\mu k_\sigma \eta_{\nu\rho} + k_\nu k_\rho \eta_{\mu\sigma} + k_\nu k_\sigma \eta_{\mu\rho}) + D \eta_{\mu\nu} \eta_{\rho\sigma} + E(\eta_{\mu\rho} \eta_{\nu\sigma} + \eta_{\mu\sigma} \eta_{\nu\rho}) \quad (3.2.3)$$

代入 (3.2.1) 得,

$$\begin{cases} 0 = -A + B + 2C = -B + D = -C + E \\ 0 = -A + 4B + 4C = -B + 4D + 2E \end{cases} \implies \frac{B = D, C = E}{A} = -\frac{1}{2}, \frac{3}{4} \quad (3.2.4)$$

因此, 这个 4 阶张量最终确定为,

$$\frac{3}{4} A \left((G_{\mu\rho} G_{\nu\sigma} + G_{\mu\sigma} G_{\nu\rho}) - \frac{2}{3} G_{\mu\nu} G_{\rho\sigma} \right) \quad (3.2.5)$$

- 所以,

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

- 计算路径积分中的 $W(T)$,

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

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,

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

考虑能量项, 可见质量互相吸引.

Appendices

Appendix A

Dirac delta function & Fourier transformation

A.1 Delta function

- 可以认为以下是定义式,

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

- 第一个常用的公式,

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

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

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

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

proof:

考虑,

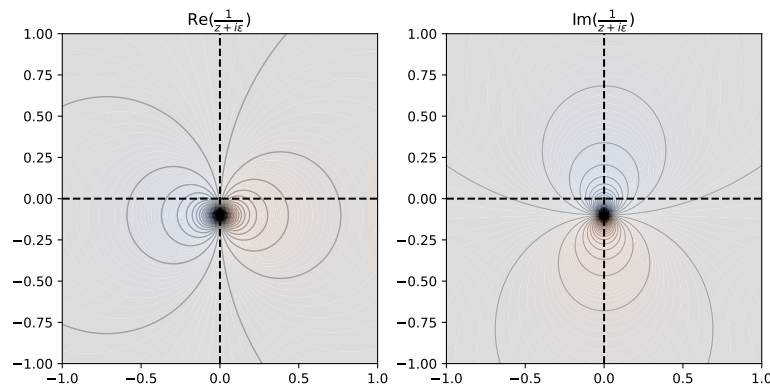
$$\frac{1}{x + i\epsilon} = \frac{x - i\epsilon}{x^2 + \epsilon^2} \quad (\text{A.1.4})$$

且注意到,

$$\int \frac{\epsilon}{x^2 + \epsilon^2} dx = 2\pi i \text{Res}(f, i\epsilon) = \pi \quad (\text{A.1.5})$$

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,

$$\begin{cases} \phi(x) = \int \frac{d^d k}{(2\pi)^d} e^{ik \cdot x} \tilde{\phi}(k) \\ \tilde{\phi}(k) = \int d^d x e^{-ik \cdot x} \phi(x) \end{cases} \quad (\text{A.2.1})$$

- 因此,

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

Appendix B

Gaussian integrals

- 最基本的几个 Gaussian integral 如下,

$$\int dx e^{-\frac{1}{2}ax^2} = \sqrt{\frac{2\pi}{a}} \quad (\text{B.0.1})$$

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

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

- 一个重要的变体如下,

$$\int dx e^{-\frac{a}{2}x^2 + Jx} = \sqrt{\frac{2\pi}{a}} e^{\frac{J^2}{2a}} \quad (\text{B.0.3})$$

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,

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

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,

$$A = O^{-1} \cdot D \cdot O \quad (\text{B.1.2})$$

其中 D 是一个 diagonal matrix. 令 $y = O \cdot x$, 那么,

$$\begin{aligned} Z(A, J) &= \int dy_1 \cdots dy_N e^{-\frac{1}{2}y^T \cdot D \cdot y + (OJ)^T \cdot y} \\ &= \prod_{i=1}^N \sqrt{\frac{2\pi}{D_{ii}}} e^{\frac{1}{2D_{ii}}(OJ)_i^2} = \sqrt{\frac{(2\pi)^N}{\det A}} e^{\frac{1}{2}J^T \cdot A^{-1} \cdot J} \end{aligned} \quad (\text{B.1.3})$$

其中, 注意到了 $\frac{1}{D_{ii}} = (O \cdot A^{-1} \cdot O^{-1})_{ii}$ 以及 $\text{tr } D = \det A$.

- 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),

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

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

其中 (B.1.5) 中有偶数个 x , 否则等于零.

calculation:

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

例如,

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

其中, 可以用 Wick contraction 计算上式, 如下,

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

Appendix C

perturbation theory in QM

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

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

其中 $\lambda \in [0, 1]$.

- 考虑 $H^{(0)}$ 的本征态为,

$$H^{(0)} |k^{(0)}\rangle = E_k^{(0)} |k^{(0)}\rangle \quad (\text{C.0.2})$$

并满足,

$$\begin{cases} \langle k^{(0)} | l^{(0)} \rangle = \delta_{kl} \\ E_0^{(0)} \leq E_1^{(0)} \leq E_2^{(0)} \leq \dots \end{cases} \quad (\text{C.0.3})$$

C.1 non-degenerate perturbation theory

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

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

– 注意, 我们可以选取修正项满足,

$$\langle k^{(0)} | k^{(n)} \rangle = 0, n = 1, 2, \dots \quad (\text{C.1.2})$$

proof:

假设我们求解得到的修正项不满足 $\langle k^{(0)} | k^{(n)} \rangle = 0, n = 1, 2, \dots$, 考虑,

$$|k^{(n)}\rangle' = |k^{(n)}\rangle + a_n |k^{(0)}\rangle \quad \text{with} \quad \langle k^{(0)} | k^{(n)} \rangle' = 0 \quad (\text{C.1.3})$$

那么, (注意到态矢量可以乘一个常数, $\frac{1}{1 - a_1 \lambda - a_2 \lambda^2 - \dots} = 1 + a_1 \lambda + (a_1^2 + a_2) \lambda^2 + \dots$),

$$\begin{aligned} |k\rangle_\lambda &= (1 - a_1 \lambda - a_2 \lambda^2 - \dots) |k^{(0)}\rangle + \lambda |k^{(1)}\rangle' + \lambda^2 |k^{(2)}\rangle' + \dots \\ |k\rangle_\lambda' &= |k^{(0)}\rangle + \frac{1}{1 - a_1 \lambda - a_2 \lambda^2 - \dots} (\lambda |k^{(1)}\rangle' + \lambda^2 |k^{(2)}\rangle' + \dots) \\ &= |k^{(0)}\rangle + \lambda |k^{(1)}\rangle' + \lambda^2 (a_1 |k^{(1)}\rangle' + |k^{(2)}\rangle') + \dots \end{aligned} \quad (\text{C.1.4})$$

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 $|k^{(0)}\rangle$),

$$\begin{aligned} {}_\lambda \langle k | k \rangle_\lambda &= \langle k^{(0)} | k^{(0)} \rangle \\ &\quad + \lambda (\langle k^{(1)} | k^{(0)} \rangle + \langle k^{(0)} | k^{(1)} \rangle) \\ &\quad + \lambda^2 (\langle k^{(2)} | k^{(0)} \rangle + \langle k^{(1)} | k^{(1)} \rangle + \langle k^{(0)} | k^{(2)} \rangle) \\ &\quad \vdots \\ &\quad + \lambda^n (\langle k^{(n)} | k^{(0)} \rangle + \langle k^{(n-1)} | k^{(1)} \rangle + \dots + \langle k^{(0)} | k^{(n)} \rangle) \end{aligned} \quad (\text{C.1.5})$$

- 将 (C.1.1) 代入 Schrodinger's eq., 得到,

$$\begin{array}{ll}
\lambda^0 & (H^{(0)} - E_k^{(0)}) |k^{(0)}\rangle = 0 \\
\lambda^1 & (H^{(0)} - E_k^{(0)}) |k^{(1)}\rangle = (E_k^{(1)} - \delta H) |k^{(0)}\rangle \\
\lambda^2 & (H^{(0)} - E_k^{(0)}) |k^{(2)}\rangle = (E_k^{(1)} - \delta H) |k^{(1)}\rangle + E_k^{(2)} |k^{(0)}\rangle \\
\vdots & \vdots \\
\lambda^n & (H^{(0)} - E_k^{(0)}) |k^{(n)}\rangle = (E_k^{(1)} - \delta H) |k^{(n-1)}\rangle + E_k^{(2)} |k^{(n-2)}\rangle + \dots + E_k^{(n)} |k^{(0)}\rangle
\end{array}$$

calculation:

Schrodinger's eq. 为,

$$(H^{(0)} + \lambda \delta H - E_k(\lambda)) |k\rangle_\lambda = 0 \quad (\text{C.1.6})$$

展开为,

$$\left((H^{(0)} - E_k^{(0)}) + \lambda(\delta H - E_k^{(1)}) - \lambda^2 E_k^{(2)} - \dots \right) (|k^{(0)}\rangle + \lambda |k^{(1)}\rangle + \lambda^2 |k^{(2)}\rangle + \dots) = 0 \quad (\text{C.1.7})$$

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

$$\begin{cases}
(E_l^{(0)} - E_k^{(0)}) \langle l^{(0)} | k^{(1)} \rangle = E_k^{(1)} \delta_{lk} - \delta H_{lk} \\
(E_l^{(0)} - E_k^{(0)}) \langle l^{(0)} | k^{(2)} \rangle = E_k^{(1)} \langle l^{(0)} | k^{(1)} \rangle - \langle l^{(0)} | \delta H | k^{(1)} \rangle + E_k^{(2)} \delta_{lk} \\
\vdots \\
(E_l^{(0)} - E_k^{(0)}) \langle l^{(0)} | k^{(n)} \rangle = E_k^{(1)} \langle l^{(0)} | k^{(n-1)} \rangle - \langle l^{(0)} | \delta H | k^{(n-1)} \rangle \\
\quad + E_k^{(2)} \langle l^{(0)} | k^{(n-2)} \rangle + \dots + E_k^{(n)} \delta_{lk}
\end{cases} \quad (\text{C.1.8})$$

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

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

并且,

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

calculation:

将 (C.1.10) 代入 (C.1.8), 得到 ($l \neq k$),

$$(E_l^{(0)} - E_k^{(0)}) \langle l^{(0)} | k^{(2)} \rangle = -E_k^{(1)} \frac{\delta H_{lk}}{E_l^{(0)} - E_k^{(0)}} + \sum_{m \neq k} \frac{\delta H_{lm} \delta H_{mk}}{E_m^{(0)} - E_k^{(0)}} \quad (\text{C.1.11})$$

所以,

$$\begin{cases}
|k^{(2)}\rangle = \sum_{l \neq k} \left(- \frac{\delta H_{00} \delta H_{lk}}{(E_l^{(0)} - E_k^{(0)})^2} + \sum_{m \neq k} \frac{\delta H_{lm} \delta H_{mk}}{E_m^{(0)} - E_k^{(0)}} \right) |l^{(0)}\rangle \\
E_k^{(3)} = \sum_{l \neq k} \left(- \frac{\delta H_{00} |\delta H_{lk}|^2}{(E_l^{(0)} - E_k^{(0)})^2} + \sum_{m \neq k} \frac{\delta H_{kl} \delta H_{lm} \delta H_{mk}}{E_m^{(0)} - E_k^{(0)}} \right)
\end{cases} \quad (\text{C.1.12})$$

计算归一化系数,

$${}_l \langle k | k \rangle_\lambda = 1 + \lambda^2 \sum_{l \neq k} \frac{|\delta H_{lk}|^2}{(E_l^{(0)} - E_k^{(0)})^2} + O(\lambda^3) \quad (\text{C.1.13})$$

C.1.1 level repulsion or the seesaw mechanism

- 能量的展开式为,

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

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

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C.2 degenerate perturbation theory