问题目标: 使用曲面线性有限元方法实现球面上的ABC-star 数值模拟

ABC-Star模型

哈密顿量

$$H = \frac{n}{V}\int \mathrm{d}r[\chi_{AB}N\rho_A\rho_B + \chi_{BC}N\rho_B\rho_C + \chi_{AC}N\rho_A\rho_C - w_A\rho_A - w_B\rho_B - w_C\rho_C - w_+(1-\rho_A-\rho_B-\rho_C)] \\ - nlogQ[w_A, w_B, w_C]$$

外场的作用力

$$\begin{aligned} w_A &= u_+ - \sigma_{1A}u_1 - \sigma_{2A}u_2 \\ w_B &= u_+ - \sigma_{1B}u_1 - \sigma_{2B}u_2 \\ w_C &= u_+ - \sigma_{1C}u_1 - \sigma_{2C}u_2 \end{aligned}$$

其中, 相关的参数

$$\begin{aligned} \sigma_{1A} &= \frac{1}{3}, \sigma_{1B} = -\frac{2}{3}, \sigma_{1C} = \frac{1}{3} \\ \sigma_{2A} &= \frac{1+\alpha}{3}, \sigma_{2B} = -\frac{1-2\alpha}{3}, \sigma_{2C} = \frac{\alpha-2}{3} \end{aligned}$$

还需要已知 u_+, u_1, u_2. 其中 $u_+ = 0$, 根据下面的 SCFT 方程求解 u_1, u_2.

$$\begin{aligned} \rho_A + \rho_B + \rho_C - 1 &= 0 \\ \frac{1}{2N\xi_1}u_1 - \sigma_{1A}\rho_A - \sigma_{1B}\rho_B - \sigma_{1C}\rho_C &= 0 \\ \frac{1}{2N\xi_2}u_2 - \sigma_{2A}\rho_A - \sigma_{2B}\rho_B - \sigma_{2C}\rho_C &= 0 \end{aligned}$$

则

$$\begin{aligned} u_1 &= 2N\xi_1(\sigma_{1A}\rho_A + \sigma_{1B}\rho_B + \sigma_{1C}\rho_C) \\ u_2 &= 2N\xi_2(\sigma_{2A}\rho_A - \sigma_{2B}\rho_B - \sigma_{2C}\rho_C) \end{aligned}$$

其中 $\xi_1 = \frac{-\Delta}{4\chi_{AC}}, \xi_2 = \chi_{AC}$.

$$\Delta = \chi_{AB}^2 + \chi_{BC}^2 + \chi_{AC}^2 - 2\chi_{AB}\chi_{AC} - 2\chi_{BC}\chi_{AC} - 2\chi_{AB}\chi_{BC}$$

根据准备的 w_A, w_B, w_C. 可以计算传播子方程. 求出 ρ_A, ρ_B, ρ_C, 和单链配分函数 Q.

ABC-star 传播子方程

$$\begin{aligned} \frac{\partial}{\partial s}q_\alpha(\mathbf{r}, s) &= \nabla_{\mathbf{S}}^2 q_\alpha(\mathbf{r}, s) - w_\alpha q_\alpha(\mathbf{r}, s), q_\alpha(\mathbf{r}, s) = 1, s \in [0, f_\alpha] \\ \frac{\partial}{\partial s}q_\alpha^+(\mathbf{r}, s) &= \nabla_{\mathbf{S}}^2 q_\alpha^+(\mathbf{r}, s) - w_\alpha q_\alpha^+(\mathbf{r}, s), q_\alpha^+(\mathbf{r}, s) = q_K(\mathbf{r}, f_K), s \in [0, f_\alpha] \end{aligned}$$

$$\rho_A + \rho_B + \rho_C = 1$$

$$
\begin{aligned}
\rho_A &= \frac{1}{Q}\int_0^{f_A} \mathrm{d}s q_A(\mathbf{r},s) q_A^{+}(\mathbf{r}, f_A - s) \\
\rho_B &= \frac{1}{Q}\int_0^{f_B} \mathrm{d}s q_B(\mathbf{r},s) q_B^{+}(\mathbf{r}, f_B - s) \\
\rho_C &= \frac{1}{Q}\int_0^{f_C} \mathrm{d}s q_C(\mathbf{r},s) q_C^{+}(\mathbf{r}, f_C - s) \\
Q &= \frac{1}{V}\int \mathrm{d}r q_\alpha(\mathbf{r},s) q_\alpha^{+}(\mathbf{r}, f_\alpha - s)
\end{aligned}
$$

其中 α是A, B, C,

根据计算的 ρ_A , ρ_B , ρ_C , 重新计算外场 w_A , w_B , w_C .

计算 u_1 , u_2 .

$$
\begin{aligned}
w_A &= \chi_{AB} N_C \rho_B(\mathbf{r}) + \chi_{AC} N_C \rho_C(\mathbf{r}) + w_+ \\
w_B &= \chi_{AB} N_C \rho_A(\mathbf{r}) + \chi_{BC} N_C \rho_C(\mathbf{r}) + w_+ \\
w_C &= \chi_{AC} N_C \rho_A(\mathbf{r}) + \chi_{BC} N_C \rho_B(\mathbf{r}) + w_+
\end{aligned}
$$

$$
w_+ = \frac{\sum_\alpha w_{\alpha,j}^k X_\alpha}{\sum_{\alpha X_\alpha}}
$$

其中,

$$
\begin{aligned}
X_A &= \chi BC(\chi AB + \chi AC - \chi BC) \\
X_B &= \chi AC(\chi BC + \chi AB - \chi AC) \\
X_C &= \chi AB(\chi AC + \chi BC - \chi AB)
\end{aligned}
$$

迭代格式, 用来计算更新后面不断迭代计算的外场作用迭代求解 PDE.

$$
w_{\alpha,j}^{k+1} = w_{\alpha,j}^k + \lambda\left(\frac{\delta H}{\delta \rho_\alpha}\right)_j^k
$$

$\frac{\delta H}{\delta \rho_\alpha}$, 对 哈密顿量的 H 关于 ρ_A , ρ_B , ρ_C , 求变分.