课堂练习

练习1：写出施密特正交化过程对应的X矩阵

解：基组变换的表达式为

$$\begin{pmatrix}|\phi_1'\rangle & |\phi_2'\rangle & \dots & |\phi_n'\rangle\end{pmatrix} = \begin{pmatrix}|\phi_1\rangle & |\phi_2\rangle & \dots & |\phi_n\rangle\end{pmatrix}\boldsymbol{X}$$

以$n=2$为例，首先将$|\phi_1\rangle$归一化，得$|\phi_1'\rangle = \frac{|\phi_1\rangle}{\langle\phi_1|\phi_1\rangle^{\frac{1}{2}}}$，其中归一化系数为$\alpha_1 = \frac{1}{\langle\phi_1|\phi_1\rangle^{\frac{1}{2}}}$，然后设$|\phi_2'\rangle = \alpha_2(|\phi_2\rangle - |\phi_1'\rangle\langle\phi_1'|\phi_2\rangle)$，则

$$\langle\phi_2'|\phi_2'\rangle = |\alpha_2|^2(\langle\phi_2|\phi_2\rangle - \langle\phi_2|\phi_1'\rangle\langle\phi_1'|\phi_2\rangle - \langle\phi_1'|\phi_2\rangle\langle\phi_2|\phi_1'\rangle + \langle\phi_2|\phi_1'\rangle\langle\phi_1'|\phi_1'\rangle\langle\phi_1'|\phi_2\rangle) = |\alpha_2|^2(\langle\phi_2|\phi_2\rangle - \langle\phi_2|\phi_1'\rangle\langle\phi_1'|\phi_2\rangle) = 1$$

解得$\alpha_2 = (\frac{\langle\phi_1|\phi_1\rangle}{\langle\phi_1|\phi_1\rangle\langle\phi_2|\phi_2\rangle - \langle\phi_1|\phi_2\rangle\langle\phi_2|\phi_1\rangle})^{\frac{1}{2}}$ （取实数解），因此

$$|\phi_2'\rangle = \alpha_2(|\phi_2\rangle - |\phi_1'\rangle\langle\phi_1'|\phi_2\rangle) = (\frac{\langle\phi_1|\phi_1\rangle}{\langle\phi_1|\phi_1\rangle\langle\phi_2|\phi_2\rangle - \langle\phi_1|\phi_2\rangle\langle\phi_2|\phi_1\rangle})^{\frac{1}{2}}|\phi_2\rangle - \frac{\langle\phi_1|\phi_2\rangle}{[\langle\phi_1|\phi_1\rangle(\langle\phi_1|\phi_1\rangle\langle\phi_2|\phi_2\rangle - \langle\phi_1|\phi_2\rangle\langle\phi_2|\phi_1\rangle)]^{\frac{1}{2}}}|\phi_1\rangle$$

$$\begin{aligned}|\phi_2'\rangle\langle\phi_2'| = &\frac{\langle\phi_1|\phi_1\rangle}{\langle\phi_1|\phi_1\rangle\langle\phi_2|\phi_2\rangle - \langle\phi_1|\phi_2\rangle\langle\phi_2|\phi_1\rangle}|\phi_2\rangle\langle\phi_2| - \frac{\langle\phi_2|\phi_1\rangle}{\langle\phi_1|\phi_1\rangle\langle\phi_2|\phi_2\rangle - \langle\phi_1|\phi_2\rangle\langle\phi_2|\phi_1\rangle}|\phi_2\rangle\langle\phi_1| \\ &- \frac{\langle\phi_1|\phi_2\rangle}{\langle\phi_1|\phi_1\rangle\langle\phi_2|\phi_2\rangle - \langle\phi_1|\phi_2\rangle\langle\phi_2|\phi_1\rangle}|\phi_1\rangle\langle\phi_2| + \frac{\langle\phi_1|\phi_2\rangle\langle\phi_2|\phi_1\rangle}{\langle\phi_1|\phi_1\rangle(\langle\phi_1|\phi_1\rangle\langle\phi_2|\phi_2\rangle - \langle\phi_1|\phi_2\rangle\langle\phi_2|\phi_1\rangle)}|\phi_1\rangle\langle\phi_1|\end{aligned}$$

接下来考虑$n=3$的情形，设$|\phi_3'\rangle = \alpha_3(|\phi_3\rangle - |\phi_2'\rangle\langle\phi_2'|\phi_3\rangle - |\phi_1'\rangle\langle\phi_1'|\phi_3\rangle)$，则

$$\begin{aligned}\langle\phi_3'|\phi_3'\rangle = &|\alpha_3|^2(\langle\phi_3|\phi_3\rangle - \langle\phi_3|\phi_2'\rangle\langle\phi_2'|\phi_3\rangle - \langle\phi_3|\phi_1'\rangle\langle\phi_1'|\phi_3\rangle \\ &- \langle\phi_2'|\phi_3\rangle\langle\phi_3|\phi_2'\rangle + \langle\phi_3|\phi_2'\rangle\langle\phi_2'|\phi_2'\rangle\langle\phi_2'|\phi_3\rangle + \langle\phi_3|\phi_2'\rangle\langle\phi_2'|\phi_1'\rangle\langle\phi_1'|\phi_3\rangle \\ &- \langle\phi_1'|\phi_3\rangle\langle\phi_3|\phi_1'\rangle + \langle\phi_3|\phi_1'\rangle\langle\phi_1'|\phi_2'\rangle\langle\phi_2'|\phi_3\rangle + \langle\phi_3|\phi_1'\rangle\langle\phi_1'|\phi_1'\rangle\langle\phi_1'|\phi_3\rangle) \\ = &|\alpha_3|^2(\langle\phi_3|\phi_3\rangle - \langle\phi_3|\phi_2'\rangle\langle\phi_2'|\phi_3\rangle - \langle\phi_3|\phi_1'\rangle\langle\phi_1'|\phi_3\rangle) \\ = &|\alpha_3|^2(\langle\phi_3|\phi_3\rangle - \frac{\langle\phi_1|\phi_1\rangle\langle\phi_3|\phi_2\rangle\langle\phi_2|\phi_3\rangle - \langle\phi_2|\phi_1\rangle\langle\phi_3|\phi_2\rangle\langle\phi_1|\phi_3\rangle - \langle\phi_1|\phi_2\rangle\langle\phi_3|\phi_1\rangle\langle\phi_2|\phi_3\rangle}{\langle\phi_1|\phi_1\rangle\langle\phi_2|\phi_2\rangle - \langle\phi_1|\phi_2\rangle\langle\phi_2|\phi_1\rangle} \\ &- \frac{\langle\phi_1|\phi_2\rangle\langle\phi_2|\phi_1\rangle\langle\phi_3|\phi_1\rangle\langle\phi_1|\phi_3\rangle}{\langle\phi_1|\phi_1\rangle(\langle\phi_1|\phi_1\rangle\langle\phi_2|\phi_2\rangle - \langle\phi_1|\phi_2\rangle\langle\phi_2|\phi_1\rangle)} - \frac{\langle\phi_3|\phi_1\rangle\langle\phi_1|\phi_3\rangle}{\langle\phi_1|\phi_1\rangle}) \\ = &|\alpha_3|^2[\frac{\langle\phi_3|\phi_3\rangle(\langle\phi_1|\phi_1\rangle\langle\phi_2|\phi_2\rangle - \langle\phi_1|\phi_2\rangle\langle\phi_2|\phi_1\rangle)}{\langle\phi_1|\phi_1\rangle\langle\phi_2|\phi_2\rangle - \langle\phi_1|\phi_2\rangle\langle\phi_2|\phi_1\rangle} - \frac{\langle\phi_3|\phi_2\rangle(\langle\phi_1|\phi_1\rangle\langle\phi_2|\phi_3\rangle - \langle\phi_1|\phi_3\rangle\langle\phi_2|\phi_1\rangle)}{\langle\phi_1|\phi_1\rangle\langle\phi_2|\phi_2\rangle - \langle\phi_1|\phi_2\rangle\langle\phi_2|\phi_1\rangle} \\ &+ \frac{\langle\phi_3|\phi_1\rangle(\langle\phi_1|\phi_2\rangle\langle\phi_2|\phi_3\rangle - \langle\phi_1|\phi_3\rangle\langle\phi_2|\phi_2\rangle)}{\langle\phi_1|\phi_1\rangle\langle\phi_2|\phi_2\rangle - \langle\phi_1|\phi_2\rangle\langle\phi_2|\phi_1\rangle}] \\ = &|\alpha_3|^2\begin{vmatrix}\langle\phi_1|\phi_1\rangle & \langle\phi_1|\phi_2\rangle & \langle\phi_1|\phi_3\rangle \\ \langle\phi_2|\phi_1\rangle & \langle\phi_2|\phi_2\rangle & \langle\phi_2|\phi_3\rangle \\ \langle\phi_3|\phi_1\rangle & \langle\phi_3|\phi_2\rangle & \langle\phi_3|\phi_3\rangle\end{vmatrix}\begin{vmatrix}\langle\phi_1|\phi_1\rangle & \langle\phi_1|\phi_2\rangle \\ \langle\phi_2|\phi_1\rangle & \langle\phi_2|\phi_2\rangle\end{vmatrix}^{-1} = 1\end{aligned}$$

解得$\alpha_3 = (\begin{vmatrix}\langle\phi_1|\phi_1\rangle & \langle\phi_1|\phi_2\rangle \\ \langle\phi_2|\phi_1\rangle & \langle\phi_2|\phi_2\rangle\end{vmatrix}\begin{vmatrix}\langle\phi_1|\phi_1\rangle & \langle\phi_1|\phi_2\rangle & \langle\phi_1|\phi_3\rangle \\ \langle\phi_2|\phi_1\rangle & \langle\phi_2|\phi_2\rangle & \langle\phi_2|\phi_3\rangle \\ \langle\phi_3|\phi_1\rangle & \langle\phi_3|\phi_2\rangle & \langle\phi_3|\phi_3\rangle\end{vmatrix}^{-1})^{\frac{1}{2}}$ （取实数解），因此

$$
\begin{aligned}
|\phi_3'\rangle &= \alpha_3(|\phi_3\rangle - |\phi_2'\rangle\langle\phi_2'|\phi_3\rangle - |\phi_1'\rangle\langle\phi_1'|\phi_3\rangle) \\
&= (\begin{vmatrix} \langle\phi_1|\phi_1\rangle & \langle\phi_1|\phi_2\rangle \\ \langle\phi_2|\phi_1\rangle & \langle\phi_2|\phi_2\rangle \end{vmatrix} \begin{vmatrix} \langle\phi_1|\phi_1\rangle & \langle\phi_1|\phi_2\rangle & \langle\phi_1|\phi_3\rangle \\ \langle\phi_2|\phi_1\rangle & \langle\phi_2|\phi_2\rangle & \langle\phi_2|\phi_3\rangle \\ \langle\phi_3|\phi_1\rangle & \langle\phi_3|\phi_2\rangle & \langle\phi_3|\phi_3\rangle \end{vmatrix}^{-1})^{\frac{1}{2}} (|\phi_3\rangle - \frac{\langle\phi_1|\phi_1\rangle\langle\phi_2|\phi_3\rangle}{\begin{vmatrix} \langle\phi_1|\phi_1\rangle & \langle\phi_1|\phi_2\rangle \\ \langle\phi_2|\phi_1\rangle & \langle\phi_2|\phi_2\rangle \end{vmatrix}}|\phi_2\rangle \\
&\quad + \frac{\langle\phi_2|\phi_1\rangle\langle\phi_1|\phi_3\rangle}{\begin{vmatrix} \langle\phi_1|\phi_1\rangle & \langle\phi_1|\phi_2\rangle \\ \langle\phi_2|\phi_1\rangle & \langle\phi_2|\phi_2\rangle \end{vmatrix}}|\phi_2\rangle + \frac{\langle\phi_1|\phi_2\rangle\langle\phi_2|\phi_3\rangle}{\begin{vmatrix} \langle\phi_1|\phi_1\rangle & \langle\phi_1|\phi_2\rangle \\ \langle\phi_2|\phi_1\rangle & \langle\phi_2|\phi_2\rangle \end{vmatrix}}|\phi_1\rangle - \frac{\langle\phi_1|\phi_2\rangle\langle\phi_2|\phi_1\rangle\langle\phi_1|\phi_3\rangle}{\langle\phi_1|\phi_1\rangle\begin{vmatrix} \langle\phi_1|\phi_1\rangle & \langle\phi_1|\phi_2\rangle \\ \langle\phi_2|\phi_1\rangle & \langle\phi_2|\phi_2\rangle \end{vmatrix}}|\phi_1\rangle - \frac{\langle\phi_1|\phi_3\rangle}{\langle\phi_1|\phi_1\rangle}|\phi_1\rangle) \\
&= (\begin{vmatrix} \langle\phi_1|\phi_1\rangle & \langle\phi_1|\phi_2\rangle \\ \langle\phi_2|\phi_1\rangle & \langle\phi_2|\phi_2\rangle \end{vmatrix} \begin{vmatrix} \langle\phi_1|\phi_1\rangle & \langle\phi_1|\phi_2\rangle & \langle\phi_1|\phi_3\rangle \\ \langle\phi_2|\phi_1\rangle & \langle\phi_2|\phi_2\rangle & \langle\phi_2|\phi_3\rangle \\ \langle\phi_3|\phi_1\rangle & \langle\phi_3|\phi_2\rangle & \langle\phi_3|\phi_3\rangle \end{vmatrix}^{-1})^{\frac{1}{2}} \begin{vmatrix} \langle\phi_1|\phi_1\rangle & \langle\phi_1|\phi_2\rangle & \langle\phi_1|\phi_3\rangle \\ \langle\phi_2|\phi_1\rangle & \langle\phi_2|\phi_2\rangle & \langle\phi_2|\phi_3\rangle \\ |\phi_1\rangle & |\phi_2\rangle & |\phi_3\rangle \end{vmatrix}
\end{aligned}
$$

一般的，记$\boldsymbol{S}_j = \begin{pmatrix} \langle\phi_1|\phi_1\rangle & \langle\phi_1|\phi_2\rangle & \dots & \langle\phi_1|\phi_j\rangle \\ \langle\phi_2|\phi_1\rangle & \langle\phi_2|\phi_2\rangle & \dots & \langle\phi_2|\phi_j\rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle\phi_3|\phi_1\rangle & \langle\phi_3|\phi_2\rangle & \dots & \langle\phi_3|\phi_j\rangle \end{pmatrix}$，对应的行列式为$D_j = \det\, \boldsymbol{S}_j$，边界条件为$\boldsymbol{S}_0 = \boldsymbol{I}$，$D_j = 1$，则

$$
|\phi_j'\rangle = \frac{1}{\sqrt{D_{j-1}D_j}} \sum_{i=1}^{j} |\phi_i\rangle \mathrm{cof}_{ji}(\boldsymbol{S}_j)
$$

其中$\mathrm{cof}_{ji}(\boldsymbol{S}_j)$为$\boldsymbol{S}_j$按$j$行$i$列展开的代数余子式，于是$\boldsymbol{X}$矩阵的矩阵元为

$$
X_{ij} = \begin{cases} \frac{1}{\sqrt{D_{j-1}D_j}} \mathrm{cof}_{ji}(\boldsymbol{S}_j) & (i \le j) \\ 0 & (i > j) \end{cases}
$$

练习2：证明按$\phi_\mu' = \sum\limits_{\nu=1}^{K} \widetilde{X}_{\nu\mu}\phi_\nu\ (\mu = 1, 2, \dots, K')$构建的基函数正交归一，其中$\widetilde{X}_{\nu\mu} = U_{\nu,\mu} s_\mu^{-\frac{1}{2}}$

证明：对于任意λ, μ，我们有：

$$
\langle\phi_\lambda'|\phi_\mu'\rangle = \sum_{\eta=1}^{K} \widetilde{X}^*_{\eta\lambda}\phi_\eta^\dagger \sum_{\nu=1}^{K} \widetilde{X}_{\nu\mu}\phi_\nu = \sum_{\eta=1}^{K}\sum_{\nu=1}^{K} \widetilde{X}^*_{\eta\lambda}\widetilde{X}_{\nu\mu}\langle\phi_\eta|\phi_\nu\rangle = \sum_{\eta=1}^{K}\sum_{\nu=1}^{K} U^*_{\eta,\lambda}(s_\lambda^*)^{-\frac{1}{2}} U_{\nu,\mu} s_\mu^{-\frac{1}{2}} S_{\eta\nu}
$$

接下来我们要利用$\boldsymbol{U}^\dagger\boldsymbol{S}\boldsymbol{U} = \boldsymbol{s}$的性质，左乘$\boldsymbol{U}$得$\boldsymbol{S}\boldsymbol{U} = \boldsymbol{U}\boldsymbol{s}$，即
$(\boldsymbol{S}\boldsymbol{U})_{ab} = \sum\limits_{i=1}^{K} S_{ai}U_{ib} = \sum\limits_{i=1}^{K} U_{ai}s_{ib} = (\boldsymbol{U}\boldsymbol{s})_{ab}$，且由于$\boldsymbol{s} = \mathrm{diag}(s_1, s_2, \dots, s_K)$，因此
$s_{ij} = s_{ij}\delta_{ij} = s_i\delta_{ij}$，从而：

$$
\begin{aligned}
\langle\phi_\lambda'|\phi_\mu'\rangle &= \sum_{\eta=1}^{K}\sum_{\nu=1}^{K} U^*_{\eta,\lambda}(s_\lambda^*)^{-\frac{1}{2}} s_\mu^{-\frac{1}{2}} S_{\eta\nu}U_{\nu,\mu} = \sum_{\eta=1}^{K}\sum_{\nu=1}^{K} U^*_{\eta,\lambda}(s_\lambda^*)^{-\frac{1}{2}} s_\mu^{-\frac{1}{2}} U_{\eta\nu}s_{\nu,\mu} = \sum_{\eta=1}^{K}\sum_{\nu=1}^{K} U^*_{\eta,\lambda}(s_\lambda^*)^{-\frac{1}{2}} s_\mu^{-\frac{1}{2}} U_{\eta\nu}s_{\nu\mu}\delta_{\nu\mu} \\
&= \sum_{\eta=1}^{K} U^*_{\eta,\lambda}(s_\lambda^*)^{-\frac{1}{2}} s_\mu^{-\frac{1}{2}} U_{\eta\mu}s_\mu = \sum_{\eta=1}^{K} U^*_{\eta,\lambda}U_{\eta\mu}(s_\lambda^*)^{-\frac{1}{2}} s_\mu^{\frac{1}{2}} = \delta_{\lambda\mu}(s_\lambda^*)^{-\frac{1}{2}} s_\mu^{\frac{1}{2}}
\end{aligned}
$$

当$\lambda \ne \mu$时，显然$\langle\phi_\lambda'|\phi_\mu'\rangle = 0$；当$\lambda = \mu$时，有$\langle\phi_\lambda'|\phi_\mu'\rangle = (s_\mu^*)^{-\frac{1}{2}} s_\mu^{\frac{1}{2}}$，而$s_\mu$为正实数，因此$\langle\phi_\lambda'|\phi_\mu'\rangle = 1$，原题得证。

练习3：证明两个1s型的Gauss函数乘积可以转化为另一个1s型的Gauss函数乘积，且满足

$$\phi_{1s}(\boldsymbol{r}-\boldsymbol{R}_A;\alpha_A)\phi_{1s}(\boldsymbol{r}-\boldsymbol{R}_B;\alpha_B)=K_{AB}\phi_{1s}(\boldsymbol{r}-\boldsymbol{R}_P;\alpha_P)$$
$$\alpha_P=\alpha_A+\alpha_B\quad K_{AB}=[\frac{2\alpha_A\alpha_B}{(\alpha_A+\alpha_B)\pi}]^{\frac{3}{4}}\mathrm{e}^{-\frac{\alpha_A\alpha_B}{\alpha_A+\alpha_B}|\boldsymbol{R}_A-\boldsymbol{R}_B|^2}\quad \boldsymbol{R}_P=\frac{\alpha_A\boldsymbol{R}_A+\alpha_B\boldsymbol{R}_B}{\alpha_A+\alpha_B}$$

证明：1s型Gauss函数的形式为$\phi_{1s}(r,\alpha)=(\frac{8\alpha^3}{\pi^3})^{\frac{1}{4}}\mathrm{e}^{-\alpha r^2}$，故代入得

$$\begin{aligned}
&\phi_{1s}(\boldsymbol{r}-\boldsymbol{R}_A;\alpha_A)\phi_{1s}(\boldsymbol{r}-\boldsymbol{R}_B;\alpha_B)\\
&=(\frac{8\alpha_A^3}{\pi^3})^{\frac{1}{4}}\mathrm{e}^{-\alpha_A|\boldsymbol{r}-\boldsymbol{R}_A|^2}\cdot(\frac{8\alpha_B^3}{\pi^3})^{\frac{1}{4}}\mathrm{e}^{-\alpha_B|\boldsymbol{r}-\boldsymbol{R}_B|^2}=(\frac{64\alpha_A^3\alpha_B^3}{\pi^6})^{\frac{1}{4}}\mathrm{e}^{-\alpha_A|\boldsymbol{r}-\boldsymbol{R}_A|^2-\alpha_B|\boldsymbol{r}-\boldsymbol{R}_B|^2}\\
&=(\frac{8\alpha_P^3}{\pi^3})^{\frac{1}{4}}(\frac{2\alpha_A\alpha_B}{\pi\alpha_P})^{\frac{3}{4}}\mathrm{e}^{-\frac{\alpha_A\alpha_B}{\alpha_A+\alpha_B}|\boldsymbol{R}_A-\boldsymbol{R}_B|^2}\cdot\mathrm{e}^{-\alpha_A|\boldsymbol{r}-\boldsymbol{R}_A|^2-\alpha_B|\boldsymbol{r}-\boldsymbol{R}_B|^2+\frac{\alpha_A\alpha_B}{\alpha_A+\alpha_B}|\boldsymbol{R}_A-\boldsymbol{R}_B|^2}\\
&=K_{AB}(\frac{8\alpha_P^3}{\pi^3})^{\frac{1}{4}}\mathrm{e}^{-\alpha_A|\boldsymbol{r}-\boldsymbol{R}_A|^2-\alpha_B|\boldsymbol{r}-\boldsymbol{R}_B|^2+\frac{\alpha_A\alpha_B}{\alpha_A+\alpha_B}|\boldsymbol{R}_A-\boldsymbol{R}_B|^2}
\end{aligned}$$

其中$\alpha_P=\alpha_A+\alpha_B$，$K_{AB}=(\frac{2\alpha_A\alpha_B}{\pi\alpha_P})^{\frac{3}{4}}\mathrm{e}^{-\frac{\alpha_A\alpha_B}{\alpha_A+\alpha_B}|\boldsymbol{R}_A-\boldsymbol{R}_B|^2}$，现在我们要证明

$$-\alpha_A|\boldsymbol{r}-\boldsymbol{R}_A|^2-\alpha_B|\boldsymbol{r}-\boldsymbol{R}_B|^2+\frac{\alpha_A\alpha_B}{\alpha_A+\alpha_B}|\boldsymbol{R}_A-\boldsymbol{R}_B|^2=-(\alpha_A+\alpha_B)|\boldsymbol{r}-\boldsymbol{R}_P|^2$$

其中$\boldsymbol{R}_P=\frac{\alpha_A\boldsymbol{R}_A+\alpha_B\boldsymbol{R}_B}{\alpha_A+\alpha_B}$，注意到$|\boldsymbol{r}|^2=\boldsymbol{r}^\dagger\boldsymbol{r}=\boldsymbol{r}^T\boldsymbol{r}$，因此两边对$\boldsymbol{r}$求导，得：

$$\begin{aligned}
&-\alpha_A(\boldsymbol{r}-\boldsymbol{R}_A)^T-\alpha_B(\boldsymbol{r}-\boldsymbol{R}_B)^T=-(\alpha_A+\alpha_B)(\boldsymbol{r}-\boldsymbol{R}_P)^T\\
&\Rightarrow-\alpha_A(\boldsymbol{r}-\boldsymbol{R}_A)^T-\alpha_B(\boldsymbol{r}-\boldsymbol{R}_B)^T=-(\alpha_A+\alpha_B)(\boldsymbol{r}-\frac{\alpha_A\boldsymbol{R}_A+\alpha_B\boldsymbol{R}_B}{\alpha_A+\alpha_B})^T\\
&\Rightarrow-(\alpha_A\boldsymbol{r}-\alpha_A\boldsymbol{R}_A)^T-(\alpha_B\boldsymbol{r}-\alpha_B\boldsymbol{R}_B)^T=-[(\alpha_A+\alpha_B)\boldsymbol{r}-(\alpha_A\boldsymbol{R}_A+\alpha_B\boldsymbol{R}_B)]^T\\
&\Rightarrow-[(\alpha_A+\alpha_B)\boldsymbol{r}-(\alpha_A\boldsymbol{R}_A+\alpha_B\boldsymbol{R}_B)]^T=-[(\alpha_A+\alpha_B)\boldsymbol{r}-(\alpha_A\boldsymbol{R}_A+\alpha_B\boldsymbol{R}_B)]^T
\end{aligned}$$

从而$\boldsymbol{R}_P=\frac{\alpha_A\boldsymbol{R}_A+\alpha_B\boldsymbol{R}_B}{\alpha_A+\alpha_B}$时，两边导数相等，而$r=0$时，代回求导前的等式，得左边为$-\alpha_A|\boldsymbol{R}_A|^2-\alpha_B|\boldsymbol{R}_B|^2+\frac{\alpha_A\alpha_B}{\alpha_A+\alpha_B}|\boldsymbol{R}_A-\boldsymbol{R}_B|^2$，右边为$-(\alpha_A+\alpha_B)|\boldsymbol{R}_P|^2$，或写作$-(\alpha_A+\alpha_B)|\frac{\alpha_A\boldsymbol{R}_A+\alpha_B\boldsymbol{R}_B}{\alpha_A+\alpha_B}|^2$，而

$$\begin{aligned}
&-(\alpha_A+\alpha_B)|\frac{\alpha_A\boldsymbol{R}_A+\alpha_B\boldsymbol{R}_B}{\alpha_A+\alpha_B}|^2=-\frac{|\alpha_A\boldsymbol{R}_A+\alpha_B\boldsymbol{R}_B|^2}{\alpha_A+\alpha_B}=-\frac{\alpha_A^2|\boldsymbol{R}_A|^2+\alpha_B^2|\boldsymbol{R}_B|^2+\alpha_A\alpha_B(\boldsymbol{R}_A^T\boldsymbol{R}_B+\boldsymbol{R}_B^T\boldsymbol{R}_A)}{\alpha_A+\alpha_B}\\
&=-\frac{\alpha_A(\alpha_A+\alpha_B)|\boldsymbol{R}_A|^2+\alpha_B(\alpha_A+\alpha_B)|\boldsymbol{R}_B|^2+\alpha_A\alpha_B(-|\boldsymbol{R}_A|^2+\boldsymbol{R}_A^T\boldsymbol{R}_B+\boldsymbol{R}_B^T\boldsymbol{R}_A-|\boldsymbol{R}_B|^2)}{\alpha_A+\alpha_B}\\
&=-\alpha_A|\boldsymbol{R}_A|^2-\alpha_B|\boldsymbol{R}_B|^2+\frac{\alpha_A\alpha_B}{\alpha_A+\alpha_B}|\boldsymbol{R}_A-\boldsymbol{R}_B|^2
\end{aligned}$$

因此求导前的等式成立，从而原题得证