介观物理第十一次作业

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Problem III.7 Verify Eq. (220).

$$T_{12} = \frac{T_1 T_2}{1 + R_1 R_2 - 2\sqrt{R_1 R_2}\cos\theta}. \tag{220}$$

Proof. 根据式 (219)，有:

$$D = \frac{e^{i\phi} t_1 t_2}{1 - e^{2i\phi} r_2 r_1'}.$$

则透射率为:

$$T_{12} = |D|^2 = \frac{T_1 T_2}{(1 - e^{2i\phi} r_2 r_1')(1 - e^{-2i\phi} r_2^* r_1^{*\prime})} = \frac{T_1 T_2}{1 + R_1' R_2 - 2\sqrt{R_1' R_2}\cos\theta}.$$

其中

$$\theta = 2\phi + \arg(r_2 r_1').$$

□

Problem III.8 Find proper conditions under which $T = 1$ in Eq. (238). Note that the 2×2 scattering matrix

$$S_i = \begin{pmatrix} r_1 & t_i' \\ t_i & r_i' \end{pmatrix}$$

must be a unitary matrix, where $i = 1, 2$.

$$T = \frac{4|A|^2}{|C|^2} = \frac{4|t_2(r_1 - 1)(1 - r_1')|^2}{|t_2^2 - (2 - r_1 - r_2)(2 - r_1' - r_2')|^2}. \tag{238}$$

Proof. 散射矩阵 S_i 满足

$$S_i^\dagger S_i = S_i S_i^\dagger = \mathbf{I};\ |r_i|^2 + |t_i|^2 = 1;\ |r_i'|^2 + |t_i'|^2 = 1;\ r_i t_i'^* + t_i r_i'^* = 0.$$

要求 $T = 1$，$t_1 = 0$，则有 $|r_1| = |r_1'| = 1$，则 r_1 和 r_1' 可以写作:

$$r_1 = e^{i\theta_1},\ r_1' = e^{i\theta_2},\ t_1 = t_1' = 0;\ r_2 = re^{i\theta_2},\ r_2' = re^{i\theta_2'},\ t_2 = t_2' = te^{i\varphi}.$$

利用 $|r_2|^2 + |t_2|^2 = r^2 + t^2 = 1$，可以将 r_2, t_2 重新写作:

$$r_2 = \cos\alpha e^{i\theta_2},\ r_2' = \cos\alpha e^{i\theta_2'};\ t_2 = t_2' = \sin\alpha e^{i\varphi} = -i\sin\alpha\sqrt{r_2 r_2'}.$$

其中，利用了 $\varphi = \frac{1}{2}(\theta_2 + \theta_2' - \pi)$。当 $T = 1$ 时，有:

$$4|t_2(r_1 - 1)(1 - r_1')|^2 = |t_2^2 - (2 - r_1 - r_2)(2 - r_1' - r_2')|^2.$$

根据讲义，θ_1 和 θ_1' 的恰当选取可以使得 $T = 1$，从而可以选取合适的 $\theta_2, \theta_2', \alpha$ 简化计算。取 $\theta_2 = \theta_2' = 0$，$\alpha = \frac{\pi}{2}$。则有:

$$r_2 = r_2' = 0;\ t_2 = t_2' = -i.$$

则 $T=1$ 得:

$$4|r_1r_1'-r_1-r_1'+1|^2=|r_1r_1'-2(r_1+r_1')+5|^2.$$

化简可得:

$$r_1r_2'+r_1^*r_1'^*-4(r_1+r_1^*)-4(r_1'+r_1'^*)+18=0.$$

即

$$\cos(\theta_1+\theta_1')-4\cos\theta_1-4\cos\theta_1'+9=0.$$

□

Problem 3. 证明贝里相位必定为实数。

Proof. 贝里相位可以写作:

$$\gamma(t)=i\int_0^{\mathbf{R}(t)}\langle n(\mathbf{R})|\,\nabla_{\mathbf{R}}\,|n(\mathbf{R})\rangle\,d\mathbf{R}.$$

由于微分算符是反厄米算符，可以计算贝里相位共轭为:

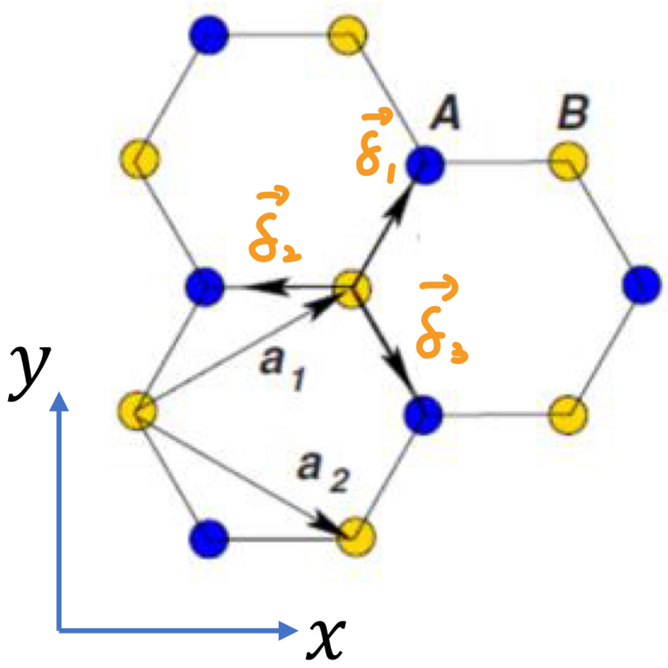
$$\begin{aligned}\gamma^*(t)=&-i\int_0^{\mathbf{R}(t)}\langle n(\mathbf{R})|\,\nabla_{\mathbf{R}}\,|n(\mathbf{R})\rangle^*\,d\mathbf{R}\\=&-i\int_0^{\mathbf{R}(t)}\langle n(\mathbf{R})|\,(\nabla_{\mathbf{R}})^\dagger\,|n(\mathbf{R})\rangle\,d\mathbf{R}\\=&i\int_0^{\mathbf{R}(t)}\langle n(\mathbf{R})|\,\nabla_{\mathbf{R}}\,|n(\mathbf{R})\rangle\,d\mathbf{R}\\=&\gamma(t).\end{aligned}$$

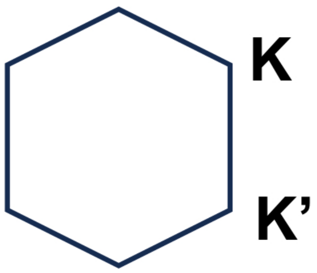
即贝里相位 $\gamma(t)$ 必定为实数。 □

Problem 4. 按照下图所示的方式选取石墨烯晶格的基矢，即

$$\mathbf{a}_1=\sqrt{3}a\left(\frac{\sqrt{3}}{2},\frac{1}{2}\right),\quad \mathbf{a}_2=\sqrt{3}a\left(\frac{\sqrt{3}}{2},-\frac{1}{2}\right),$$

其中 a 为最近邻原子的间距。利用紧束缚模型，写出只考虑最近邻相互作用的哈密顿量，给出第一布里渊区高对称点 K 和 K' 附近的近似形式，并求解出相应的本征值和本征函数，计算波函数对应的贝里相位；与课堂上给出的结果进行比较，并讨论其异同。





Proof. 考虑二次量子化，只考虑近邻相互作用的哈密顿量可以写作:

$$\hat{H} = -t \sum_{<i,j>\delta} \hat{a}_i^\dagger \hat{b}_j - t' \sum_i (\hat{a}_i^\dagger \hat{a}_i + \hat{b}_i^\dagger \hat{b}_i) + h.c.$$

为了简化记号，以下的算符不再写算符记号ˆ，但仍表示算符。两套湮灭算符的展开可以写作:

$$a_i = \sum_k a_k e^{-\vec{k}\cdot\vec{r}_i^A}; \quad b_j = \sum_k b_k e^{i\vec{k}\cdot\vec{r}_j^B}.$$

则哈密顿量非对角元项可以写作:

$$\begin{aligned}\sum_{<i,j>,\vec{\delta}} a_i^\dagger b_j &= \sum_{<i,j>,\vec{\delta}} \sum_k a_k^\dagger e^{-i\vec{k}\cdot\vec{r}_i^A} \sum_{k'} b_{k'} e^{i\vec{k}'\cdot(\vec{r}_i^A+\vec{\delta})} \\ &= \sum_{kk'} a_k^\dagger b_{k'} \sum_{\vec{\delta}} e^{i\vec{k}'\cdot\vec{\delta}} \sum_i e^{i\vec{r}_i^A\cdot(\vec{k}'-\vec{k})} \\ &= \sum_k a_k^\dagger b_k \sum_{\vec{\delta}} e^{i\vec{k}\cdot\vec{\delta}}.\end{aligned}$$

其中，在计算过程中忽略了归一化常数 $\frac{1}{N}$，但由于 $\sum_i e^{i\vec{r}_i^A\cdot(\vec{k'}-\vec{k})} = N\delta(\vec{k}-\vec{k}')$，所以归一化常数被抵消，从而不影响计算结果。

取 $t'=0$，则哈密顿量可以写作:

$$H = -t\sum_k \begin{pmatrix} a_k^\dagger & b_k^\dagger \end{pmatrix} \begin{pmatrix} 0 & \sum_{\vec{\delta}} e^{i\vec{k}\cdot\vec{\delta}} \\ \sum_{\vec{\delta}} e^{-i\vec{k}\cdot\vec{\delta}} & 0 \end{pmatrix} \begin{pmatrix} a_k \\ b_k \end{pmatrix}$$

记

$$\vec{H} = (H_x, H_y, H_z).$$

其中 H_x, H_y, H_z 满足:

$$H = -t\sum_k \begin{pmatrix} a_k^\dagger & b_k^\dagger \end{pmatrix} \begin{pmatrix} H_z & H_x - iH_y \\ H_x + iH_y & H_z \end{pmatrix} \begin{pmatrix} a_k \\ b_k \end{pmatrix}$$

结合

$$\vec{\delta}_1 = a\left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right);\ \vec{\delta}_2 = a\left(-1, 0\right);\ \vec{\delta}_1 = a\left(\frac{1}{2}, -\frac{\sqrt{3}}{2}\right);$$

可以计算:

$$\begin{aligned} H_x =& \cos\left[\frac{a}{2}(k_x+\sqrt{3}k_y)\right] + \cos(ak_x) + \cos\left[\frac{a}{2}(k_x-\sqrt{3}k_y)\right] \\ =& \cos(ak_x) + 2\cos(ak_x/2)\cos(\sqrt{3}ak_y/2); \\ H_y =& \sin(ak_x) - \sin\left[\frac{a}{2}(k_x+\sqrt{3}k_y)\right] - \sin\left[\frac{a}{2}(k_x-\sqrt{3}k_y)\right] \\ =& \sin(ak_x) - 2\sin(ak_x/2)\cos(\sqrt{3}ak_y/2); \\ H_z =& 0. \end{aligned}$$

在 K 和 K' 点，倒空间中坐标为:

$$K = \left(\frac{2\pi}{3a}, \frac{2\pi}{3\sqrt{3}a}\right);\ K' = \left(\frac{2\pi}{3a}, -\frac{2\pi}{3\sqrt{3}a}\right).$$

在 K 点的近似形式为:

$$H_x = -\frac{1}{2} - \frac{\sqrt{3}}{2}a\delta k_x + 1 - \frac{1}{2} - \frac{\sqrt{3}}{2}\left(\frac{\sqrt{3}}{2}a\delta k_y - \frac{1}{2}a\delta k_x\right) = \frac{3a}{4}(-\sqrt{3}\delta k_x - \delta k_y);$$

$$H_y = \frac{\sqrt{3}}{2} - \frac{1}{2}a\delta k_x - \frac{\sqrt{3}}{2} + \frac{1}{2}\left(\frac{1}{2}a\delta k_x + \frac{\sqrt{3}}{2}a\delta k_y\right) - \frac{1}{2}a(\delta k_x - \sqrt{3}\delta k_y) = \frac{3a}{4}(-\delta k_x + \sqrt{3}\delta k_y);$$

$$H_z = 0.$$

本征值为

$$\lambda = \pm|-t\vec{H}| = \pm\frac{3}{2}at|\delta\vec{k}|.$$

其中，对哈密顿量的相似变换矩阵为:

$$U = \frac{1}{\sqrt{2}}\begin{pmatrix} \frac{H_z-H}{H_x+iH_y} & \frac{H_z+H}{H_x+iH_y} \\ 1 & 1 \end{pmatrix}.$$

则两个本征波函数分别为:

$$\psi_1 = \begin{pmatrix} \frac{H_z - H}{H_x + iH_y} \\ 1 \end{pmatrix}; \text{对应本征值 } \frac{3}{2}at|\delta\vec{k}|;$$

$$\psi_2 = \begin{pmatrix} \frac{H_z + H}{H_x + iH_y} \\ 1 \end{pmatrix}; \text{对应本征值 } -\frac{3}{2}at|\delta\vec{k}|.$$

从而可以计算贝里相位:

$$\gamma_1 = \oint i \langle\psi_1| \nabla_k |\psi_1\rangle \cdot d\vec{l} = -\pi;\ \gamma_2 = \oint i \langle\psi_2| \nabla_k |\psi_2\rangle \cdot d\vec{l} = -\pi.$$

类似的对于 K' 点，近似形式为:

$$\begin{aligned} H_x =& 1 - \frac{1}{2} - \frac{\sqrt{3}}{2}a\delta k_x - \frac{1}{2} - \frac{\sqrt{3}}{2}\frac{1}{2}a(\delta k_x - \sqrt{3}\delta k_y) = \frac{3}{4}a(-\sqrt{3}\delta k_x + \delta k_y); \\ H_y =& \frac{\sqrt{3}}{2} - \frac{1}{2}a\delta k_x - \frac{a}{2}(\delta k_x + \sqrt{3}\delta k_y) - \frac{\sqrt{3}}{2} + \frac{1}{2}\frac{a}{2}(\delta k_x - \sqrt{3}\delta k_y) = \frac{3}{4}a(-\delta k_x - \sqrt{3}\delta k_y); \\ H_z =& 0. \end{aligned}$$

类似的，本征值为:

$$\lambda = \pm| - t\vec{H}| = \pm\frac{3}{2}at|\delta\vec{k}|.$$

其中，对哈密顿量的相似变换矩阵为:

$$U = \frac{1}{\sqrt{2}} \begin{pmatrix} \frac{H_z - H}{H_x + iH_y} & \frac{H_z + H}{H_x + iH_y} \\ 1 & 1 \end{pmatrix}.$$

则两个本征波函数分别为:

$$\psi_3 = \begin{pmatrix} \frac{H_z - H}{H_x + iH_y} \\ 1 \end{pmatrix}; \text{对应本征值 } \frac{3}{2}at|\delta\vec{k}|;$$

$$\psi_4 = \begin{pmatrix} \frac{H_z + H}{H_x + iH_y} \\ 1 \end{pmatrix}; \text{对应本征值 } -\frac{3}{2}at|\delta\vec{k}|.$$

从而可以计算贝里相位:

$$\gamma_1 = \oint i \langle\psi_1| \nabla_k |\psi_1\rangle \cdot d\vec{l} = -\pi;\ \gamma_2 = \oint i \langle\psi_2| \nabla_k |\psi_2\rangle \cdot d\vec{l} = -\pi.$$

综上所述，与上课结果给出的贝里相位不同，但差值为 2π，所以在物理上等价。 □