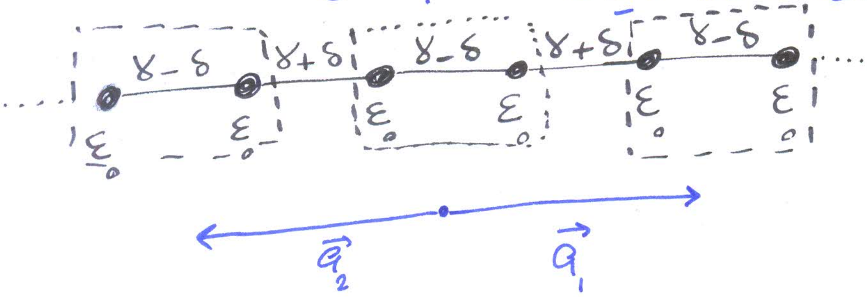
طیف پاشیدگی زنجیر مولکولی زیر را حساب کنید.



$\vec a = 2a_0$

$$|\psi_k\rangle = \frac{1}{\sqrt N}\sum_R \sum_{n=1}^{2} e^{i\vec k\cdot\vec R} A_{n,k}\, |\vec R_n\rangle$$

$$E(k)\, A_{n',\vec k} = \sum_R \sum_n^{2} e^{ik\cdot(R-R')} A_{n,k} \langle R'n'|\mathcal H|Rn\rangle$$

1) on site-energy

$$\langle R'n'|H|R'n\rangle = \begin{pmatrix} \varepsilon_0 & \gamma-\delta \\ \gamma-\delta & \varepsilon_0 \end{pmatrix} \qquad e^{ik\cdot(R'-R')} = 1$$

2) $\vec a_1$ ناحیه $\quad \langle R'n'|H|R'+a\,n\rangle = \begin{pmatrix} 0 & 0 \\ \gamma+\delta & 0 \end{pmatrix} \qquad e^{i\vec k\cdot(R'+a-R')} = e^{ik\cdot a}$

3) $-\vec a_1 = \vec a_2$ ناحیه $\quad \langle R'n'|\mathcal H|R'+a\,n\rangle = \begin{pmatrix} 0 & \gamma+\delta \\ 0 & 0 \end{pmatrix} \qquad e^{-ik\cdot a}$

ماتریس

$$\begin{pmatrix} \varepsilon_0 & (\gamma-\delta)+e^{-ika}(\gamma+\delta) \\ (\gamma-\delta)+e^{ika}(\gamma-\delta) & \varepsilon_0 \end{pmatrix}$$

$$\det\begin{vmatrix} (\varepsilon_0-E) & (\gamma-\delta)+e^{-ika}(\gamma+\delta) \\ (\gamma-\delta)+e^{ika}(\gamma+\delta) & (\varepsilon_0-E) \end{vmatrix} = 0$$

$$(\varepsilon_0-E)^2-\left((\gamma-\delta)+e^{ika}(\gamma+\delta)\right)\left((\gamma-\delta)+e^{-ika}(\gamma+\delta)\right)=0$$

$$(\varepsilon_0-E)^2-\left[(\gamma+\delta)^2+(\gamma-\delta)^2+(\gamma-\delta)(\gamma+\delta)\left(e^{ika}+e^{-ika}\right)\right]=0$$

$$E=\varepsilon_0\pm\sqrt{(\gamma+\delta)^2+(\gamma-\delta)^2+2(\gamma-\delta)(\gamma+\delta)\cos ka}$$

$\delta=0$ $\quad E=\varepsilon_0\pm\sqrt{2\gamma^2+2\gamma^2\cos ka}$

$$E=\varepsilon_0\pm\sqrt{2\gamma^2(1+\cos 2ka_0)}$$

$\vec{a}=2a_0$

$\cos 2ka_0=2\cos^2 ka_0-1$

$E=\varepsilon_0\pm 2\gamma\cos ka_0 \longrightarrow$ شکل زیر را می

$k=0 \longrightarrow E=\varepsilon_0\pm\sqrt{(\gamma-\delta)^2+(\gamma+\delta)^2+2(\gamma-\delta)(\gamma+\delta)}$

$$E=\varepsilon_0\pm\sqrt{(\gamma-\delta+\gamma+\delta)^2}=\varepsilon_0\pm 2\gamma$$

$k=\frac{\pi}{a}=\frac{\pi}{2a_0} \Rightarrow E=\varepsilon_0\pm 2\delta$

رسم بصورت تقریبی