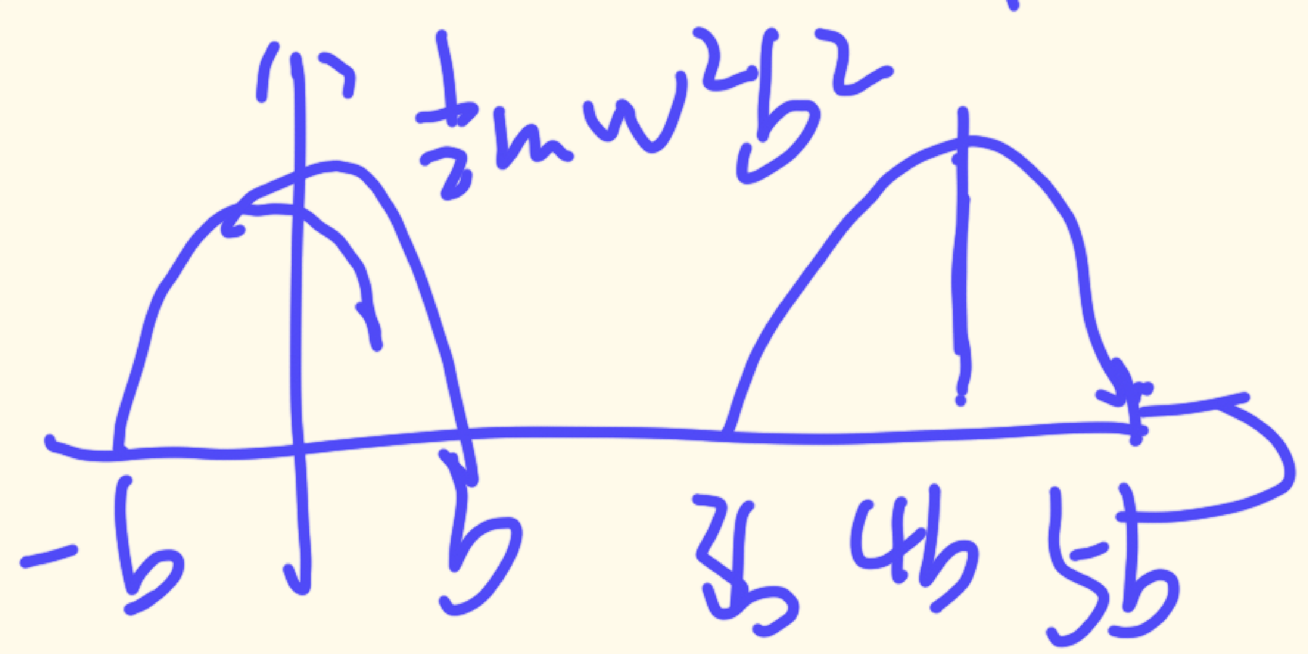
由 $E(\vec{k})=\varepsilon_s-J_0-J_1\sum e^{i\vec{k}\cdot\vec{R}_s}$ 面心立方 $(\frac{a}{2},\frac{a}{2},0)$ $(-\frac{a}{2},-\frac{a}{2},0)$ $(\frac{a}{2},-\frac{a}{2},0)$
$(-\frac{a}{2},\frac{a}{2},0)$ $(\frac{a}{2},0,\frac{a}{2})$ $(\frac{a}{2},0,-\frac{a}{2})$ $(-\frac{a}{2},0,\frac{a}{2})$ $(-\frac{a}{2},0,-\frac{a}{2})$ $(0,\frac{a}{2},\frac{a}{2})$ $(0,-\frac{a}{2},-\frac{a}{2})$ $(0,-\frac{a}{2},\frac{a}{2})$ $(0,\frac{a}{2},-\frac{a}{2})$

$$E(\vec{k})=\varepsilon_s-J_0-4J_1\left(\cos\frac{k_xa}{2}\cos\frac{k_ya}{2}+\cos\frac{k_xa}{2}\cos\frac{k_za}{2}+\cos\frac{k_ya}{2}\cos\frac{k_za}{2}\right)$$

体心立方 $(\frac{a}{2},\frac{a}{2},\frac{a}{2})$ $(-\frac{a}{2},-\frac{a}{2},\frac{a}{2})$ $(\frac{a}{2},-\frac{a}{2},\frac{a}{2})$ $(-\frac{a}{2},\frac{a}{2},\frac{a}{2})$ $(\frac{a}{2},\frac{a}{2},-\frac{a}{2})$ $(\frac{a}{2},-\frac{a}{2},-\frac{a}{2})$
$(\frac{a}{2},\frac{a}{2},-\frac{a}{2})$ $(-\frac{a}{2},-\frac{a}{2},-\frac{a}{2})$ $E(\vec{k})=\varepsilon_s-J_0-8J_1\cos\frac{k_xa}{2}\cos\frac{k_ya}{2}\cos\frac{k_za}{2}$

2、a. 势能曲线

$$\bar{V}=\frac{1}{T}\int_0^T V(x)\,dx=\frac{1}{4b}\int_{-b}^{b}\frac{m\omega^2}{2}(b^2-x^2)\,dx=\frac{m\omega^2b^2}{6}$$



b. $V(x)$ 为偶函数 $\therefore V(x)=V_0+\sum_{n=1}^{\infty}V_n\cos\frac{n\pi x}{2b}$

$$V_n=\frac{2}{4b}\int_0^{2b}V(x)\cos\frac{n\pi x}{2b}\,dx=\frac{1}{2b}\int_0^{b}\frac{m\omega^2}{2}(b^2-x^2)\cos\frac{n\pi x}{2b}\,dx=-\frac{2m\omega^2b^2}{n^2\pi^2}\cos\frac{n\pi}{2}+\frac{4m\omega^2b^2}{n^3\pi^3}\sin\frac{n\pi}{2}$$

$\therefore$ 第一禁带宽 $E_{g_1}=\frac{8m\omega^2b^2}{\pi^3}$ 第二禁带宽 $E_{g_2}=\frac{m\omega^2b^2}{\pi^3}$