PHYS 563 HW #4

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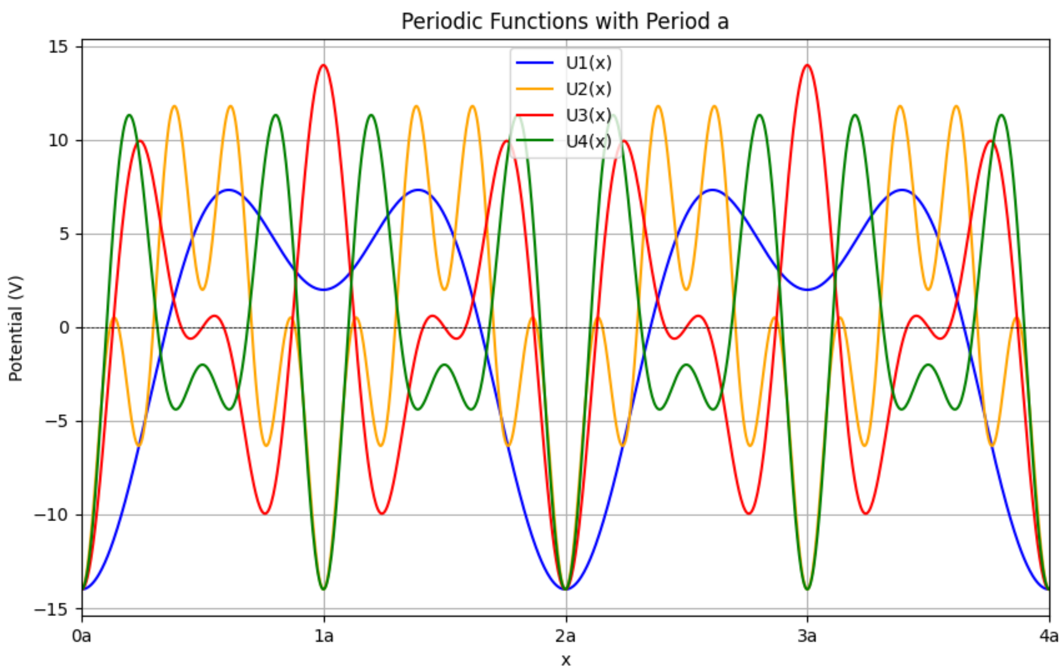
Problem 1

We plotted the potential functions with python and have the following graph.



We can see clearly that U2, U4 are periodic function with period of a,

$$U_2(x+a) = U_2(x), U_4(x+a) = U_4(x)$$

But U1 and U3 have a larger period of 2a.

The reason is that U2 and U4 only have even integers multiplied with $\pi x/a$ in their cosine functions, and we know that $\cos\left(n \times \frac{2\pi a}{a}\right) = 1$, so after a period of a, U2 and U4 can return to the original value.

But for U1 and U3, they have odd numbers integers multiplied with $\pi x/a$ in their cosine functions, which will have a larger period of 2a.

And since the one dimensional chain has a lattice constant of a, its potential must also have a period of a.

Thus only U2 and U4 satisfy the condition.

Problem 2

(a) From the discussion of Kronig-Penney (KP) model in A&M exercise , we know that the energy dissigation of the lattice is:

From A&M (8.76)

$$\Rightarrow \cos ka = \frac{\cos\left(\sqrt{\frac{2mE}{\hbar^2}}\,a+\delta\right)}{|t|} := \frac{\cos(sa+\delta)}{|t|}$$

Where $|t|$ is the absolute value of amplitude transmission coefficient through a lattice unit.

To determine $|t|$ in KP model with the given Hamiltonian H

$$H = \frac{p^2}{2m} + \sum_n g\delta(x-na)$$

We can try to determine t and r (reflection coef. of amplitude) by the continuity of the wavefunction and its differentiation across $x = na$

We now restrict to discussing the unit lattice where $n=0$, so that

$$U(x) = g\delta(x) \quad \text{for } \frac{-a}{2} \le x \le \frac{a}{2}$$

And wave function is

$$\psi(x) = \begin{cases} e^{isx} + re^{-isx}, & x<0 \\ te^{+isx}, & x>0 \end{cases}$$

① Continuity of $\psi(x)$ at $x=0$ From A&M (8.75) $\Downarrow$

$$\Rightarrow 1+r = t \Rightarrow |t|e^{+i\delta} = 1 - i|r|e^{+i\delta}$$

$$\Rightarrow |t| = e^{-i\delta} - i|r|$$

And since

$$|t|^2 + |r|^2 = 1 \Rightarrow e^{-2i\delta} - 2i|r|e^{-i\delta} = 1$$

$$\Rightarrow e^{-i\delta} - e^{+i\delta} - 2i|r| = 0 \Rightarrow |r| = -\sin\delta, \; |t| = \cos\delta$$

② Continuity of $\frac{d}{dx}\psi(x)$ at $x=0$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + U(x)\psi(x) = \mathcal{E}\psi(x)$$

$$\Rightarrow \int_{-\Delta}^{+\Delta} -\frac{\hbar^2}{2m}\psi''(x)\,dx = \int_{-\delta}^{+\delta} (\mathcal{E} - U(x))\psi(x)\,dx$$

$$\Rightarrow -\frac{\hbar^2}{2m}\psi'(x)\Big|_{-\delta}^{+\Delta} = \int_{-\delta}^{+\delta} (\mathcal{E} - U(x))\psi(x)\,dx$$

Take limit $\Delta \to 0^+$,

$$\lim_{x\to 0^+} -\frac{\hbar^2}{2m}\psi'(x) - \lim_{x\to 0^-}\left(-\frac{\hbar^2}{2m}\right)\psi'(x) = -g\psi(x)$$

$$\Rightarrow -\frac{\hbar^2}{2m}\left[(is)\cdot t - (is)\cdot(1-r)\right] = -tg$$

$$\left(\because \psi(x) = \begin{cases} e^{+isx} + re^{-isx} & x<0 \\ te^{isx} & x>0 \end{cases}\right)$$

$$\Rightarrow -\frac{\hbar^2}{2m}\cdot(is)\left(\cos\delta\, e^{+i\delta} - 1 + i\sin\delta\, e^{+i\delta}\right)$$

$$= g\cos\delta\, e^{+i\delta}$$

$$\Rightarrow \frac{i\hbar^2 s}{2m}\left(e^{+i\delta} - e^{-i\delta}\right) = g\cos\delta$$

$$\Rightarrow \cot\delta = \frac{-\hbar^2 s}{mg} \Rightarrow \cos\delta = |t| = \frac{\hbar^2 s}{\sqrt{(\hbar^2 s)^2 + (mg)^2}}$$

$$\therefore \cos ka = \frac{\cos(sa+\delta)}{|t|} \qquad s := \sqrt{\frac{2m\mathcal{E}}{\hbar^2}}$$

$$= \frac{\cos\left(sa + \cot^{-1}\left(-\frac{\hbar^2 s}{mg}\right)\right)}{\hbar^2 s}\cdot\sqrt{(\hbar^2 s)^2 + (mg)^2} \qquad (2.1)$$

$\therefore$ We can use (2.1) to plot the dispersion relationship for $g=0$ and $g=$ finite value cases.

Problem 2b

Here we set $a = 20$ Å, and $g = 0.1eV \times a$, $g = 0$ (free electron case). We plotted the first three bands of the confined case ($g = 0.1eV \times a$) and free electron case ($g = 0$).

We can see that the confined case have significant band gaps near the Brillioun Zone edge while the free electron case has continuous dispersion curve following the free-electron Hamiltonian:

$$E = H = \frac{\hbar^2 k^2}{2m_e}$$