Matrix Method for Periodic Potential

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Course: Quantum and Wave Phenomenon (EE683A)
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Problem Statement

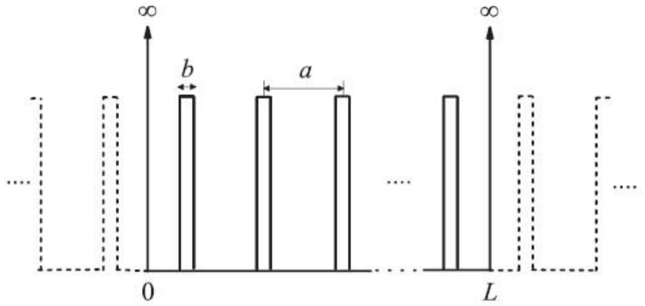


Fig. 1. The true potential $V(x)$ (dashed) and the auxiliary potential $V_{\inf}(x) + V(x)$ (solid) for the Kronig-Penney model.

Periodic Potential Barrier
Physically such a system is seen in Metallic and Semiconductor Lattice

Problem 1: Compute the Energy Eigenvalues of the Hamiltonian corresponding to this potential

Problem 2: Variation of these Energy Eigenvalues on application of an external field to this system

Image Source: https://arxiv.org/pdf/1606.00211.pdf

Matrix Formalism of Hamiltonian

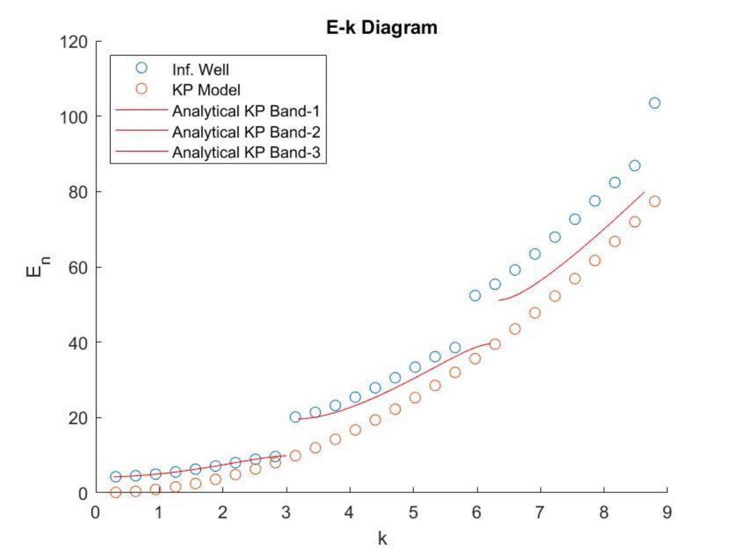
$$\sum_{m=1}^{\infty} H_{nm} c_m = E c_n$$

$$H_{nm} = \delta_{nm} E_n^0 + \frac{2}{L} \int_0^L sin(\frac{n\pi x}{L}) V_{KP}(x) sin(\frac{m\pi x}{L}) dx$$

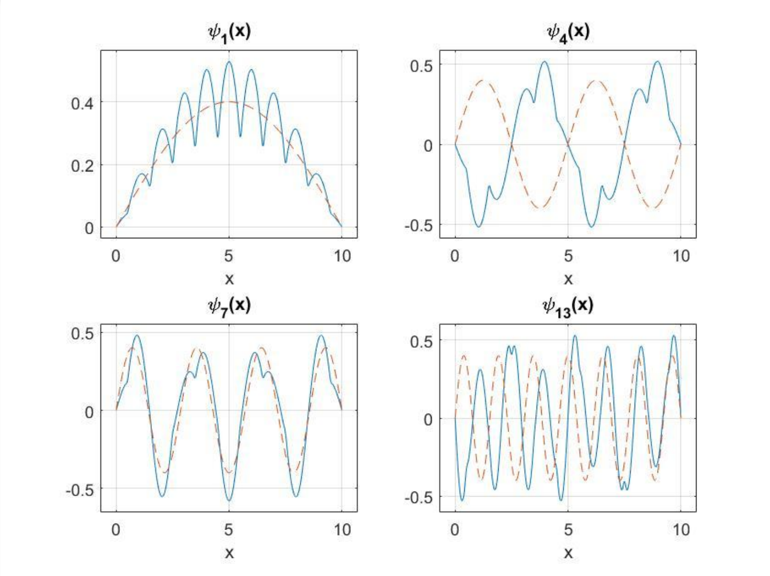
The above expression resorts to an infinite dimension matrix equation in C. Truncating it at m=150, further computations were made. Basically, we have to find the eigenvalues of H-matrix.

Computational Results

V0=100 N=150 nb=10 a=1 b=1/16 L=nb*a



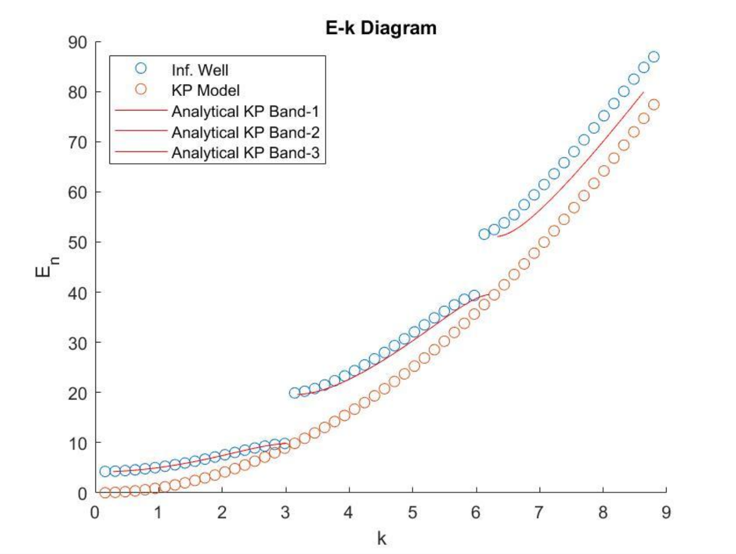
Bandgap-1=10.48 units
Bandgap-2=13.82units



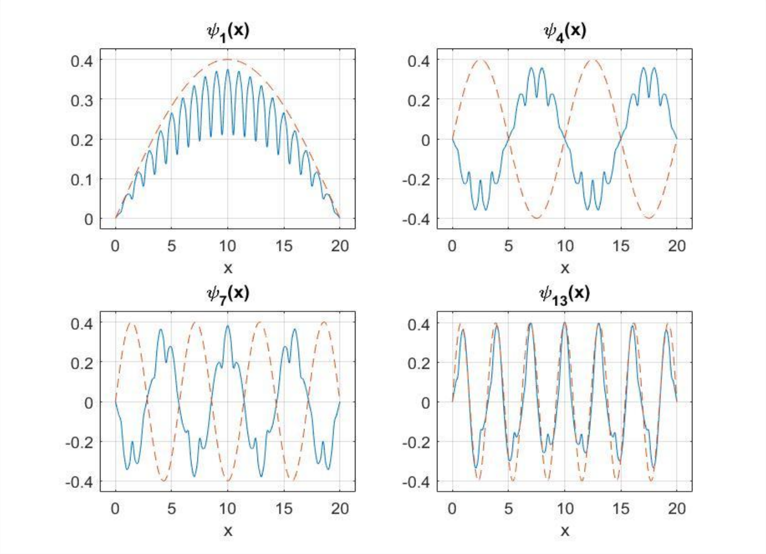
Wavefunction

Computational Results

V0=100 N=150 nb=20 a=1 b=1/16 L=nb*a



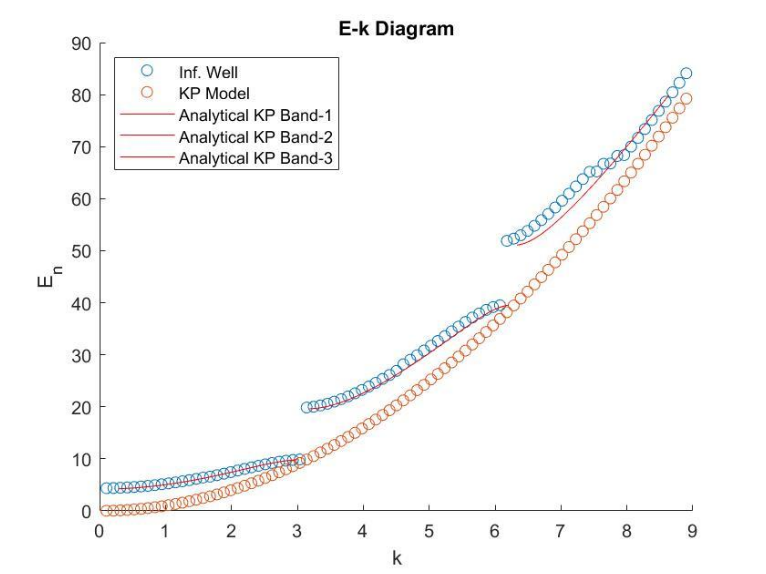
Bandgap-1=10.07 units
Bandgap-2=12.21 units



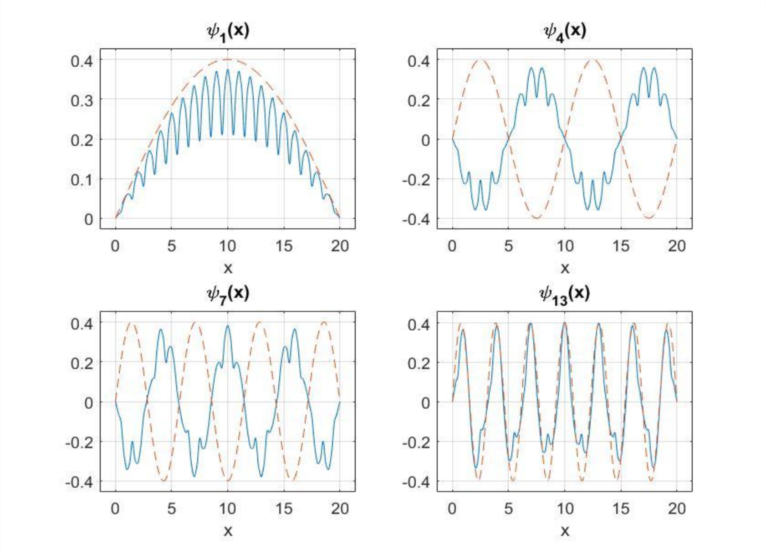
Wavefunction

Computational Results

V0=100 N=150 nb=30 a=1 b=1/16 L=nb*a



Bandgap-1=10.00 units
Bandgap-2=12.39 units



Wavefunction

External Field

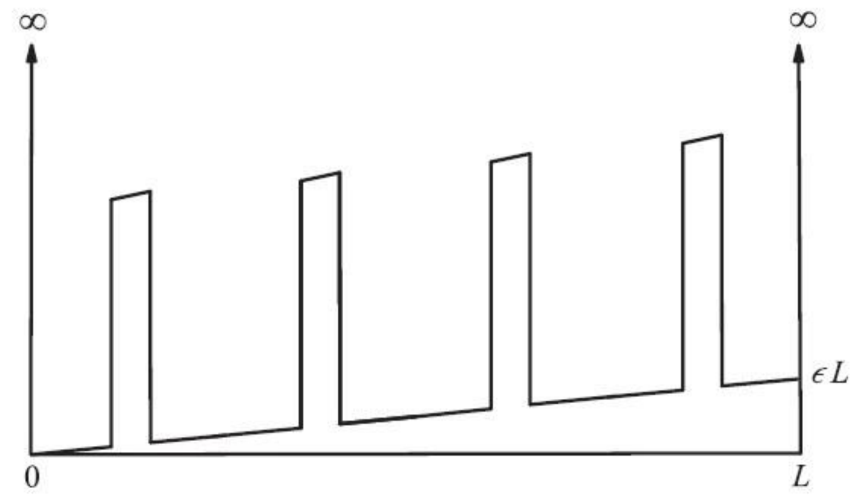


Fig. 9. Potential for a Kronig-Penney solid with a constant electric field ϵ.

$$V(x) = V_{KP}(x) + \epsilon x$$

$$H^e_{nm} = \frac{2\epsilon}{L}\int_0^L sin(\frac{n\pi x}{L})x sin(\frac{m\pi x}{L})dx$$

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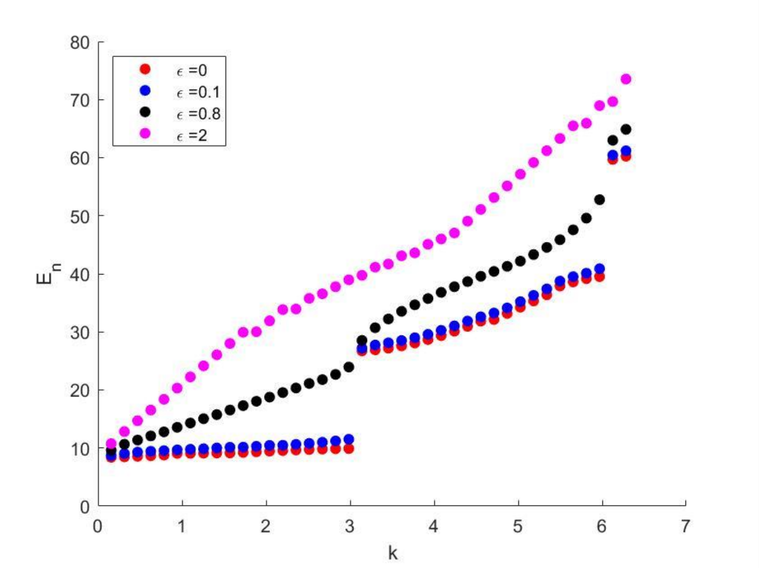
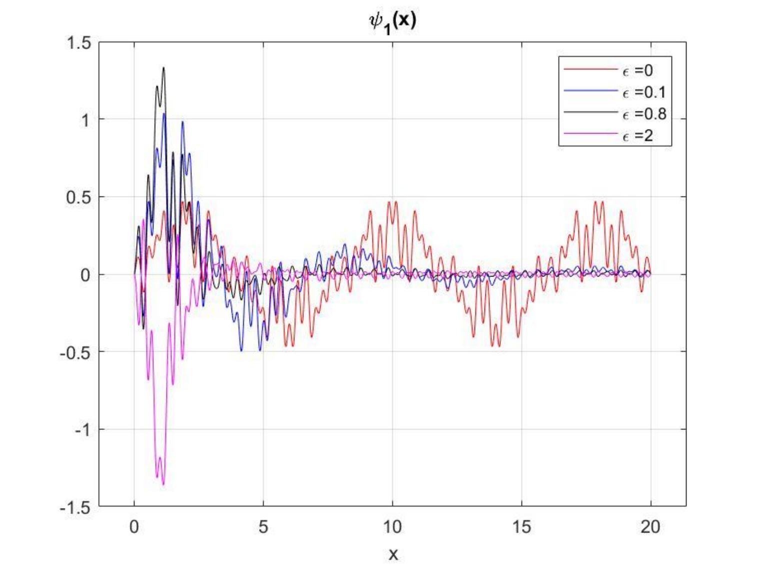
Computational Results

V0=100 N=150 nb=10 a=1 b=1/16 L=nb*a



E-k Band Diagram



Wavefunction

Analytical Model

Bloch's Theorem:

$$\psi(x) = e^{ix}u(x)$$

$$u(x) = u(x+a)$$

K-P Model:

$$\frac{\partial^2\psi}{\partial x^2} + \alpha^2\psi = 0; \alpha^2 = \frac{2mE}{\hbar^2}$$

$$\frac{\partial^2\psi}{\partial x^2} - \beta^2\psi = 0; \beta^2 = \frac{2m(V_o - E)}{\hbar^2}$$

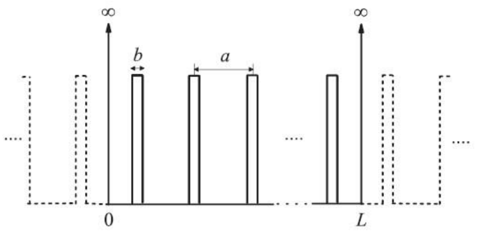


Fig. 1. The true potential $V(x)$ (dashed) and the auxiliary potential $V_{\text{inf}}(x) + V(x)$ (solid) for the Kronig-Penney model.

Analytical Model

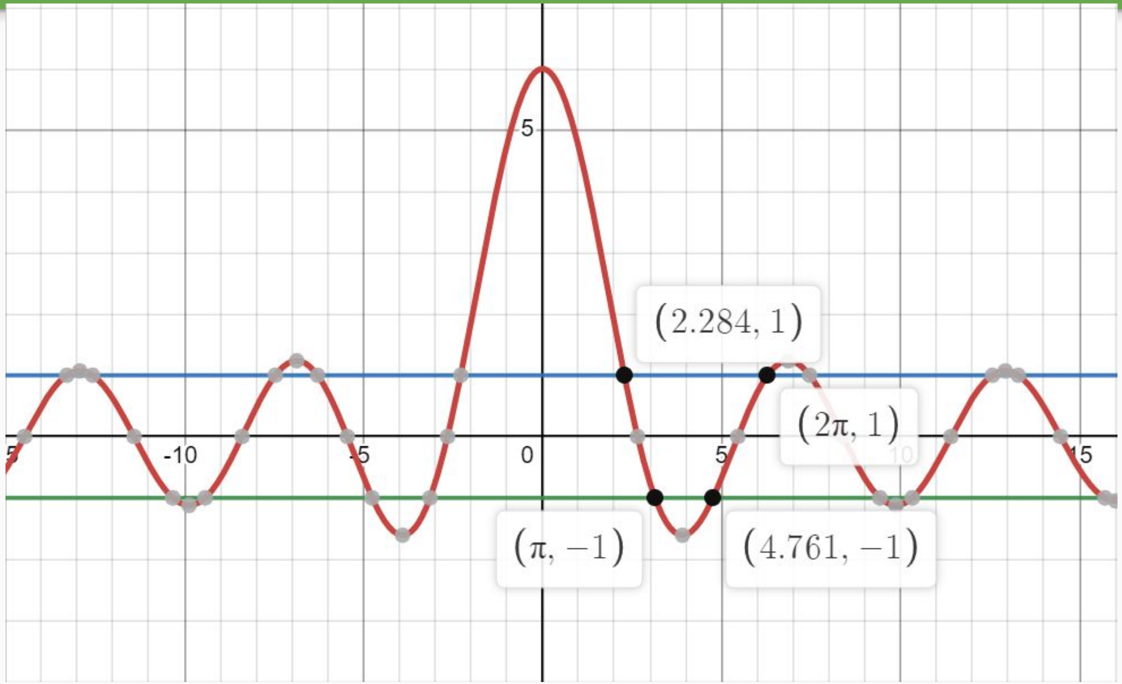
Applying Boundary Condition:

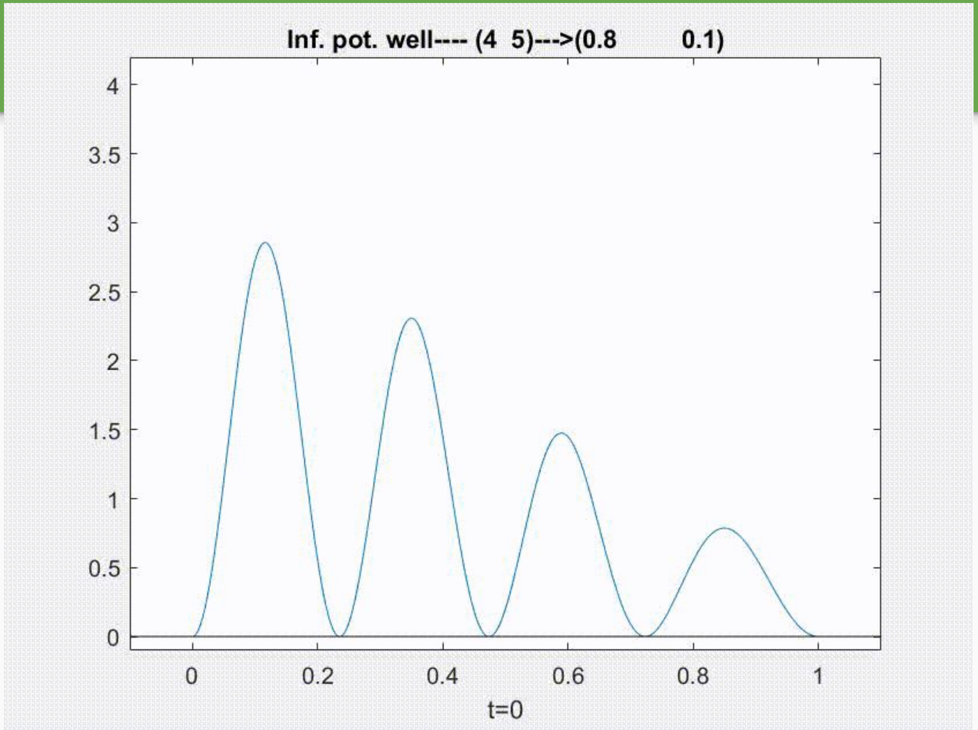
$$\frac{\beta^2 - \alpha^2}{2\alpha\beta} sinh(\beta b) sin(\alpha(a-b)) + cosh(\beta b) cos(\alpha(a-b)) = cos(ka)$$

Assuming V>>1 and b<<1

$$P\frac{sin(\alpha a)}{\alpha a} + cos(\alpha a) = cos(ka); P = \frac{mV_o ab}{\hbar^2}$$

Formation of Band Gaps





THANK YOU