The Kronig-Penney model extended to arbitrary potentials via numerical matrix mechanics

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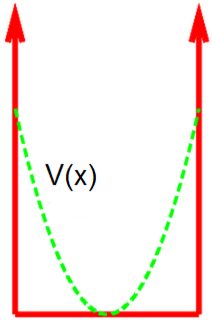
1. Solving the ODE with Hermite polynomials
2. Using Dirac's raising and lowering operators
3. Matrix diagonalization with an infinite square well basis

Hamiltonian matrix elements are divided into kinetic diagonal terms and potential-dependent terms

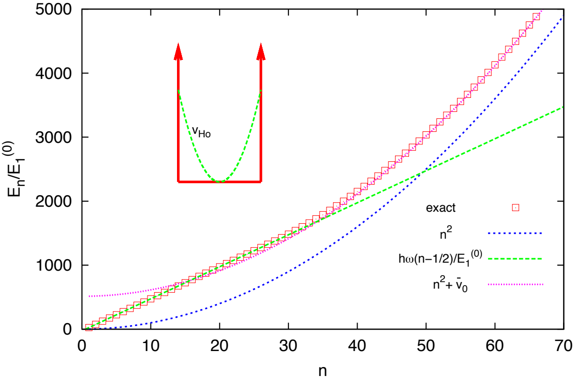


$$
\begin{aligned}
H_{nm} &= \langle \psi_n | \left(H_0 + V \right) | \psi_m \rangle \\
&= \delta_{nm} E_n^{(0)} + H_{nm}^{V}
\end{aligned}
$$

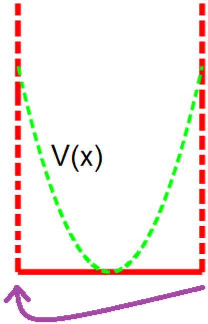
And the potential terms are computed in the usual way

$$
\begin{aligned}
H^V_{nm} &= \langle \psi_n | \, V(x) \, | \psi_m \rangle \\
&= \frac{2}{a} \int_0^a \, \mathrm{d}x \;\; \sin\left(\frac{n\pi x}{a}\right) V(x) \sin\left(\frac{m\pi x}{a}\right)
\end{aligned}
$$

This method gives excellent agreement with analytical solutions at low energies



But what about another potential? We try periodic boundary conditions (*à la* a particle on a ring)



$$\phi(x + a) = \phi(x)$$

This gives plane wave basis states...

$$\phi_n^{(0)}(x) = \sqrt{\frac{1}{a}}\, e^{i\frac{2\pi n}{a}x}$$

… with similar energies to the infinite square well

$$ka = 2\pi n$$

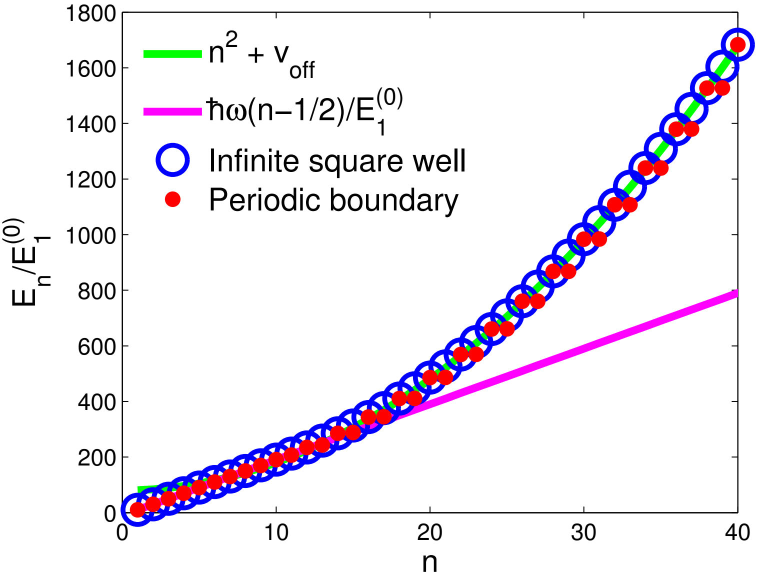
or

$$E_n = 4\left(\frac{n^2\pi^2\hbar^2}{2ma^2}\right) = 4n^2 E_1^{(0)} = (2n)^2 E_1^{(0)}$$

We now compute our matrix elements in the new basis

$$
\begin{aligned}
H^V_{nm} &= \langle \phi^{(0)}_n | \, V \, | \phi^{(0)}_m \rangle \\
&= \frac{1}{a} \int_0^a \mathrm{d}x \, e^{-i2\pi nx/a} \, V(x) \, e^{i2\pi mx/a}
\end{aligned}
$$

We can recreate the results in the 2008 paper in the new basis easily!



But we want to go beyond a single unit cell, so the boundary condition we actually want is the Bloch condition

$$\phi(x + a) = e^{iKa}\phi(x)$$

Given our plane wave basis states, we are essentially just multiplying exponentials so the Bloch contribution to the energy is merely additive

$$ka = 2\pi n + Ka$$

Further, this only affects the main diagonal kinetic energy terms as the potential terms in the Hamiltonian are unaffected

$$\frac{1}{a}\int_0^a \mathrm{d}x\, \cancel{e^{-iKx}} e^{-i2\pi nx/a}\, V(x)\, e^{i2\pi mx/a} \cancel{e^{+iKx}}$$

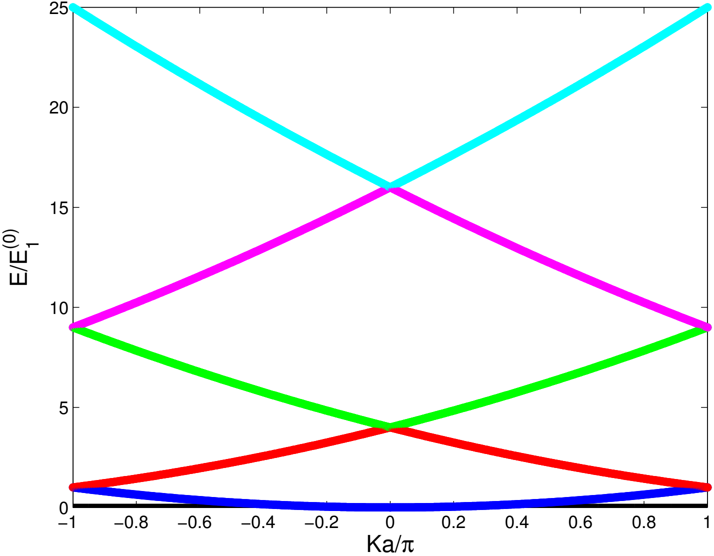
Thus our procedure is to first populate our Hamiltonian matrix ignoring the Bloch contribution

$$\frac{H_{nm}}{E_1^{(0)}} = \begin{pmatrix} (2\cdot 0)^2 + h_{00}^V & h_{01}^V & h_{02}^V & \cdots \\ h_{10}^V & (2\cdot 1)^2 + h_{11}^V & h_{12}^V & \cdots \\ h_{20}^V & h_{21}^V & (2\cdot 2)^2 + h_{22}^V & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

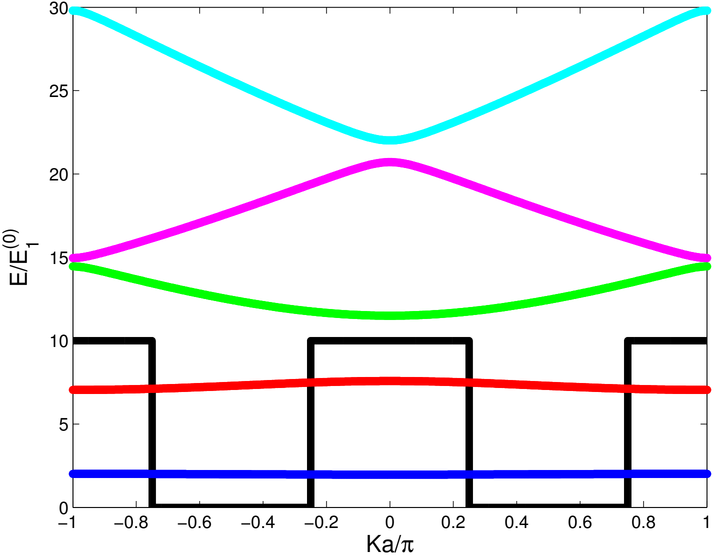
Then we iteratively introduce Bloch terms to the main diagonal, ranging from $Ka \in (-\pi, \pi)$, diagonalizing each to get a new set of eigenvalues

$$\begin{pmatrix} (0 + Ka/\pi)^2 + h^V_{00} & h^V_{01} & h^V_{02} & \dots \\ h^V_{10} & (2 + Ka/\pi)^2 + h^V_{11} & h^V_{12} & \dots \\ h^V_{20} & h_{21} & (4 + Ka/\pi)^2 + h^V_{22} & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

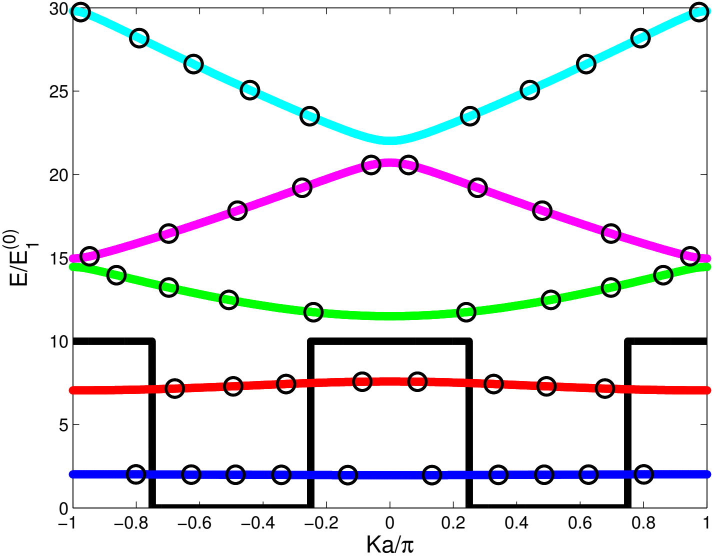
With no potential, these solutions recapitulate the expected free electron parabolic bands



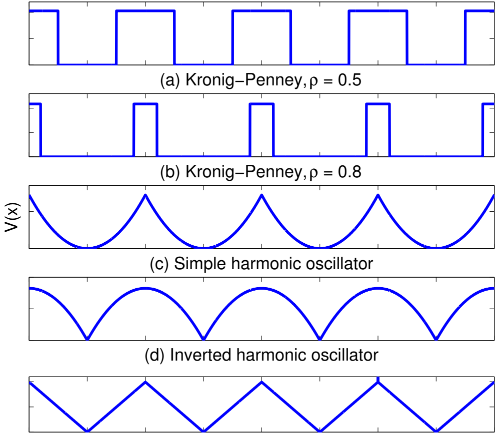
As we introduce the actual potential, there is a lifting of degeneracies and band gaps appear...



... and these solutions exactly match up with the known analytic solutions to the Kronig-Penney model

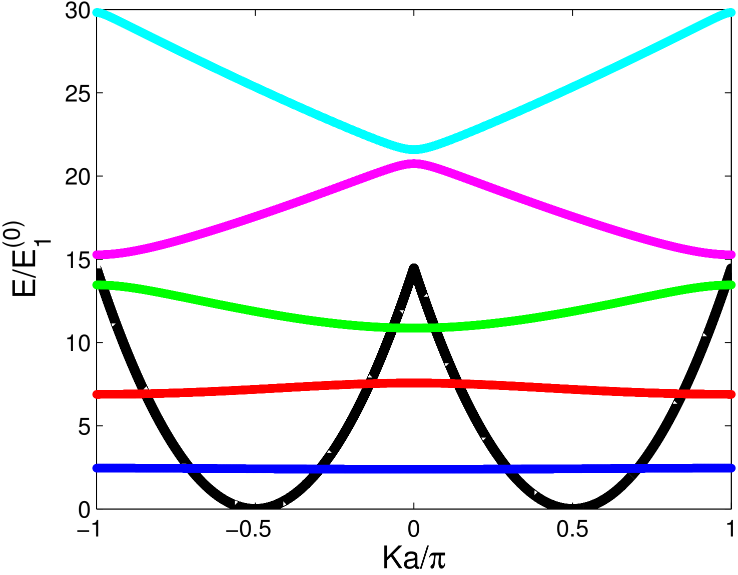


But the method is general enough to handle any repeating 1D potential; here we investigated several for which we could compute analytical matrix elements

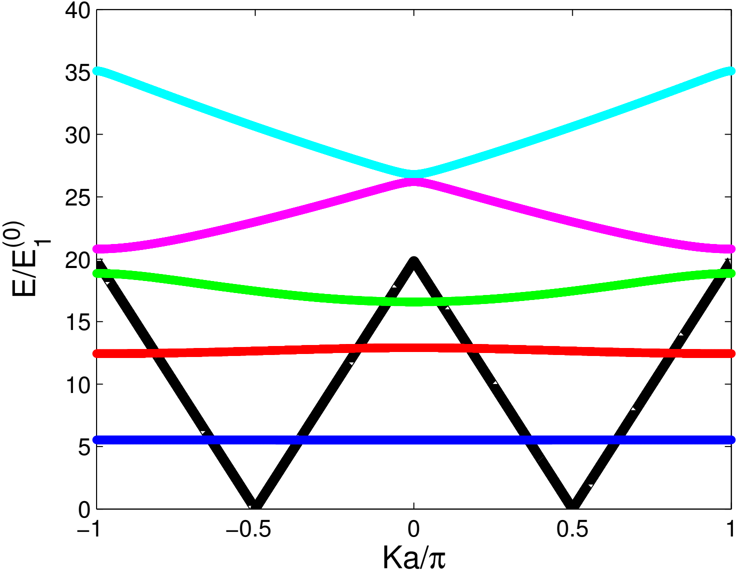


(a) Kronig–Penney, ρ = 0.5
(b) Kronig–Penney, ρ = 0.8
(c) Simple harmonic oscillator
(d) Inverted harmonic oscillator
(e) Linear well

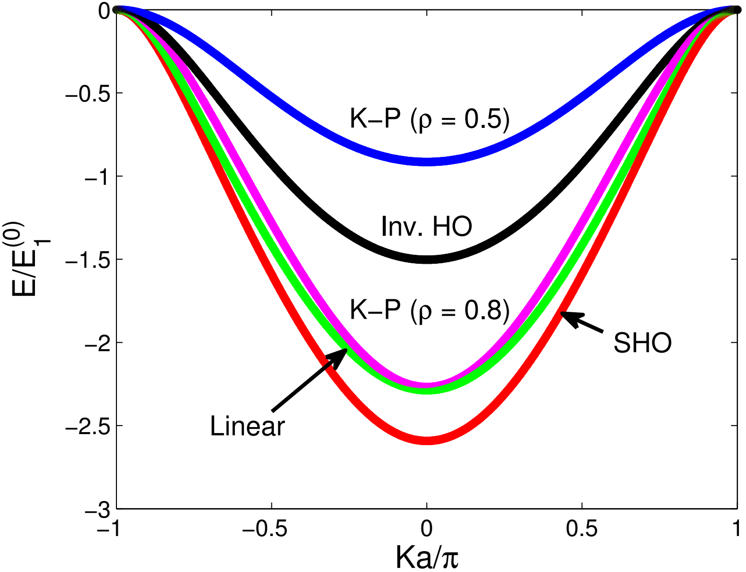
For example periodic harmonic oscillators...



... or the so-called linear well



We can compare the bandstructure by making the third band in each case “similarly bounded”



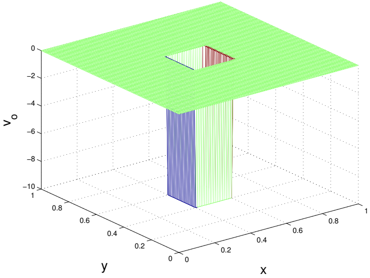
Further, we can use the second derivatives of these bands as a measure of the effective mass of the electrons/holes

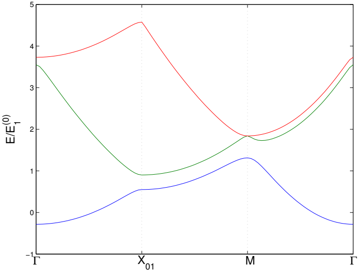
$$\frac{1}{m^*_{\substack{\mathrm{ele}\\ \mathrm{hol}}}} \equiv \frac{1}{\hbar^2}\frac{\mathrm{d}^2 E(K)}{\mathrm{d}K^2}\bigg|_{\substack{K_{\mathrm{min}}\\ K_{\mathrm{max}}}} \equiv \frac{E_1^{(0)}}{\hbar^2}e''_{\substack{\mathrm{ele}\\ \mathrm{hol}}}$$

We find that potentials with more realistic "cusp-like" potentials have lower hole effective masses (there's less of a potential "seen" by the higher energy band states)

Potential	e''_{ele}	e''_{hol}	$e''_{\text{ele}}/e''_{\text{hol}}$ $= m_{\text{hol}}/m_{\text{ele}}$
K-P ($\rho = 0.5$)	13.83	−25.35	−0.55
K-P ($\rho = 0.8$)	39.09	−70.61	−0.55
Simple HO	37.84	−121.80	−0.31
Inverted HO	19.83	−55.96	−0.35
Linear	31.63	−102.23	−0.31

Work in progress: 2D bandstructures





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