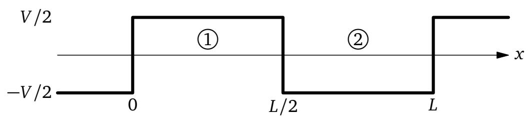
SPECTRAL WEIGHT OF BACKFOLDED BANDS



Consider an electron in the one-dimensional square-periodic potential of amplitude V and period L. This is a variant of the Kronig-Peney model. In units such that $\hbar^2/(2m) = 1$, the Schrödinger equation reads

$$-\psi''(x) + V(x)\psi(x) = \varepsilon\psi(x). \tag{1}$$

The solutions in the domains ① and ② may be written, up to a normalization, as

$$\begin{aligned}\psi_{①}(x) &= \left(Qe^{-iQL} + qe^{iqL} - q_+e^{ikL}\right)e^{iq_-x}\\ &\quad - \left(Qe^{iQL} + qe^{-iqL} - q_+e^{ikL}\right)e^{-iq_-x} \end{aligned}\tag{2}$$

$$\begin{aligned}\psi_{②}(x) &= -\left(Qe^{iQL} - qe^{iqL} - q_-e^{-ikL}\right)e^{ikL}e^{iq_+(x-L)}\\ &\quad + \left(Qe^{-iQL} - qe^{-iqL} - q_-e^{-ikL}\right)e^{ikL}e^{-iq_+(x-L)} \end{aligned}\tag{3}$$

with

$$q_\pm = \sqrt{\varepsilon \pm V/2}, \quad Q = \frac{q_+ + q_-}{2}, \quad q = \frac{q_+ - q_-}{2} \tag{4}$$

and k in the first Brillouin zone $[0, 2\pi/L[$. These solutions satisfy the matching conditions

$$\psi_{①}(L/2) = \psi_{②}(L/2), \quad \psi'_{①}(L/2) = \psi'_{②}(L/2), \tag{5}$$

as well as the Bloch theorem

$$\psi_{②}(L) = \psi_{①}(0)e^{ikL}, \quad \psi'_{②}(L) = \psi'_{①}(0)e^{ikL}, \tag{6}$$

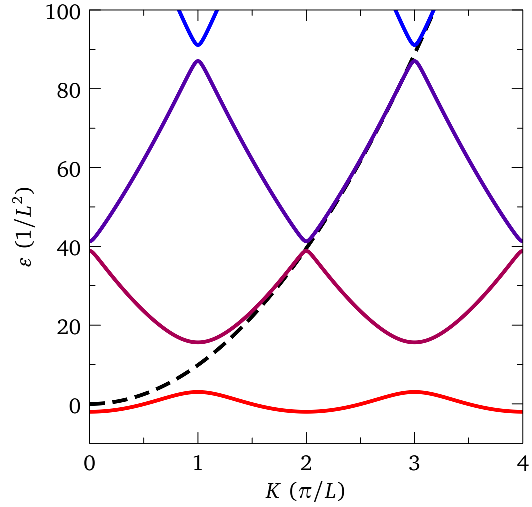
if and only if the energies obey the equation

$$\cos(kL) = \cos\left(\frac{q_+L}{2}\right)\cos\left(\frac{q_-L}{2}\right) - \varepsilon\frac{\sin\left(\frac{q_+L}{2}\right)}{q_+}\frac{\sin\left(\frac{q_-L}{2}\right)}{q_-}. \tag{7}$$

The normalization is fixed via the relation

$$\begin{aligned}&\int_0^{L/2} dx\,|\psi_{①}(x)|^2 + \int_{L/2}^{L} dx\,|\psi_{②}(x)|^2 =\\ &\frac{LV}{2}\left[\cos(q_+L) - \cos(q_-L)\right] + 2L\varepsilon\left[1 - \cos(q_+L)\cos(q_-L)\right]\\ &\quad + L\left[1 + \frac{\varepsilon^2}{\varepsilon^2 - (V/2)^2}\right]q_+\sin(q_+L)q_-\sin(q_-L)\\ &\quad + \frac{2(V/2)^2}{\varepsilon^2 - (V/2)^2}\Big\{\left[\cos(q_+L) - 1\right]q_-\sin(q_-L) +\\ &\qquad \left[\cos(q_-L) - 1\right]q_+\sin(q_+L)\Big\}. \end{aligned}\tag{8}$$

The figure shows the free dispersion K^2 in dashed-black and the solutions ε_{kn} of Eq. (7) for $V = 20$ in colors, which are periodic functions of K in extended-zone scheme with period $2\pi/L$. We denote K an arbitrary wave vector and keep the notation k for the first Brillouin zone.



We are interested in the spectral function

$$\begin{aligned}A(K,E) &= \frac{1}{L}\int_0^L dR\\ &\times\left(-\frac{1}{\pi}\right)\mathrm{Im}\int_{-\infty}^{\infty} d\rho\, e^{-iK\rho}G(R+\rho/2, R-\rho/2, E). \end{aligned}\tag{9}$$

$G(x, x', E)$ is the retarded Green's function, with $x = R + \rho/2$ and $x' = R - \rho/2$ expressed in terms of the center-of-mass and relative coordinates R and ρ, respectively. The second line in Eq. (9) expresses the Fourier transform of G with respect to the relative coordinate, while the first line performs a spatial average due to broken translational symmetry. The Green's function is

$$G(x, x', E) = \int_0^{\frac{2\pi}{L}} \frac{dk}{2\pi}\sum_n \frac{\psi_{kn}(x)\psi^*_{kn}(x')}{E - \varepsilon_{kn} + i0}. \tag{10}$$

In order to perform the Fourier transform and the spatial average, we use the representation

$$\psi_{kn}(x) = \sum_G u_{kn}(G)e^{i(k+G)x} \quad \text{with} \quad e^{iGL} = 1 \tag{11}$$

$$u_{kn}(G) = \frac{1}{L}\int_0^L dx\,\psi_{kn}(x)e^{-i(k+G)x}. \tag{12}$$

The consistency of this representation may be checked by using the identity

$$\sum_G e^{iGx} = L\sum_{m\in\mathbb{N}}\delta(x + mL). \tag{13}$$

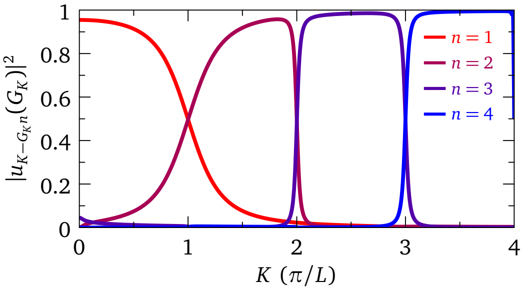
We are lead to the integral

$$\begin{aligned}&\frac{1}{L}\int_0^L dR\int_{-\infty}^{\infty} d\rho\, e^{-iK\rho}e^{i(k+G)(R+\rho/2)}e^{-i(k+G')(R-\rho/2)}\\ &\qquad = 2\pi\delta_{GG'}\delta(k + G - K). \end{aligned}$$

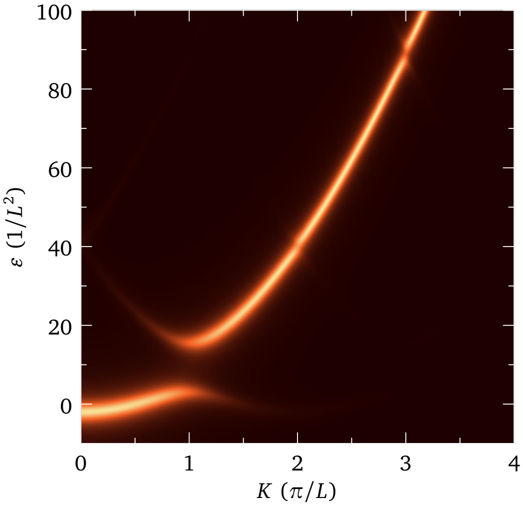
The spectral function results as

$$A(K,E) = \int_0^{\frac{2\pi}{L}} dk \sum_{nG} |u_{kn}(G)|^2 \delta(k+G-K)\delta(E-\varepsilon_{kn}) \\ = \sum_n |u_{K-G_K n}(G_K)|^2 \delta(E-\varepsilon_{K-G_K n}), \tag{14}$$

where G_K is the unique reciprocal-lattice vector such that $K-G_K \in [0, 2\pi/L[$. The figure shows $|u_{K-G_K n}(G_K)|^2$ as a function of K for the first four bands.



These amplitudes add to unity at each K, as required by the sum rule $\int_{-\infty}^{\infty} dE\, A(K,E) = 1$. It is seen that the spectral weight of the backfolded band extends up to the zone boundary and even beyond for the fundamental gap. Note also that the second band has zero weight at $K=0$ while the third band as a finite weight there. The figure shows Eq. (14) with the delta function replaced by a Lorentzian of width $2/L^2$.



The weak spectral weight on the Umklapp bands is better visualized if the intensity is plotted on a log scale as below.