Box Quantization
Observed by Photoemission

(For photoemission see Lect. 18.)

\[ p = \frac{h}{\lambda} \]

\[ E = \frac{p^2}{2m} = \frac{h^2}{2m} \cdot \frac{1}{\lambda^2} \]

- Then quantize: \( \lambda_n = \frac{2d}{n} \)

\[ E_n \propto n^2, \quad E_n \propto d^{-2} \]
Quantization in k-Space

Consider a thin film of thickness $d$ containing $N$ atomic layers spaced by the lattice constant $a$: $d = N \cdot a$

$$\lambda_n = \frac{2d}{n}$$

$$k_n = \frac{n \cdot \pi}{d}$$

$$n = 1, \ldots, N$$

Grid of discrete states in k-space.

N states per band for N atomic layers
Analogous to Bohr’s quantization condition an integer number of electron wavelengths needs to fit around the circumference of the nanotube. Otherwise the electron waves would interfere destructively.

This leads to discrete wavelengths $\lambda_n = \pi d/n$ ($d =$ diameter of the tube). The corresponding wave vectors are $k_n = n \cdot 2/d$ (along the circumference).

Electrons can move freely parallel to the nanotube, forming a band for each quantized state. The kinetic energy $p^2/2m$ of the motion along the tube is added to the quantized energy level.
Tailoring the Density of States by Quantization

The one-dimensional density of states for motion along a nanotube exhibits \(1/\sqrt{E}\) singularities at the onsets of the quantized energy levels (see Lect. 13). Their energy positions can be varied by changing the diameter \(d\) of the tube.
Density of States of a Nanotube

Calculated Density of States \( D(E) \):

\[ D(E) \text{ Measured by Scanning Tunneling Spectroscopy (STS):} \]

\[ \frac{dI/dV}{I/V} \propto D(E) \]

\[ \rightarrow 1 \text{ for } V \rightarrow 0 \text{ for metallic tubes} \]
Distinguishing Nanotubes by their Quantized States

“Two-dimensional” spectroscopy:
Measure both photon absorption (x-axis) and photon emission (y-axis).
Indices \((m,n)\) of Nanotubes

Unwrap a nanotube into planar graphene

Circumference vector \(c_r = m a_1 + n a_2\)