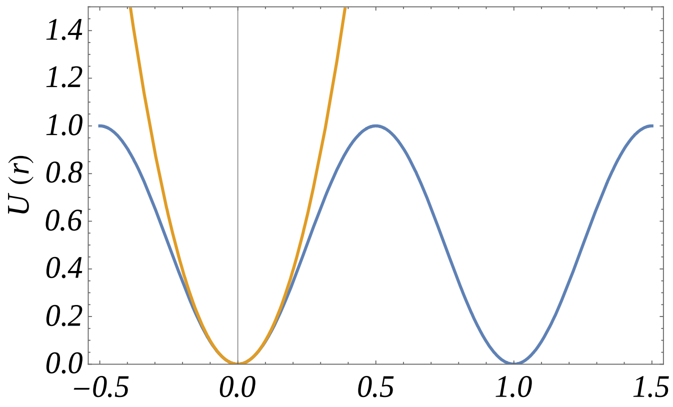
Lectures:

Thursday, 23.5.: Tight binding model; optical lattices

Exercises:

All solutions must be handed in by **Tue. 28.5.** noon in box on 5th floor of Building 46 or electronically to laschwar@rptu.de



Consider particles of mass m in the following one-dimensional periodic potential[1]

$$U(r) = U \sin^2 k_a r$$

where $k_a = \pi / a$ in terms of the lattice constant a (see figure). The kinetic energy at the Bragg-planes is $E_r = \hbar^2 k_a^2 / 2m$, which should be used as the overall unit, i.e. $s = U / E_r$ can be used as a dimensionless parameter for the potential amplitude.

8) Determine the Fourier-components $U_n = \frac{1}{a}\int_0^a U(r) e^{i2\pi n r/a} dr$ for $n = \pm 1$ and calculate the approximate dispersion relation $\varepsilon(k)$ by diagonalizing the 2x2 matrix for the lowest band and the next lowest band around $k = k_a$. Plot the dispersion as a function of k / k_a for s=0.5 and for s=1., which is the approximate value for Cu.

9) In the atomic limit of large s>>1 the potential can be approximated by harmonic oscillators at each lattice site. Express the effective frequency ω in terms of $s = U / E_r$ so that $U(r) \approx U_{osc}(r) = \frac{1}{2} m\omega^2 r^2$ (see figure). Hence at each lattice site n the Wannier function (or "atomic orbitals") can be approximated as the ground state of an harmonic oscillator, which is known to be $\tilde{\psi}_n(r) = (d^2\pi)^{-1/4} e^{-\frac{(r-na)^2}{2d^2}}$ with $d^2 = \dfrac{\hbar}{m\omega}$.
The nearest-neighbor hopping matrix element is therefore given by

$$t(1) = \int_{-\infty}^{\infty} dr\, \tilde{\psi}_{n=1}^*(r) \big(U(r) - U_{osc}(r)\big) \tilde{\psi}_{n=0}(r) .$$

Verify that in the limit of a large potential $d^2 \propto 1/\sqrt{s} << 1$ the product of wave-functions becomes sharply peaked and can be approximated by a delta-function $\tilde{\psi}_0^*(r-a)\tilde{\psi}_0(r) \approx \exp[-(a/2d)^{-2}]\delta(x - a/2)$.
Using this approximation determine the hopping integral for s=3 and s=1. and plot the resulting cosine dispersion. Compare the latter with the results from 8) (the ground state energy at k =0 can be subtracted in both cases).

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[1] In optical lattices for ultra-cold atoms such a potential is produced by standing waves of interfering lasers with wavelength $\lambda = 2a$. In this case $E_r = \hbar^2 k_a^2 / 2m$ is exactly the so-called recoil energy from the momentum transfer of one photon.