Lectures:

Monday, 27.5.: Optical lattice. The Hydrogen Molecule.

Exercises:

All solutions must be handed in by **Tue. 4.6.** noon in box on 5th floor of Building 46 or electronically to laschwar@rptu.de

10) In 1D Wannier orbitals around the origin are defined by $\widetilde{\psi}_m(x) = \sqrt{\frac{a}{2\pi}} \int_{-\pi/a}^{\pi/a} dk\, \psi_{k,m}(x)$ where m is the Band index and $-\frac{\pi}{a} < k \le \frac{\pi}{a}$. We know that the Bloch solutions $\psi_{k,m}(x)$ are orthonormal wavefunctions.

Show that the Wannier orbitals form an orthonormal basis, i.e.

$$\int_{-\infty}^{\infty} \widetilde{\psi}_m^*(x-na)\widetilde{\psi}_l(x)dx = \delta_{n,0}\delta_{m,l}$$

11) In the tight binding approximation often normalized atomic orbitals φ_m are used as approximations, which are *not* orthogonal on nearest neighboring sites

$$\int_{-\infty}^{\infty} \varphi_m^*(x-a)\varphi_m(x)dx = \int_{-\infty}^{\infty} \varphi_m(x+a)\varphi_m^*(x)dx = \gamma$$

Find a suitable orthonormal linear combination $\widetilde{\varphi}_m$ of $\varphi_m(x)$ with $\varphi_m(x \pm a)$, so that all overlap integrals of the $\widetilde{\varphi}_m$ between nearest neighboring sites vanish. What is the expression for the nearest neighbor hopping integral in this case?