Homework Set 3.

Problem 1. The quantum-mechanical momentum operator $\hat{\vec{p}} = -i\hbar\nabla$ does not commute with the effective single-particle Hamiltonian of solid, $\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + U(\vec{r})$ where $U(\vec{r}+\vec{R}) = U(\vec{r})$, since $[\hat{H},\hat{\vec{p}}] = i\hbar\nabla U(\vec{r})$. Therefore, the momentum $\vec{p}$ (i.e., the eigevalue of $\hat{\vec{p}}$) is not the constant of motion (i.e., it is not a "good" quantum number). Nevertheless, it is possible to construct a quasi-momentum operator $\hat{\vec{P}}$ which will commute with $\hat{H}$ and whose eigenvalue is the quasi-momentum (or crystalline momentum) $\hbar\vec{k}$

$$[\hat{H},\hat{\vec{P}}] = 0; \quad \hat{\vec{P}}\Psi_{n\vec{k}}(\vec{r}) = \hbar\vec{k}\Psi_{n\vec{k}}(\vec{r}),$$

where $\Psi_{n\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}u_{n\vec{k}}(\mathbf{r})$ is the Bloch state (eigenstate of $\hat{H}$). Since $\hat{\vec{P}} \to \hat{\vec{p}}$ when $U(\mathbf{r}) = const$, we can assume that quasi-momentum operator can be expressed as $\hat{\vec{P}} = \hat{\vec{p}} + i\hbar\hat{\vec{F}}$. Find the unknown operator $\hat{\vec{F}}$.

Problem 2. Suppose that a small amount of damping changes the semiclassical equations of motion for tightly bound electron in one dimension to

$$\begin{aligned} \frac{dx}{dt} &= \frac{2\epsilon_0 a}{\hbar}\sin ka \\ \hbar\frac{dk}{dt} &= -eE - \frac{m}{\tau}\frac{dx}{dt}. \end{aligned}$$

Take $\epsilon_0 = 1$ eV, $a = 2$Å, $E = 10^6$V/cm, and $\tau = 10^{-14}$s.

(a) Put these equations in dimensionless form, measuring distance in units of a and measuring time in units of τ.

(b) Integrate the equations numerically and examine the effect of the damping upon dynamics of electrons (i.e., Bloch oscillations when $m/\tau \to 0$) in 1D solid.

(c) Describe the final state of the system analytically.

Problem 3. The tight binding Hamiltonian for spinless particle propagating through one-dimensional or square lattice (spacing a), where each lattice site contains a single s-orbitals, is given by

$$\hat{H} = \sum_m \epsilon_0|m\rangle\langle m| - t\sum_{\langle m,m'\rangle}|m\rangle\langle m'|.$$

The sum in the second term runs over the nearest neighbors pairs and $t > 0$.

(a) Using the fact that the eigenvalues (i.e., the "energy band") of this Hamiltonian in 1D are $\varepsilon(k) = \varepsilon_0 - 2t\cos(ka)$, find the effective mass of the Bloch electron and plot this function in the first Brillouin zone $k \in [-\pi/a, \pi/a)$.

(b) The eigenvalues of the 2D tight-binding Hamiltonian are $\varepsilon(\mathbf{k}) \equiv \varepsilon(k_x, k_y) = \varepsilon_0 - 2t[\cos(k_x a) + cos(k_y a)]$. Find the effective mass *tensor* of the Bloch electron in one of the energy eigenstates [labeled by (k_x, k_y)], i.e., evaluate the 2×2 matrix as a function of k_x, k_y

$$\left(\frac{1}{m^*}\right)_{ij} = \frac{1}{\hbar^2}\frac{\partial^2 \varepsilon(\mathbf{k})}{\partial k_i \partial k_j},$$

where $i, j \in \{x, y\}$.

(c) How does the effective mass vary with the hopping parameter t? Why?