

5.1 Quasi-momentum operator of Bloch electrons.

As mentioned in the class, the quantum-mechanical momentum operator $\hat{p} = -i\hbar\nabla$ does not commute with the effective single-electron Hamiltonian of a solid, $\hat{H} = -\frac{\hbar^2\nabla^2}{2m} + U(\vec{r})$, where $U(\vec{r} + \vec{R}) = U(\vec{r})$ with \vec{R} a lattice vector. However, it is possible to construct a quasi-momentum operator \hat{P} that commutes with \hat{H} and whose eigenvalue is the quasi-momentum (or crystal momentum) $\hbar k$, so that

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

where $\psi_k(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}u_k(\vec{r})$ is the Bloch function. Since $\hat{P} \rightarrow \hat{p}$ for $U(\vec{r}) = \text{const}$, we can express quasi-momentum operator \hat{P} as $\hat{P} = \hat{p} + i\hbar\hat{F}$.

- (1) Evaluate the commutator $[\hat{H}, \hat{p}]$.
- (2) Find the unknown operator \hat{F} .

习题

5.2 阎书3.1：电子在周期场中的势能函数

$$V(x) = \begin{cases} \frac{1}{2}m\omega^2[b^2 - (x - na)^2], & na - b \leq x \leq na + b \\ 0, & (n-1)a + b \leq x \leq na - b \end{cases}$$

其中 $a=4b$ ， ω 为常数，

- (1) 画出此势能曲线，并求其平均值；
- (2) 用近自由电子近似模型求出晶体的第一个和第二个禁带的宽度。

5.3 黄书4.1

5.4 黄书4.2