k.p Perturbation Theory

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1 Introduction

Suppose we have a periodic potential function. That is

$$V(\mathbf{r}) = V(\mathbf{r} + \mathbf{R}) \tag{1}$$

The vector $\mathbf{R} = n_1\mathbf{a_1} + n_2\mathbf{a_2} + n_3\mathbf{a_3}$ is a linear combination the primitive lattice vectors, $\{\mathbf{a_1}, \mathbf{a_2}, \mathbf{a_3}\}$, and $n_1, n_2, n_3 \in \mathcal{Z}$. Bloch's theorem applies and we can write the spacial wave-function as

$$\psi_{n,\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{n,\mathbf{k}}(\mathbf{r}) \tag{2}$$

where $\mathbf{k}$ is in the first Brillouin zone.

The Block wave-function satisfy then energy-eigenvalue equation.

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right)\psi_{n,\mathbf{k}}(\mathbf{r}) = E_{n,\mathbf{k}}\psi_{n,\mathbf{k}}(\mathbf{r}) \tag{3}$$

and the Bloch wave functions satisfy the energy eigenvalue equation. Using the vector identity

$$\nabla^2(fg) = \nabla^2 f + 2\nabla f \cdot \nabla g + \nabla^2 g \tag{4}$$

we find

$$\begin{aligned} \nabla^2\psi_{n,\mathbf{k}}(\mathbf{r}) &= e^{i\mathbf{k}\cdot\mathbf{r}}\left(\nabla^2 u_{n,\mathbf{k}}(\mathbf{r}) + 2i\mathbf{k}\cdot\nabla u_{n,\mathbf{k}}(\mathbf{r}) - k^2 u_{n,\mathbf{k}}(\mathbf{r})\right) \\ &= -e^{i\mathbf{k}\cdot\mathbf{r}}\left(\left(\frac{\hat{\mathbf{p}}}{\hbar}\right)^2 + 2\frac{\mathbf{k}\cdot\hat{\mathbf{p}}}{\hbar} + k^2\right)u_{n,\mathbf{k}}(\mathbf{r}) \end{aligned} \tag{5}$$

using the operator identity $\hat{\mathbf{p}} = -i\hbar\nabla$. Not the the momentum operator, $\hat{\mathbf{p}}$, has already acted on the phase factor, $e^{\mathbf{k}\cdot\mathbf{r}}$, and does not commute. Plugging in Eq. **??** to Eq. **??** we find

$$\begin{aligned} \left(\frac{\hat{\mathbf{p}}^2}{2m} + \hbar\frac{\mathbf{k}\cdot\hat{\mathbf{p}}}{m} + \frac{\hbar^2k^2}{2m} + V(\mathbf{r})\right)u_{n,\mathbf{k}}(\mathbf{r}) &= E_{n,\mathbf{k}}u_{n,\mathbf{k}}(\mathbf{r}) \\ \left(\frac{(\hat{\mathbf{p}} + \hbar\mathbf{k})^2}{2m} + V(\mathbf{r})\right) &= E_{n,\mathbf{k}}u_{n,\mathbf{k}}(\mathbf{r}) \end{aligned} \tag{6}$$

that the phase factor $e^{i\mathbf{k}\cdot\mathbf{r}}$ cancels out.

We can now define an new Hamiltonian that depends on $\mathbf{k}$.

$$H_{\mathbf{k}} = H_0 + H'_{\mathbf{k}} \tag{7}$$

$$H_0 = \frac{p^2}{2m} + V(\mathbf{r}) \tag{8}$$

$$H'_{\mathbf{k}} = \hbar\frac{\mathbf{k}\cdot\hat{\mathbf{p}}}{m} + \frac{\hbar^2 k^2}{2m} \tag{9}$$

Clearly the perturbation is zero when $\mathbf{k} = 0$, and for small $\mathbf{k}$ us can use perturbation theory.

$$E_{n,\mathbf{k}} = E_{n,\mathbf{0}} + E^{(1)}_{n,\mathbf{k}} + E^{(2)}_{n,\mathbf{k}} \tag{10}$$