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Theoretical Solid-State Physics, Herbstsemester 2012

Blatt 0

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(1) **Hellman-Feynman theorem and its implications for Bloch electrons**
Consider a Hamiltonian that depends on parameters $\lambda \equiv \{\lambda_i | i = 1, 2, \ldots\}$. Let $|\Psi_n(\lambda)\rangle$ be the orthonormal eigenstates of this Hamiltonian, i.e., assume that

$$H(\lambda)|\Psi_n(\lambda)\rangle = E_n(\lambda)|\Psi_n(\lambda)\rangle, \qquad \langle\Psi_m(\lambda)|\Psi_n(\lambda)\rangle = \delta_{mn} \, .$$

(a) Prove the Hellman-Feynman theorem

$$\left\langle \Psi_n(\lambda) \left| \frac{\partial H(\lambda)}{\partial \lambda_i} \right| \Psi_n(\lambda) \right\rangle = \frac{\partial E_n(\lambda)}{\partial \lambda_i}$$

and its "off-diagonal" generalization:

$$\left\langle \Psi_m(\lambda) \left| \frac{\partial H(\lambda)}{\partial \lambda_i} \right| \Psi_n(\lambda) \right\rangle = -(E_m - E_n) \left\langle \Psi_m(\lambda) \middle| \frac{\partial \Psi_n(\lambda)}{\partial \lambda_i} \right\rangle \quad (m \neq n) \, .$$

(b) Consider an electron in a periodic potential $V(\mathbf{r}) = V(\mathbf{r} + \mathbf{a})$, that is, with the Hamiltonian

$$H_e = \frac{\mathbf{p}^2}{2m} + V(\mathbf{r}) \, .$$

Show that the Bloch eigenvalue problem $H_e \Psi_{n,\mathbf{k}}(\mathbf{r}) = E_{n,\mathbf{k}} \Psi_{n,\mathbf{k}}(\mathbf{r})$, where $\langle \mathbf{r}|\Psi_{n,\mathbf{k}}\rangle \equiv \Psi_{n,\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{n,\mathbf{k}}(\mathbf{r})$ are Bloch functions with the crystal-periodic parts $u_{n,\mathbf{k}}(\mathbf{r})$, can be recast as an equivalent eigenvalue problem

$$H_e^{(\mathbf{k})} u_{n,\mathbf{k}}(\mathbf{r}) = E_{n,\mathbf{k}} u_{n,\mathbf{k}}(\mathbf{r}) \, .$$

Here

$$H_e^{(\mathbf{k})} \equiv H_e + \frac{\hbar}{m} \mathbf{k} \cdot \mathbf{p} + \frac{\hbar^2 \mathbf{k}^2}{2m}$$

is a Hamiltonian that depends parametrically on the electron quasimomentum $\mathbf{k}$, with $\mathbf{p} \equiv (\hbar/i)\partial_{\mathbf{r}}$ being the electron momentum operator.

(c) Demonstrate that the expectation value

$$\mathbf{v}_{n,\mathbf{k}} \equiv \left\langle \Psi_{n,\mathbf{k}} \left| \frac{\mathbf{p}}{m} \right| \Psi_{n,\mathbf{k}} \right\rangle$$

of the electron velocity operator is given by

$$\mathbf{v}_{n,\mathbf{k}} = \int d\mathbf{r} \, u^*_{n,\mathbf{k}}(\mathbf{r}) \frac{1}{m} (\mathbf{p} + \hbar\mathbf{k}) u_{n,\mathbf{k}}(\mathbf{r}) \, .$$

Then, by applying the (diagonal) Hellman-Feynman theorem to the Hamiltonian $H_e^{(\mathbf{k})}$, derive the following expression for $\mathbf{v}_{n,\mathbf{k}}$ used in semiclassical transport theories:

$$\mathbf{v}_{n,\mathbf{k}} = \frac{1}{\hbar} \frac{\partial E_{n,\mathbf{k}}}{\partial \mathbf{k}} \, .$$