

HOMEWORK SET 02
 Theory of Condensed Matter
 UFV/TKL1/99 lecture by Martin Gmitra
 Winter Semester 2021, room KNKTFA(Pa9-PKn)

1. A Bloch state $\psi_{nk}(x) = u_{nk}(x)\exp(ikx)$ satisfy the eigenvalue equation $H\psi_{nk}(x) = \varepsilon_{nk}\psi_{nk}(x)$ has the expectation value of the velocity given by

$$v_{nk} = \frac{1}{i\hbar} \int dx \psi_{nk}^*(x)[x, H]\psi_{nk}(x) = \frac{\partial \varepsilon_{nk}}{\partial \hbar k}$$

a) [3 points] using the fact that ψ_{nk} is the eigenstate of H and that H is hermitian, we could write

$$v_{nk} = \frac{1}{i\hbar} \int dx \psi_{nk}^*(x)(xH - Hx)\psi_{nk}(x) = \frac{1}{i\hbar} \varepsilon_{nk} \int dx \psi_{nk}^* x \psi_{nk} - \frac{1}{i\hbar} \varepsilon_{nk} \int dx \psi_{nk}^* x \psi_{nk} = 0$$

The velocity in general is not zero. What is wrong here?

b) [1 point] Using Bloch state $\psi_{nk}(x) = u_{nk}(x)\exp(ikx)$ and Schrödinger equation for a periodic potential $U(x)$ show that eigenvalue problem can be considered in the form

$$H(k)u_{nk}(x) = \varepsilon_{nk}u_{nk}(x) \text{ and } H(k) = \frac{\hbar^2}{2m}(-i\nabla + k)^2 + U(x).$$

2. Free electron band structure calculations (empty lattice approximation) for monoatomic 2D square lattice with lattice vectors $\mathbf{a}_1 = a\hat{x}$, $\mathbf{a}_2 = a\hat{y}$ along the high symmetry lines connecting the following points in the reciprocal space

$$\Gamma = (0, 0), \mathbf{X} = \frac{2\pi}{a} \left(\frac{1}{2}, 0 \right) \text{ and } \mathbf{M} = \frac{2\pi}{a} \left(\frac{1}{2}, \frac{1}{2} \right).$$

a) [4 points] Calculate free electron band structure using your favorite software or write a computer program, specifically for each momentum k along the high symmetry lines using

$$\varepsilon_{n,\mathbf{k}}^0 = \frac{\hbar^2}{2m}(\mathbf{k} + \mathbf{G}_n)^2, \text{ where } \mathbf{G}_n = m_1\mathbf{b}_1 + m_2\mathbf{b}_2, \text{ and } m_1 \text{ and } m_2 \text{ are integers. For calculations include reciprocal lattice vectors that satisfy } |\varepsilon_{\mathbf{k}}^0 - \varepsilon_{\mathbf{k}+\mathbf{G}}^0| < \varepsilon_{\text{cutoff}} \text{ such that reduced energy } \varepsilon_{n,\mathbf{k}} \text{ in relative units } \varepsilon_{n,\mathbf{k}} = \varepsilon_{n,\mathbf{k}} / \left(\frac{\hbar^2}{2ma^2} \right) \text{ is below 100.}$$

b) [1 point] Identify degeneracy of the bands (write numbers to the plot).

c) [1 point] Derive Fermi momentum and Fermi energy.

d) [2 extra points] Plot Fermi contours (Fermi surfaces) for one and two conduction electrons.

3. [2 extra points] Using Green's theorem for periodic functions (see Appendix I in Ashcroft and Mermin book) prove that

$$\int dx u_{nk}^*(x) H(k) \frac{\partial u_{nk}(x)}{\partial k} = N \int_{\text{cell}} dx u_{nk}^*(x) H(k) \frac{\partial u_{nk}(x)}{\partial k} = \varepsilon_{nk} \int dx u_{nk}^*(x) \frac{\partial u_{nk}(x)}{\partial k}$$

where N is total number of cells.

4. [4 extra points] Generalize prove and calculate the general matrix element of the velocity

$$\text{operator } v_{n,n'}(k) = \frac{1}{i\hbar} \int dx \psi_{nk}^*(x)[x, H]\psi_{n'k}(x) = \frac{\partial \varepsilon_{nk}}{\partial \hbar k} \delta_{n,n'} + \frac{i}{\hbar}(\varepsilon_{nk} - \varepsilon_{n'k})A_{n,n'}(k)$$

where the off-diagonal elements are given by

$$A_{n,n'}(k) = i \int dx u_{nk}^*(x) \frac{\partial u_{n'k}(x)}{\partial k} = i \langle u_{nk} | \nabla u_{n'k} \rangle.$$

The diagonal elements $A_{n,n}(k) = i \langle u_{nk} | \nabla u_{nk} \rangle$ do not contribute to the Bloch velocity and are called Berry connectivity contributing to an anomalous velocity when Bloch electrons are subject to an external field.

5. [2 extra points] Prove Hellmann-Feynman theorem which states that

$$\frac{\partial E(\lambda)}{\partial \lambda} = \langle n(\lambda) | \frac{\partial H(\lambda)}{\partial \lambda} | n(\lambda) \rangle,$$

use the fact that the norm of the eigenfunction is unity implying that $(\partial/\partial \lambda) \langle n(\lambda) | n(\lambda) \rangle = 0$.

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