HOMEWORK SET 02

Theory of Condensed Matter
UFV/TKL1/99 lecture by Martin Gmitra
Winter Semester 2024, room KNKTFA

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. Consider free electron band structure calculations (empty lattice approximation) for monoatomic two-dimensional square lattice with lattice vectors $\mathbf{a}_1 = a\hat{\mathbf{x}}$, $\mathbf{a}_2 = a\hat{\mathbf{y}}$ along the high symmetry lines connecting the following points in the reciprocal space
$\mathbf{\Gamma} = (0, 0)$, $\mathbf{X} = \frac{2\pi}{a}\left(\frac{1}{2}, 0\right)$ 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 $\epsilon^0_{n,\mathbf{k}} = \frac{\hbar^2}{2m}(\mathbf{k} + \mathbf{G}_n)^2$, where $\mathbf{G}_n = m_1\mathbf{b}_1 + m_2\mathbf{b}_2$, and m_1 and m_2 are integers. For calculations include reciprocal lattice vectors that satisfy $|\epsilon^0_{\mathbf{k}} - \epsilon^0_{\mathbf{k}+\mathbf{G}}| < \epsilon_{\mathrm{cutoff}}$ such that reduced energy $\varepsilon_{n,\mathbf{k}}$ in relative units $\varepsilon_{n,\mathbf{k}} = \epsilon_{n,\mathbf{k}} / \left(\frac{\hbar^2}{2ma^2}\right)$ 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
$$\int dx\, u^*_{nk}(x)H(k)\frac{\partial u_{nk}(x)}{\partial k} = N\int_{\mathrm{cell}} dx\, u^*_{nk}(x)H(k)\frac{\partial u_{nk}(x)}{\partial k} = \varepsilon_{nk}\int dx\, u^*_{nk}(x)\frac{\partial u_{nk}(x)}{\partial k}$$
where N is total number of cells.

4. [*4 extra points*] Generalize prove and calculate the general matrix element of the velocity 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 $(\partial/\partial\lambda)\langle n(\lambda)|n(\lambda)\rangle = 0$.

HOMEWORK SET 02

Theory of Condensed Matter

UFV/TKL1/99 lecture by Martin Gmitra

Winter Semester 2024, room KNKTFA