PROBLEM SHEET 5

Introduction to Condensed Matter Theory

(To be submitted on Wednesday, 29.06.2015)

1(a). Schrödinger equation for Bloch wave-functions: Derive explicitly the time independent Schrödinger equation, $H\psi = \varepsilon\psi$, for the normalized Bloch waves, $\psi_{nk}(\mathbf{r}) = \frac{1}{\sqrt{V}} e^{i\mathbf{k}.r} u_{nk}(\mathbf{r})$, including a lattice-periodic potential $U(\mathbf{r}), U(\mathbf{r}+\mathbf{t}) = U(\mathbf{r})$ for $\mathbf{t} \in \beta$.
Use the Fourier series expansions,
$u_{nk}(\mathbf{r}) = \sum_{G_j \in \Re} c_{nk}(G_j) e^{iG_j.\mathbf{r}}$ and $u(\mathbf{r}) = \sum_{G_j \in \Re} U(G_j) e^{iG_j.\mathbf{r}}; U(\mathbf{G}_j = 0) = 0.$

1(b) Empty lattice approximation. Consider the derived equation in 1(a) in the asymptotic limit $U = 0$. Show that the solution is
$c_{nk}(\mathbf{G}_i) = 0$ or $\varepsilon_{nk} = E^{(0)}_{k+\mathbf{G}_i} := \frac{\hbar^2}{2m_e}(\mathbf{k}+\mathbf{G}_i)^2$,
with a normalized Bloch wave, $\psi_{nk}(\mathbf{r}) = \frac{1}{\sqrt{V}} e^{i\mathbf{k}.\mathbf{r}} e^{i\mathbf{G}_i.r}$. This procedure establishes a one-to-one correspondence between the band indices n and reciprocal lattice vectors $\mathbf{G}_i$.

1(c) 1d lattice: As a concrete example, consider a 1d chain of length L = Na(a is the lattice constant and N number of lattice sites) Imposing periodic boundary conditions, show that the wave vectors k can only take values $k = \frac{2\pi}{L}m = \frac{2\pi}{Na}m, m \in \mathbb{Z}$. Derive also the reciprocal lattice vectors as $G = \frac{2\pi}{a}n, n \in \mathbb{Z}$. Then by taking the k-vectors in the first Brillouin zone, $-\frac{\pi}{a} \leq k \leq \frac{\pi}{a}$, show that when U = 0, the energy eigen values are given by
$\varepsilon_{nk} = \frac{\hbar^2}{2m_e}(k + \frac{2\pi}{a}n)^2 = \frac{\hbar^2}{2m_e}(\frac{2\pi}{Na})^2(m+nN)^2$.
Obtain the band structure by plotting the energy eigen values in the first Brillouin zone.

2. Band structure: Tight-Binding Method Consider the follwoing Hamiltonian for an electron on a lattice

$$H = -\frac{\hbar^2}{2m}\nabla^2 + U(r), \tag{1}$$

with periodic potential $U(r) = \sum_{\mathbf{R}_i \in \beta} V(\mathbf{r} - \mathbf{R}_i \in \beta)$, the lattice vectors of the Bravais lattice β. We denote the complete basis of wannier states by $\mathscr{W} = |n,i\rangle | \mathbf{R}_i \in \beta, n = 0,1,2,...$; the wave function of $|n,i\rangle$ in position representation is the Wannier function,
$W_{n\mathbf{R}_i}(\mathbf{r}) \equiv \langle r|n,i\rangle = \sum_{\mathbf{k}\in R} B_{nk}(\mathbf{r}) e^{-ik.\mathbf{R}_i}$, where $B_{nk}(\mathbf{r})$ are the Bloch functions.
(a) Give the representation of H in the Wannier basis; i.e. write down the matrix elements of H in the Wannier basis, $\varepsilon_{nm,i} = \langle n,i|H|m,i\rangle, t_{nm,ij} = \langle n,i|H|m,j\rangle, i \neq j$. Are $\varepsilon_{nm,i}$ and $t_{nm,ij}$ diagonal in the band indices n,m? Give reason.

(b) We assume now that the Wannier function $W_{n\mathbf{R}_i}$ are strongly localized around the lattice site $\mathbf{R}_i$ ("tight-binding"), so that their overlap is non-vanishing only for the on-site and nearest neighbour matrix elements. Write down the Hamiltonian for this tight-binding assumption in terms of the parameters $E_n = \varepsilon_{n,i}$ and $t_n = t_{n,ij}$,where i,j are nearest neighbours. Use the operator notation $|n,i\rangle\langle m,j|$.

(c) Show that H is diagonalised by the transformation

$|n,i\rangle = \sum_{\mathbf{k}} e^{-i\mathbf{k}.\mathbf{R}_i}|n,\mathbf{k}\rangle$, for any $n = 0,1,2,..$

What is the meaning of the new basis states $|n,\mathbf{k}\rangle$? Obtain the dispersion (eigen energies) of the tight-binding Hamiltonian $\varepsilon_{n,\mathbf{k}}$ as

$\varepsilon_{n,\mathbf{k}} = E_n + 2t \sum_{i=1}^{d} cos(k_i a)$ for a cubic lattice in d dimensions, $d = 1,2,3,..$