Solid State Physics

Homework Ch2 No.2, Due on Mar 22nd, Friday

1. (a) From the relation between the Wannier function and the Bloch eigenstates: $f_n(\mathbf{R},\mathbf{r}) = \frac{1}{v_0}\int d^3\mathbf{k}e^{-i\mathbf{k}\cdot\mathbf{R}}\Psi_{n\mathbf{k}}(\mathbf{r})$, show that $\int f_n^*(\mathbf{R},\mathbf{r})f_{n'}(\mathbf{R}',\mathbf{r})d^3\mathbf{r} \propto \delta_{nn'}\delta_{\mathbf{R}\mathbf{R}'}$, where the orthogonality of the Bloch states $\Psi_{n\mathbf{k}}(\mathbf{r})$ can be applied.
   (b) In particular, find the proper normalization factor so that $\int f_n^*(\mathbf{R},\mathbf{r})f_{n'}(\mathbf{R}',\mathbf{r})d^3\mathbf{r} = \delta_{nn'}\delta_{\mathbf{R}\mathbf{R}'}$.

2. Problem No.2 in Chapter 10 of "Solid State Physics" by Ashcroft/Mermin, "Tight-Binding p-Bands in Cubic Crystals". Questions (a)-(d).

3. Consider a one-dimensional lattice Hamiltonian $H = -\frac{1}{2}\nabla_x^2 + U(x)$, with $U(x) = -V_0\cos^2(k_0 x)$, where the constant $V_0 > 0$ denotes the amplitude of periodic lattice potential and $k_0 = \pi/a$, with a the lattice constant. For simplicity, here we take that the mass $m = 1$ and $\hbar = 1$. Thus the recoil energy reads $E_R = \hbar^2 k_0^2/2m = k_0^2/2$. The Bloch states of the Hamiltonian can be solved by plane-wave expansion

$$\Psi_k = \sum_l c_l e^{ikx + i\frac{2l\pi}{a}x}, \tag{1}$$

   where $-k_0 \leq k < k_0$ and l sums over all integers. Note that $2l\pi/a$ is a just reciprocal lattice vector.
   (a) Find the secular equation for the coefficients c_l.
   (b) Numerically solve the Bloch energy $\mathcal{E}_k$ for the lowest band under certain value of V_0 and plot $\mathcal{E}_k$ as a function of k. This can be done by taking a cut-off l_0 for the summation of l, namely, l sums from $l = -l_0$ to $l = l_0$. For simplicity, you can take $a = 1$ so that $k_0 = \pi$ and then $E_R = \pi^2/2$. For $V_0 = 3E_R$, you can see that by taking $l_0 = 5$, the numerically solved $\mathcal{E}_k$ of the lowest band is already very close to the exact solution (that's to say, if you increase the value of the cut-off l_0 the solution almost does not change). In your calculation and plot, you can take say 30 values of k within $[-k_0, k_0]$, namely, let $k = -\pi, -14\pi/(15), ..., 14\pi/(15), \pi$.

4. **(This is not a homework problem, but you can choose to study).**–For problem No. 3, Find the Wannier function $f(x,R)$ for $R = 0$ for the lowest band. On the other hand, expand the potential $U(x)$ around $x = 0$ and keep the harmonic term, i.e. up to x^2. Solve the lowest eigen-function $\phi_0(x)$ for the harmonic potential. Then calculate the overlapping integral $\langle f(x,R)|\phi_0(x)\rangle$ and compare it with unity. Check the cases with $V_0 \gg E_R$ and $V_0 \sim E_R$.