Solid State Physics Homework

Chapter2 No.2, Due on Mar 25th 2022, Friday

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Problem1

(a) From the relation

$$f_n(\boldsymbol{R},\boldsymbol{r}) = \frac{1}{v_0}\int d^3\boldsymbol{k} e^{-i\boldsymbol{k}\cdot\boldsymbol{R}}\Psi_{n\boldsymbol{k}}(\boldsymbol{r}) \tag{1}$$

it can be proved that

$$\begin{aligned}
\int f_n^*(\boldsymbol{R},\boldsymbol{r}) f_{n'}(\boldsymbol{R'},\boldsymbol{r}) d^3\boldsymbol{r} &= \frac{1}{v_0^2}\int d^3\boldsymbol{k}\int d^3\boldsymbol{k'} e^{i\boldsymbol{k}\cdot\boldsymbol{R}-i\boldsymbol{k'}\cdot\boldsymbol{R'}}\int d^3\boldsymbol{r}\Psi_{n\boldsymbol{k}}^*(\boldsymbol{r})\Psi_{n'\boldsymbol{k'}}(\boldsymbol{r}) \\
&= \frac{1}{v_0^2}\int d^3\boldsymbol{k}\int d^3\boldsymbol{k'} e^{i\boldsymbol{k}\cdot\boldsymbol{R}-i\boldsymbol{k'}\cdot\boldsymbol{R'}}\delta_{nn'}\delta_{\boldsymbol{k}\boldsymbol{k'}} \\
&= \frac{1}{v_0^2}\frac{v_0}{N}\int d^3\boldsymbol{k} e^{i\boldsymbol{k}\cdot(\boldsymbol{R}-\boldsymbol{R'})}\delta_{nn'} \\
&= \frac{1}{N}\delta_{nn'}\delta_{\boldsymbol{R}\boldsymbol{R'}}
\end{aligned}$$

Note that the normalization of Bloch eigenstates is defaulted. So

$$\int f_n^*(\boldsymbol{R},\boldsymbol{r}) f_{n'}(\boldsymbol{R'},\boldsymbol{r}) d^3\boldsymbol{r} \propto \delta_{nn'}\delta_{\boldsymbol{R}\boldsymbol{R'}} \tag{2}$$

(b) According to the derivation of formulas in (a), **the normalization factor is $\boldsymbol{N^{-1}}$**, which is the reciprocal of the number of inequivalent $\boldsymbol{k}$.This is because $\boldsymbol{k}$ is quasi-continuous in first Brillouin zone, whose volume is v_0, so

$$\begin{aligned}
\int d^3\boldsymbol{k'} e^{i\boldsymbol{k}\cdot\boldsymbol{R}-i\boldsymbol{k'}\cdot\boldsymbol{R'}}\delta_{\boldsymbol{k}\boldsymbol{k'}} &= \frac{v_0}{N}\sum_{\boldsymbol{k'}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}-i\boldsymbol{k'}\cdot\boldsymbol{R'}}\delta_{\boldsymbol{k}\boldsymbol{k'}} \\
&= \frac{v_0}{N} e^{i\boldsymbol{k}\cdot(\boldsymbol{R}-\boldsymbol{R'})}
\end{aligned}$$

Then follow the derivation and we can get the result.

Problem2

(a) According to (10.31)

$$\beta_{xx} = -\int d\boldsymbol{r}\psi_x^*(\boldsymbol{r})\psi_x(\boldsymbol{r})\Delta U(\boldsymbol{r}) = -\int d\boldsymbol{r}x^2|\phi(\boldsymbol{r})|^2\Delta U(\boldsymbol{r}) \tag{3}$$

Obviously, the symmetry of x,y,z qualifies that

$$\beta_{xx} = \beta_{yy} = \beta_{zz} = \beta \tag{4}$$

and it can be proved that

$$\begin{aligned} 0 = \beta_{xx} - \beta_{yy} &= -\int d\boldsymbol{r}(x^2 - y^2)|\phi(\boldsymbol{r})|^2\Delta U(\boldsymbol{r}) \\ &= -\int d\boldsymbol{r}(x-y)(x+y)|\phi(\boldsymbol{r})|^2\Delta U(\boldsymbol{r}) \\ &= -\frac{1}{2}\int d\boldsymbol{r}x'y'|\phi(\boldsymbol{r})|^2\Delta U(\boldsymbol{r}) \\ &= \frac{1}{2}\beta_{x'y'} \end{aligned} \tag{5}$$

where we use a transformation $\binom{x'}{y'} = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & -1\\ 1 & 1\end{pmatrix}\binom{x}{y}$

(b) For simple cubic Bravais lattice, we only take into 6 nearest neighbors account

$$\boldsymbol{R} = a(\pm 1, 0, 0); a(0, \pm 1, 0); a(0, 0, \pm 1) \tag{6}$$

So because of the symmetry of rotation, $\widetilde{\gamma}_{ij}(\boldsymbol{k})$ should be diagonal

$$\begin{aligned} \widetilde{\gamma}_{xy}(\boldsymbol{k}) = &-\sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}}\int d\boldsymbol{r}\psi_x^*(\boldsymbol{r})\psi_y(\boldsymbol{r}-\boldsymbol{R})\Delta U(\boldsymbol{r}) \\ = &- e^{ik_xa}\int d\boldsymbol{r}xy\phi(\boldsymbol{r})\phi(\boldsymbol{r}-a\widehat{x})\Delta U(\boldsymbol{r}) \\ &- e^{-ik_xa}\int d\boldsymbol{r}xy\phi(\boldsymbol{r})\phi(\boldsymbol{r}+a\widehat{x})\Delta U(\boldsymbol{r}) \\ &- e^{ik_ya}\int d\boldsymbol{r}x(y-a)\phi(\boldsymbol{r})\phi(\boldsymbol{r}-a\widehat{y})\Delta U(\boldsymbol{r}) \\ &- e^{-ik_ya}\int d\boldsymbol{r}x(y+a)\phi(\boldsymbol{r})\phi(\boldsymbol{r}+a\widehat{y})\Delta U(\boldsymbol{r}) \\ &- e^{ik_za}\int d\boldsymbol{r}xy\phi(\boldsymbol{r})\phi(\boldsymbol{r}-a\widehat{z})\Delta U(\boldsymbol{r}) \end{aligned} \tag{7}$$

$$
\begin{aligned}
& - e^{-ik_z a} \int d\boldsymbol{r} xy\phi(\boldsymbol{r})\phi(\boldsymbol{r}+a\widehat{z})\Delta U(\boldsymbol{r}) \\
=& 0
\end{aligned}
$$

(c) Completely similar way like (b). We only take into 12 nearest neighbors account

$$
\boldsymbol{R} = \frac{a}{2}(\pm 1, \pm 1, 0); \frac{a}{2}(0, \pm 1, \pm 1); \frac{a}{2}(\pm 1, 0, \pm 1) \tag{8}
$$

$$
\widetilde{\gamma}_{xx}(\boldsymbol{k}) = -\sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}} \int d\boldsymbol{r} \psi_x^*(\boldsymbol{r})\psi_x(\boldsymbol{r}-\boldsymbol{R})\Delta U(\boldsymbol{r}) \tag{9}
$$

Use (8) and (9), we can get

$$
\begin{aligned}
\widetilde{\gamma}_{xx}(\boldsymbol{k}) =& 4\cos k_x a/2(\cos k_y a/2 + \cos k_z a/2)\gamma_2 \\
& + 4\cos k_y a/2 \cos k_z a/2(\gamma_2 + \gamma_0)
\end{aligned} \tag{10}
$$

in which

$$
\gamma_2 = -\int d\boldsymbol{r} x(x - a/2)\phi(\boldsymbol{r})\phi(\boldsymbol{r} - a/2(\widehat{x}+\widehat{y})\Delta U(\boldsymbol{r}) \tag{11}
$$

$$
\gamma_2 + \gamma_0 = -\int d\boldsymbol{r} x^2\phi(\boldsymbol{r})\phi(\boldsymbol{r} + a/2(\widehat{y}+\widehat{z})\Delta U(\boldsymbol{r}) \tag{12}
$$

so we can get the matrix element

$$
\varepsilon(\boldsymbol{k}) - E_p + \beta + \widetilde{\gamma}_{xx}(\boldsymbol{k}) = \varepsilon(\boldsymbol{k}) - \varepsilon^0(\boldsymbol{k}) + 4\gamma_0 \cos k_y a/2 \cos k_z a/2 \tag{13}
$$

The same way we can verify other elements of matrix (10.33) in Ashcroft.
(d) For $\boldsymbol{k} = 0$, all three bands are degenerate

$$
\varepsilon_0 = E_p - \beta - 12\gamma_2 - 4\gamma_0 \tag{14}
$$

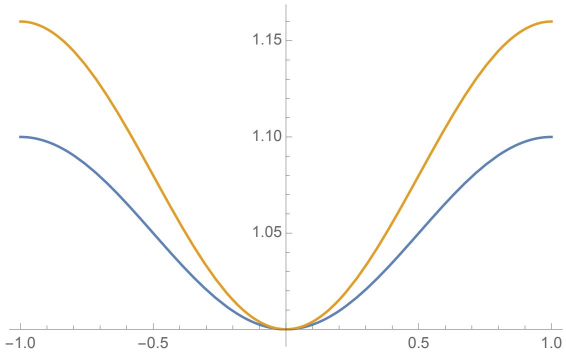
For ΓX, $\boldsymbol{k} = \pi/a(\mu, 0, 0), |\mu| \leq 1$. There are two bands

$$
\varepsilon'(\mu)/\varepsilon_0 = 1 + 8\gamma_2/\varepsilon_0(1 - \cos\pi\mu) \tag{15}
$$

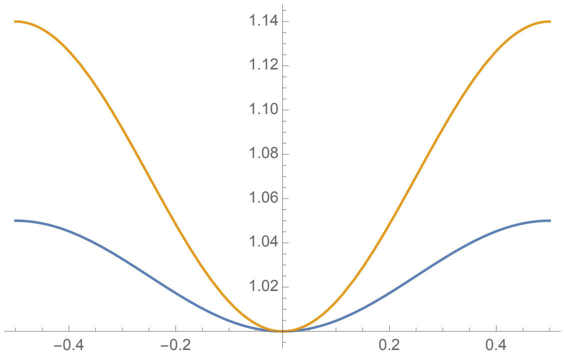
$$
\varepsilon(\mu)/\varepsilon_0 = 1 + (8\gamma_2 + 4\gamma_0)/\varepsilon_0(1 - \cos\pi\mu) \tag{16}
$$

the band in (15) is double degenerate.
For ΓL, $\boldsymbol{k} = 2\pi/a(\zeta, \zeta, \zeta), |\zeta| \leq \frac{1}{2}$. There are two bands

$$
\varepsilon'(\zeta)/\varepsilon_0 = 1 + (12\gamma_2 + 4\gamma_0 - 4\gamma_1)/\varepsilon_0 \sin^2\pi\zeta \tag{17}
$$



Schematic diagram of ΓX bands. The lower is double degenerate.



Schematic diagram of ΓL bands. The lower is double degenerate.

$$\varepsilon(\zeta)/\varepsilon_0 = 1 + (12\gamma_2 + 4\gamma_0 + 8\gamma_1)/\varepsilon_0 \sin^2 \pi\zeta \tag{18}$$

the band in (17) is double degenerate.

Problem3

(a) The Schrodinger Equation

$$[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} - V_0 \cos^2(k_0 x)]\Psi_k = \varepsilon_k \Psi_k \tag{19}$$

can be rewrite as

$$[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} - \frac{V_0}{4}(e^{2ik_0x} + e^{-2ik_0x})]\Psi_k = E_k \Psi_k \tag{20}$$

in which $E_k = \varepsilon_k + V_0/2$. Applying the plane wave method

$$\Psi_k = \sum_l c_l e^{i(k+2lk_0)x} \tag{21}$$

we can get

$$\sum_l [\frac{\hbar^2}{2m}(k+2lk_0)^2 - \frac{V_0}{4}(e^{2ik_0x} + e^{-2ik_0x})]c_l e^{i(k+2lk_0)x} = \sum_l E_k c_l e^{i(k+2lk_0)x} \tag{22}$$

If we donote $|\psi_l\rangle = c_l e^{i(k+2lk_0)x}$, then multiply (6) by $\langle\psi_{l'}|$

$$[\frac{\hbar^2}{2m}(k+2l'k_0)^2 - E_k]c_{l'}^2 - \frac{V_0}{4}(c_{l'+1} + c_{l'-1})c_{l'} = 0 \tag{23}$$

For c_l isn't equal to zero, we can write the equations in matrix form

$$H \begin{pmatrix} \cdots \\ c_{l-1} \\ c_l \\ c_{l+1} \\ \cdots \end{pmatrix} = 0, \quad \langle l|H|l'\rangle = [\frac{\hbar^2}{2m}(k+2lk_0)^2 - E_k]\delta_{ll'} - \frac{V_0}{4}(\delta_{ll'-1}+\delta_{ll'+1}) \quad (24)$$

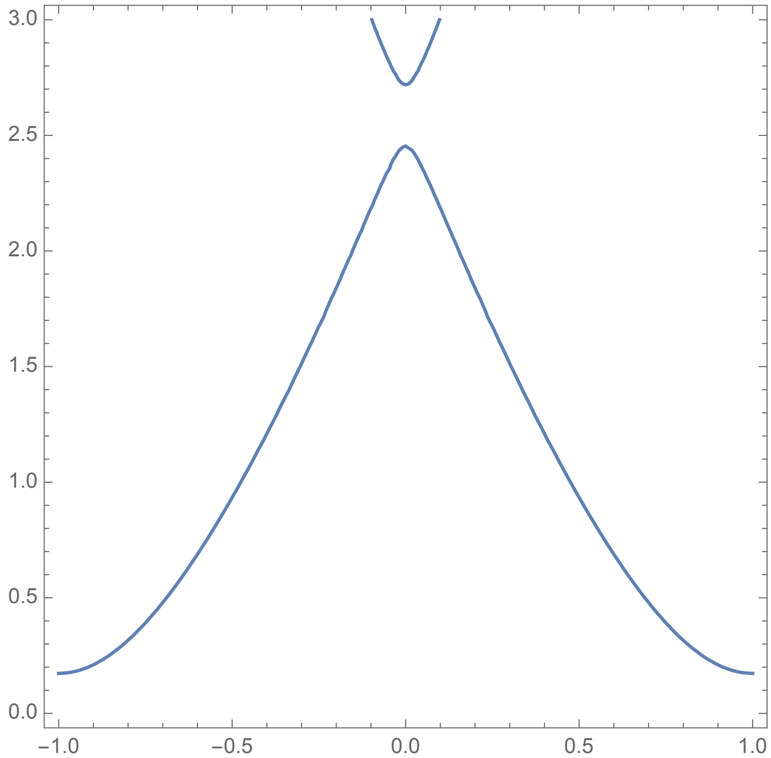
and the secular equation for the coefficients is

$$det(H) = 0 \quad (25)$$

(b) To numerically solve the Bloch energy, simplify the matrix elements

$$h_{ll'} = [(k/k_0+2l)^2 - \varepsilon_k/E_R - \frac{3}{2}]\delta_{ll'} - \frac{3}{4}(\delta_{ll'-1}+\delta_{ll'+1}) \quad (26)$$

in which $E_R = \hbar^2 k_0^2/2m, V_0 = 3E_R$.Use k/k_0 and ε_k/E_R as independent variables and solve this secular equation numerically in Mathematica by taking a cut-off $l_0 = 5$ in the summation, the result of energy band figure is below



The lowest band: the abscissa is k/k_0, the ordinate is ε_k/E_R

We can see that in the lowest band, $\varepsilon_{max} \approx 2.5E_R, \varepsilon_{min} \approx 0.2E_R$. And it's easy to verify that a bigger l_0 almost doesn't change the result.