A simple semiconductor and the formation of excitons

Band Structure

We consider the following Hamiltonian:

$$H = -t \sum_{j=1}^{N} \left(c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j \right) + v \sum_{j=1}^{N} (-1)^j n_j \ . \tag{1}$$

(a) Notice that $(-1)^j = e^{i\pi j}$, so by taking the Fourier transformation $c_j = \frac{1}{\sqrt{N}} \sum_{k\in(-\pi,\pi]} e^{-ikj} c_k$ where N is the total number of sites, we get

$$\begin{aligned} H &= -2t \sum_k \cos(k) c_k^\dagger c_k + \frac{v}{N} \sum_{k,k'} \underbrace{\sum_j e^{i(k-k'+\pi)j}}_{\Rightarrow N\delta_{k-k'+\pi}} c_k^\dagger c_{k'} \\ &= -2t \sum_{k\in(-\pi,\pi]} \cos(k) c_k^\dagger c_k + v \sum_{k\in(-\pi,\pi]} c_k^\dagger c_{k+\pi} \\ &= -2t \sum_{\#k} \cos(k) c_k^\dagger c_k + 2t \sum_{\#k} \cos(k) c_{k+\pi}^\dagger c_{k+\pi} + v \sum_{\#k} (c_k^\dagger c_{k+\pi} + \text{h.c.}) \\ &= \sum_{\#k} \bar{c}_k^\dagger H(k) \bar{c}_k \ , \end{aligned} \tag{2}$$

where

$$H(k) = \begin{pmatrix} -2t\cos(k) & v \\ v & 2t\cos(k) \end{pmatrix} \tag{3}$$

(b) According to your knowledge of linear algebra, choose the technique you like (e.g. multiply directly $UHU^\dagger$ to get the result or solve the eigenvalue problem first) and you should find that

$$u_k = \sin(\theta),\ v_k = \cos(\theta) \tag{4}$$

where the parameter θ is determined by

$$\tan(2\theta) = -\frac{v}{2t\cos(k)}. \tag{5}$$

The band gap Δ is calculated from the two eigenvalues $E_\pm(k)$ of $H(k)$:

$$E_\pm(k) = \pm\sqrt{v^2 + 4t^2\cos^2(k)} \equiv \pm E_k. \tag{6}$$

from which we conclude that $\Delta = 2|v|$.

(c) It is straightforward to see that

$$
\begin{aligned}
H = \sum_{\# k} \bar{c}_k^\dagger H(k) \bar{c}_k &= \sum_{\# k} \bar{c}_k^\dagger U^\dagger \underbrace{U H(k) U^\dagger}_{\begin{pmatrix} E_-(k) & 0 \\ 0 & E_+(k) \end{pmatrix}} U \bar{c}_k \\
&= \sum_{\# k} \left[-E_k a_k^\dagger a_k + E_k b_k^\dagger b_k \right]
\end{aligned} \tag{7}
$$

(d) At half-filling, the system reaches its lowest energy when the lower band is fully occupied while the upper band has no fermion, i.e.

$$
|\Omega\rangle = \prod_{\# k} a_k^\dagger |0\rangle \tag{8}
$$

Wigner crystallization

(a) Calculate the charge density ρ and the electric field $\mathbf{E}_p(r)$.

- charge density ρ:

$$
\rho = \frac{e}{V_s} = \frac{e}{\frac{4}{3}\pi R^3} = \frac{e}{\frac{4}{3}\pi r_s^3 a_B^3} = \frac{3e}{4\pi r_s^3 a_B^3} \tag{9}
$$

- Electric field $\mathbf{E}_p(r)$
  - Within the sphere:

$$
\begin{aligned}
4\pi Q &= \oint \mathbf{E} \cdot \mathrm{d}\mathbf{A} \\
\Rightarrow 4\pi \times \rho \times \frac{4}{3}\pi r^3 &= E_p(r) \times 4\pi r^2 \\
\Rightarrow E_p(r) &= \frac{er}{r_s^3 a_B^3}
\end{aligned} \tag{10}
$$

  - Outside the sphere:

$$
\begin{aligned}
4\pi e &= E_p(r) \times 4\pi r^2 \\
\Rightarrow E_p(r) &= \frac{e}{r^2}.
\end{aligned} \tag{11}
$$

In the equations (10) and (11), we used the fact that the electric field is isotropic and the area of a sphere of radius r is $4\pi r^2$.

(b) Compute the potential $V_p(r)$ and make it continuos.

- Inside the sphere:

$$
V_p(r) = -\int \frac{er}{r_s^3 a_B^3} \mathrm{d}r = -\frac{er^2}{2 r_s^3 a_B^3} + C_1 \tag{12}
$$

- Outside the sphere:

$$
V_p(r) = -\int \frac{e}{r^2} \mathrm{d}r = \frac{e}{r} + C_2 \tag{13}
$$

Now if we choose the convention that $V_p(+\infty) = 0$ and require $V_p(r)$ is continous at the sphere, then we can get

$$
V_p(r) = \begin{cases} \frac{e}{2 r_s a_B} \left(3 - \frac{r^2}{(r_s a_B)^2} \right), & r \le r_s a_B \\ \frac{e}{r}, & r > r_s a_B\,. \end{cases} \tag{14}
$$

(c) Compute the self-energy of the charged background.

$$
\begin{aligned}
U_{pp} &= \frac{1}{2}\int_{\text{within sphere}} \mathrm{d}^3\mathbf{r}\rho(\mathbf{r})V_p(\mathbf{r}) \\
&= 2\pi\int_0^{r_s a_B} \mathrm{d}r r^2 \frac{3e}{4\pi r_s^3 a_B^3} \times \frac{e}{2r_s a_B}\left(3 - \frac{r^2}{(r_s a_B)^2}\right) \\
&= \frac{3e^2}{5r_s a_B}
\end{aligned}
\tag{15}
$$

(d) Compute the potential energy between the background and the electron.

$$
\begin{aligned}
U_{ep} &= \int_{\text{within sphere}} \mathrm{d}^3\mathbf{r}\rho(\mathbf{r})V_e(\mathbf{r}) \\
&= 4\pi\int_0^{r_s a_B} \mathrm{d}r r^2 \frac{3e}{4\pi r_s^3 a_B^3} \times \frac{-e}{r} \\
&= -\frac{3e^2}{2r_s a_B} = -eV_p(r=0)
\end{aligned}
\tag{16}
$$

(e) Kinetic energy and the total energy for an electron in the Wigner crystal.

According to the basic quantum machanics, the wave vector $k = \frac{2\pi}{\lambda}$ and the momentum $p = \hbar k$. So for the electron, its kinetic energy is

$$
E_k = \frac{\hbar^2 k^2}{2m} = \frac{2\pi^2\hbar^2}{m\lambda^2} \approx \frac{2\pi^2\hbar^2}{m(r_s a_B)^2}. \tag{17}
$$

Then the total energy is

$$
E_{\text{Wigner}} = E_k + U_{pp} + U_{ep} = \frac{2\pi^2\hbar^2}{m_e(r_s a_B)^2} - \frac{9e^2}{10r_s a_B} \tag{18}
$$

(f) Since $n(E) = \frac{3}{2\varepsilon_F^{3/2}}E^{1/2}$, we can calculate the average energy per electron:

$$
\begin{aligned}
E_{\text{Fermi}} &= \int_0^{\varepsilon_F} n(E)E\mathrm{d}E \\
&= \frac{3}{2\varepsilon_F^{3/2}}\int_0^{\varepsilon_F} E^{3/2}\mathrm{d}E. \\
&= \frac{3}{5}\varepsilon_F
\end{aligned}
\tag{19}
$$

Then let's see when the energy of electron in Wigner crystall becomes smaller than that in Fermi sea. Notice that

$$
\begin{aligned}
E_{\text{Wigner}} - E_{\text{Fermi}} &= \frac{2\pi^2\hbar^2}{m_e(r_s a_B)^2} - \frac{9e^2}{10r_s a_B} - \frac{3}{5}\varepsilon_F \\
&= \frac{me^4}{\hbar^2 r_s}\left(\frac{2\pi^2 - \frac{3}{10}\alpha^2}{r_s} - \frac{9}{10}\right)
\end{aligned}
\tag{20}
$$

where $\alpha = (\frac{9\pi}{4})^{1/3}$. So when $r_s \gtrapprox 20$, $E_{\text{Wigner}} - E_{\text{Fermi}} < 0$, which means there Wigner crystal has a lower energy.