Condensed Matter Physic

Electron in periodic field

Istvan Groma

ELTE

December 27, 2018

Electron periodic potential

$$\left[-\frac{\hbar^2}{2m_e}\nabla^2+V(\underline{r})\right]\psi=E\psi$$

Periodic potential

$$V(\underline{r}+\underline{R}_n)=V(\underline{r})$$

We consider

$$\psi(\underline{r}+\underline{R}_n)\neq\psi(\underline{r})$$

If

$$\psi(\underline{r}+\underline{R}_n)\quad=e^{i\underline{k}\underline{R}_n}\psi(\underline{r})$$

The mean value

$$\int\psi^*(\underline{r})A(\underline{r}+\underline{R}_n)\psi(\underline{r})dV=\int\psi^*(\underline{r}+\underline{R}_n)A(\underline{r}+\underline{R}_n)\psi(\underline{r}+\underline{R}_n)dV$$

Electron periodic potential

So

$$< A(\underline{R}_n) >=< A >$$

Translation operator

$$T(\underline{R}_n)\psi^*(\underline{r}) = \psi(\underline{r} + \underline{R}_n)$$

$$T(\underline{R}_n)\left\{H(\underline{r})\psi(\underline{r})\right\} = H(\underline{r} + \underline{R}_n)\psi(\underline{r} + \underline{R}_n) = H(\underline{r})T(\underline{R}_n)\psi(\underline{r})$$

So

$$[T(\underline{R}_n)H(\underline{r})] = 0$$

It has common equine states!

Translation operator

$$T(\underline{R})\phi(\underline{r}) = C(\underline{R})\phi(\underline{r})$$

Since

$$T(\underline{R}_1)T(\underline{R}_2) = T(\underline{R}_2)T(\underline{R}_1)$$

The different translations have common equine states
Moreover

$$T(\underline{R}_1)T(\underline{R}_2) = T(\underline{R}_1 + \underline{R}_2)$$

So

$$C(\underline{R}_1)C(\underline{R}_2) = C(\underline{R}_1 + \underline{R}_2)$$

Leading to

$$C(\underline{R}_n) = e^{i\underline{k}\underline{R}_n}$$

$\underline{k}$ is in the Brilluen zone!

Bloch equation

equine states

$$\psi(\underline{r}) = e^{i\underline{kr}}u(\underline{r})$$

where

$$u(\underline{r}) = u(\underline{r} + \underline{R}_n)$$

is a periodic function.

$$\bigtriangledown\left\{e^{i\underline{kr}}u(\underline{r})\right\} = \left\{i\underline{k}u(\underline{r})e^{i\underline{kr}} + e^{i\underline{kr}}\bigtriangledown u(\underline{r})\right\} = e^{i\underline{kr}}(i\underline{k} + \bigtriangledown)u(\underline{r})$$

Bloch equation

$$\left[-\frac{\hbar^2}{2m_e}(i\underline{k} + \bigtriangledown)^2 + V(\underline{r})\right]u_{\underline{k},n}(\underline{r}) = E_n(\underline{k})u_{\underline{k},n}(\underline{r})$$

Quantum states $\longleftrightarrow$ $u_{\underline{k},n}(\underline{r}) = u_{\underline{k},n}(\underline{r} + \underline{R}_l)$
The Bloch functions corresponding to different $\underline{k}$ values are orthogonal

$$\int \psi^*_{\underline{k}_1}(\underline{r})\psi_{\underline{k}_2}(\underline{r})dV = \int \psi^*_{\underline{k}_1}(\underline{r} + \underline{R}_l)\psi_{\underline{k}_2}(\underline{r} + \underline{R}_l)dV = e^{i(\underline{k}_1 - \underline{k}_2)\underline{R}_l}\int \psi^*_{\underline{k}_1}(\underline{r})\psi_{\underline{k}_2}(\underline{r})dV$$

Periodic boundary conditions

$$\psi(\underline{r} + N_i \underline{a}_i) = \psi(\underline{r}) \qquad i = 1, 2, 3$$

There is no phase shift!

$$\psi(\underline{r}) = e^{i\underline{kr}} u(\underline{r})$$

Let us take

$$\underline{k} = k_1 \underline{b}_1 + k_2 \underline{b}_2 + k_3 \underline{b}_3$$

Since

$$\underline{k} N_i \underline{b}_i = 2\pi k_i$$

one obtains

$$k_i = \frac{n_i}{N_i} \qquad i = 1, 2, 3$$

$$|\triangle \underline{k}| = \frac{(\underline{b}_1 \times \underline{b}_2)\underline{b}_3}{N_1 N_2 N_3} = \frac{(2\pi)^3}{v_c N}$$

Quasi free electron

Week potential

$$-\frac{\hbar^2}{2m_e}(i\underline{k}+\bigtriangledown)^2 u_{\underline{k}}(\underline{r}) = E(\underline{k})u_{\underline{k}}(\underline{r})$$
$$u(\underline{r}) = u(\underline{r}+\underline{R}_l)$$

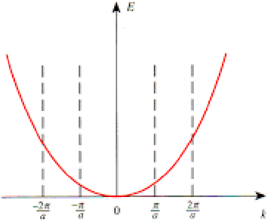
The solution is

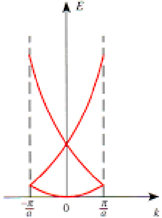
$$u(\underline{r}) = e^{i\underline{G}_l\underline{r}}$$

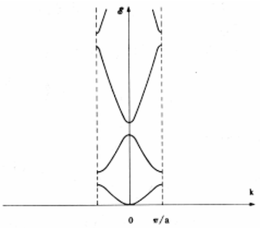
Energy

$$E_l(\underline{k}) = \frac{\hbar^2}{2m_e}(\underline{k}+\underline{G}_l)^2$$

Quasi free electron







Many electron systems

If we neglect electron-electron interaction we can take

$$\psi(\underline{r}_1, \underline{r}_2, ...\underline{r}_N) = \psi_1(\underline{r}_1)\psi_2(\underline{r}_2)...\psi_N(\underline{r}_N)$$

Pauli principle

$$\psi(\underline{r}_1, \underline{r}_2, ...\underline{r}_i...\underline{r}_j...\underline{r}_N) = -\psi(\underline{r}_1, \underline{r}_2, ...\underline{r}_j...\underline{r}_i...\underline{r}_N)$$

Slater determinant

$$\psi(\underline{r}_1, \underline{r}_2, ...\underline{r}_N) = \begin{vmatrix} \psi_1(\underline{r}_1), & \psi_1(\underline{r}_2) & ... & \psi_1(\underline{r}_N) \\ \psi_2(\underline{r}_1), & \psi_2(\underline{r}_2) & ... & \psi_2(\underline{r}_N) \\ ... & ... & ... & ... \\ ... & ... & ... & ... \\ \psi_N(\underline{r}_1), & \psi_N(\underline{r}_2) & ... & \psi_N(\underline{r}_N) \end{vmatrix}$$

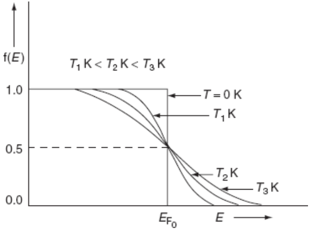
So if $i \neq j$ one cannot have that

$$\psi_i(\underline{r}) = \psi_j(\underline{r})$$

So 2 electrons cannot have in the same state
If spin does not matter 2 electrons can have the same energy.

Fermi-Dirac distribution

$$f_0(E_n(\underline{k})) = \frac{1}{e^{\frac{E_n(\underline{k})-\mu(T)}{k_B T}} + 1}$$



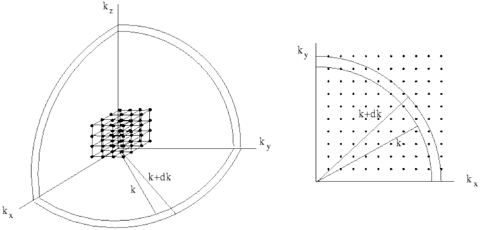
where $\mu(T)$ is the chemical potential determined by

$$2 \sum_{\underline{k}} \sum_{n} f_0(E_n(\underline{k})) = N$$

Várható érték

$$\sum_{\underline{k}} \to \frac{V}{(2\pi)^3}\int d^3k$$

Density of states



$$\triangle N = \rho(E) \triangle E$$

From this

$$\sum_n \sum_{\underline{k}} g(E_n(\underline{k})) = \sum_n \frac{V}{(2\pi)^3}\int g(E_n(\underline{k}))d^3k = V\int g(E)\rho(E)dE$$

Density of states, quasi free electron

$$E = \frac{\hbar^2}{2m_e}k^2 \qquad \longrightarrow \qquad k = \sqrt{\frac{2m_e}{\hbar^2}E}$$

The volume is

$$dN = 4\pi k^2 dk$$

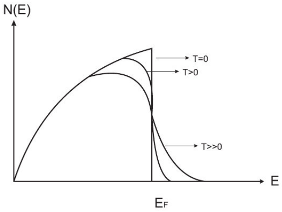
From this

$$\rho(E) = 2\frac{4\pi}{(2\pi)^3}\frac{2m_e}{\hbar^2}E \;\; \frac{1}{2}\frac{\sqrt{\frac{2m_e}{\hbar^2}}}{\sqrt{E}}$$

So

$$\rho(E) = \frac{1}{2\pi^2}\left(\frac{2m_e}{\hbar^2}\right)^{3/2}\sqrt{E}$$

Fermi energy, quasi free elektron



$$N = V \int_0^{E_f} \rho(E) dE$$

From this

$$\frac{N}{V} = n_e = \frac{2}{3} \frac{1}{2\pi^2} \left(\frac{2m_e}{\hbar^2} \right)^{3/2} E_f^{3/2}$$

$$n_e = \frac{1}{3\pi^2} \left(\frac{2m_e}{\hbar^2} E_f \right)^{3/2}$$

Fermi energy, quasi free electron

$$E_f = \frac{\hbar^2}{2m_e}\left(3\pi^2 n_e\right)^{2/3}$$

Finite temperature

$$n_e = \int_0^\infty \frac{\sqrt{E}}{e^{\frac{E-\mu}{k_B T}}+1}\frac{1}{2\pi^2}\left(\frac{2m_e}{\hbar^2}\right)^{3/2} dE$$

$$n_e = 2\left(\frac{m_e k_B T}{2\pi\hbar^2}\right)^{3/2} F_{1/2}\left(\frac{\mu}{k_B T}\right)$$

where

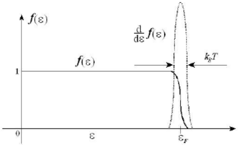
$$F_{1/2}(x) = \frac{2}{\sqrt{\pi}}\int_0^\infty \frac{y^{1/2}}{exp(y-x)+1} dy \approx \frac{4}{3\sqrt{\pi}} x^{3/2}\left[1+\frac{\pi^2}{8}\frac{1}{x^2}\right]$$

$$\mu(T) = E_f\left[1-\frac{\pi^2}{12}\left(\frac{T}{T_f}\right)^2\right], \qquad k_B T_f = E_f$$

Sommerfeld expansion

$$\int_0^\infty g(E) f_0(E) dE = \int_0^\infty G(E) \left(-\frac{df_0}{dE} \right) dE$$

where $G' = g$, and $G(0) = 0$



$$G(E) \approx G(\mu) + (E - \mu) G'(\mu) + \frac{1}{2}(E - \mu)^2 G''(\mu) + ...$$

The leading term is

$$< g > \approx G(\mu) + \frac{\pi^2}{6} (k_B T)^2 G''(\mu) + ...$$

$$< g > \approx \int_0^\mu g(E) dE + \frac{\pi^2}{6} (k_B T)^2 \left. \frac{dg}{dE} \right|_\mu + ...$$

Energy of an electron

$$\frac{< E >}{V} = \int_0^{\mu} E\rho(E)dE + \frac{\pi^2}{6}(k_B T)^2 \left.\frac{d}{dE}(E\rho(E))\right|_{\mu}$$

Since

$$\rho(E) = \frac{1}{2\pi^2}\left(\frac{2m_e}{\hbar^2}\right)^{3/2}\sqrt{E}$$

one gets

$$\frac{< E >}{V} = \frac{1}{5\pi^2}\left(\frac{2m_e}{\hbar^2}\right)^{3/2}\mu^{5/2} + \frac{1}{8}\left(\frac{2m_e}{\hbar^2}\right)^{3/2}(k_B T)^2\mu^{1/2}$$

Heat capacity is

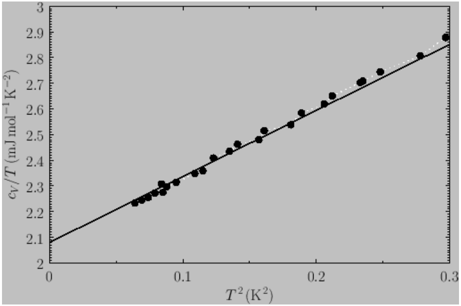
$$c_V^e(T) = \gamma T$$

Teljes

$$c_V(T) = c_V^e(T) + c_V^l(T) = \gamma T + AT^3$$

Energy of an electron

$$\frac{c_V(T)}{T} == \gamma + AT^2$$

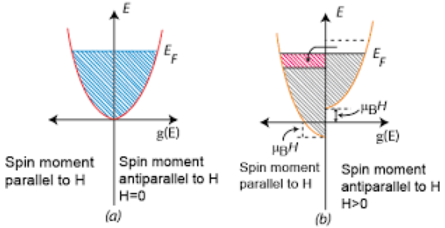


Energia mágneses térben

$$\triangle E = \pm \frac{1}{2} g_e \mu_B B$$

Ekkor az állapotsűrűség

$$\rho_\downarrow(E) = \frac{1}{2}\rho(E + \frac{1}{2} g_e \mu_B B)$$
$$\rho_\uparrow(E) = \frac{1}{2}\rho(E - \frac{1}{2} g_e \mu_B B)$$



Pauli szuszceptibilitás

Kis mágneses tér esetén

$$\rho_\downarrow(E) = \frac{1}{2}\rho(E + \frac{1}{2}g_e\mu_B B) \approx \frac{1}{2}\rho(E) + \frac{1}{4}g_e\mu_B B\frac{d\rho(E)}{dE}$$
$$\rho_\uparrow(E) = \frac{1}{2}\rho(E - \frac{1}{2}g_e\mu_B B) \approx \frac{1}{2}\rho(E) - \frac{1}{4}g_e\mu_B B\frac{d\rho(E)}{dE}$$

Innen a betöltött állapotok száma a két irányben

$$\begin{aligned} n_{\downarrow\uparrow} &= \int \rho_{\downarrow\uparrow}(E) f_0(E) dE \\ &= \frac{1}{2}\int \rho(E) f_0(E) dE \pm \frac{1}{4}g_e\mu_B B \int \frac{d\rho(E)}{dE} f_0(E) dE \end{aligned}$$

Mivel

$$n = n_\downarrow + n_\uparrow = \int \rho(E) f_0(E) dE$$

A kémiai potenciál nem változik

Pauli szuszceptibilitás

A mágnesezettség

$$M = \frac{1}{2} g_e \mu_B (n_\downarrow - n_\uparrow) = \frac{1}{4} g_e^2 \mu_B^2 B \int \frac{d\rho(E)}{dE} f_0(E) dE$$

Innen

$$M = \frac{1}{4} g_e^2 \mu_B^2 B \int \rho(E) \left(-\frac{df_0(E)}{dE} \right) dE = \frac{1}{4} g_e^2 \mu_B^2 B \rho(E_f)$$

Tehát

$$\chi_P = \frac{1}{4} g_e^2 \mu_B^2 \mu_0 \rho(E_f)$$

Amely

$$\chi_P = \frac{3}{8} \mu_0 \frac{g_e^2 n_e \mu_B^2}{E_f}$$