Disclaimer

The solution at hand was written in the course of the respective class at the University of Bonn. If not stated differently on top of the first page or the following website, the solution was prepared and handed in solely by me, Marvin Zanke. Anything in a different color than the ball pen blue is usually a correction that I or a tutor made. For more information and all my material, check:
https://www.physics-and-stuff.com/

I raise no claim to correctness and completeness of the given solutions! This equally applies to the corrections mentioned above.

31.05.'16

Condensed Matter Exercise 3

2.a. Quantum well : $V(x) = \begin{cases} V_0 & \text{for } -L/2 \le x \le L/2 \\ \infty & \text{else} \end{cases}$

S.E yields: $-\frac{\hbar^2}{2m}\vec{\nabla}^2\psi(\vec r) + V(x)\psi(\vec r) = E\psi(\vec r)$

Ansatz; Sep. of variables? $\Phi_1\Phi_2\Phi_3 \to A+B+C = E = \text{const}$

with Ansatz: $\psi(\vec r) = \phi_n(x)\, e^{i(k_y y + k_z z)} = \phi_n(x)\, e^{i\vec k_\parallel \vec r}$

$\vec{k}_\parallel$? parallel to the potential barriers

$$\Rightarrow -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\phi_n(x)e^{i\vec k_\parallel \vec r} + V(x)\phi_n(x)e^{i\vec k_\parallel \vec r} - E\phi_n(x)e^{i\vec k_\parallel\cdot\vec r}$$

Seperation of variables

$V(y)=V(z)=0$ constant potential in y and z → shift

$$\Rightarrow -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)e^{i\vec k_\parallel \vec r} = E_\parallel e^{i\vec k_\parallel \vec r} \qquad (1)$$

and $$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\phi_n(x) + V(x)\phi_n(x) = E_x\phi_n(x) \qquad (2)$$

Ansatz for this seperation? No wavefunction split in product? e-vec is split in product!

(1) $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2}e^{ik_y y} = E_y e^{ik_y y}$ | $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2}e^{ik_z z} = E_z e^{ik_z z}$

$\Leftrightarrow \frac{\hbar^2}{2m}k_y^2 = E_y$ | $\Leftrightarrow \frac{\hbar^2}{2m}k_z^2 = E_z$

$$\Rightarrow E_\parallel = \frac{\hbar^2}{2m}\vec{k}_\parallel^2$$

(2) $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\phi_n(x) = (E_x - V(x))\,\phi_n(x)$

$\phi_n(x) = 0$ for $x < -L/2,\ x > L/2$

$V(x) = V_0$ for $-L/2 \le x \le L/2$

$$\Rightarrow \frac{\partial^2}{\partial x^2}\phi_n(x) = -\frac{2m(E_x - V_0)}{\hbar^2}\phi_n(x)$$

Ansatz: $\phi_n(x) = A e^{\lambda x} \Rightarrow \phi_n''(x) = \lambda^2 e^{\lambda x}$

$$\lambda^2 = -\frac{2m(E_x-V_0)}{\hbar^2} \Leftrightarrow \lambda = \pm i\underbrace{\frac{\sqrt{2m(E_x-V_0)}}{\hbar}}_{=k_x}$$

$$\Rightarrow \phi_n(x) = A e^{ik_x x} + B e^{-ik_x x}$$

boundary conditions : $\phi_n(-L/2) = \phi_n(L/2) = 0$

$\phi_n(-L/2) = A e^{-ik_x L/2} + B e^{ik_x L/2} = 0$

$\Leftrightarrow A = -B e^{ik_x L}$

$\Phi_n(L/2) = A e^{ik_x L/2} + B e^{-ik_x L/2} = 0$

$\Leftrightarrow \quad A + B e^{-ik_x L} = 0$

$\Leftrightarrow \quad B\left(e^{-ik_x L} - e^{ik_x L}\right) = 0$

$\Leftrightarrow \quad -B \cdot 2i \sin(k_x L) = 0$

$\Leftrightarrow \quad \sin(k_x L) = 0 \quad \Leftrightarrow \quad k_x L = n\pi \Leftrightarrow k_x = \frac{n\pi}{L} = \frac{\sqrt{2m(E_x - V_0)}}{\hbar}$

$\Leftrightarrow \quad E_x' = \frac{\hbar^2 n^2 \pi^2}{2mL^2} = E_x - V_0$

$\Rightarrow$ Total Energy yields: $E(\vec{k}_n, n) = \frac{\hbar^2}{2m}\vec{k}_n^2 + \frac{\hbar^2 n^2 \pi^2}{2mL^2}$

Volume of k-space: $\Delta_k = \frac{\pi^2}{L^2}$

2D Sub band: minimum $E(0,n)$ for $\vec{k}_n = 0$

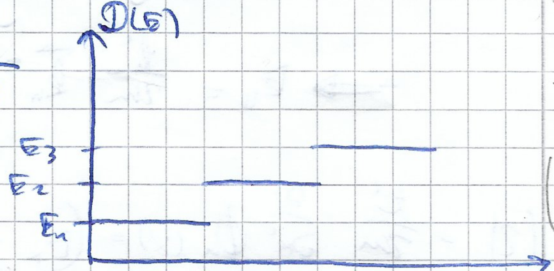
$dN = \frac{2}{4} 2\pi k \frac{dk}{\frac{\pi^2}{L^2}} = \frac{L^2}{\pi} k\, dk \quad , \quad k \left(= \frac{n\pi}{L}\right) = \frac{\sqrt{2mE}}{\hbar}$

$[L^2 = L_x L_y]$

$= \frac{L^2}{\pi} \frac{\sqrt{2mE}}{\hbar} \frac{dk}{dE} dE = \frac{L^2}{\pi} \frac{\sqrt{2mE}}{\hbar} \frac{1}{2} \sqrt{\frac{2m}{\hbar^2}} \frac{1}{\sqrt{E}} dE$

$= \frac{L^2}{\pi} \frac{1}{\hbar^2} \frac{1}{2} \sqrt{4m^2 E} \cdot \frac{1}{\sqrt{E}} dE = \frac{L^2 m}{\hbar^2 \pi} dE$

$\frac{dN}{V} = \frac{m}{\hbar^2 \pi} dE \quad \Rightarrow \quad D(E) = \frac{m}{\hbar^2 \pi}$



free + bound states?

bound in ⊥ direction, free in 2dim.

Why E_x'! not E_x'! total energy

Subband minimum? fixed n (new plane with energy levels) and first energy level of that

$\Delta_k = \frac{\pi^2}{L^2}$? k-volume

(L^2) $V = L_y L_z$ Volume

E of confined area in 2D

b) Quantum Wire 1D:

$$V(x,y) = \begin{cases} V_0 & \text{for } -L/2 \leq x \leq L/2 \text{ and } -L/2 \leq y \leq L/2 \\ 0 & \text{else} \end{cases}$$

Calculation analogous to a) but $\Delta k = \frac{\pi}{L}$ (k-space volume)

$$E = \frac{\hbar^2 \pi^2}{2mL^2}(n_x^2 + n_y^2) + \frac{\hbar^2 k_z^2}{2m}$$

$L \to L_y$ and L_z

2 for spin, but $\frac{1}{2}$, positive and negative numbers have to be taken out of calculation

Spin

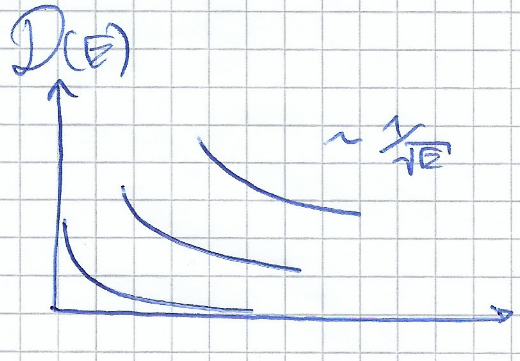
$$dN = \frac{2}{2} \frac{dk}{\pi/L} = \frac{L}{\pi} dk \quad \text{with } k = \sqrt{\frac{2mE}{\hbar^2}}$$

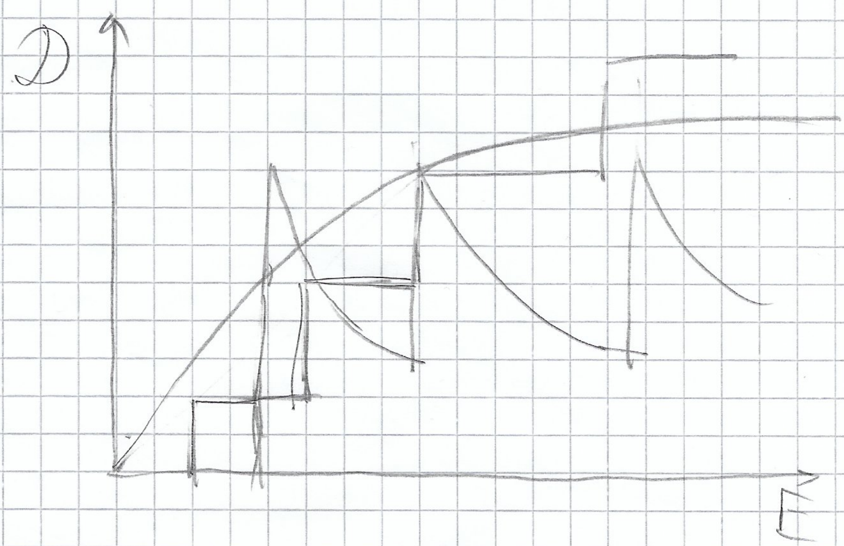
$$= \frac{L}{\pi} \frac{dk}{dE} dE = \frac{L}{\pi} \frac{1}{\hbar} \sqrt{2m} \cdot \frac{1}{2} \frac{1}{\sqrt{E}} dE$$

$$= \frac{L}{\pi} \frac{1}{\hbar} \sqrt{\frac{m}{2E}} dE.$$

$$\Rightarrow \frac{dN}{V} = \frac{1}{\pi\hbar} \sqrt{\frac{m}{2E}} dE$$

$$\rightarrow D(E) = \frac{1}{\pi\hbar} \sqrt{\frac{m}{2E}}$$





4. Chemical potential in lower dimensions

Where from $D(E)$, $f(E)$?

$$n = \int_0^\infty D(E)\, f(E)\, dE \quad \text{with} \quad D(E) = \frac{m}{\pi \hbar^2} \text{ in 2D}$$

$$f(E) = \frac{1}{e^{\frac{E-\mu}{k_B T}} + 1} \quad \text{Fermi-Distribution}$$

$$n = \frac{m}{\pi \hbar^2} \int_0^\infty \frac{1}{e^{\frac{E-\mu}{k_B T}} + 1}\, dE = \frac{m}{\pi \hbar^2} \int_0^\infty \frac{e^{-\frac{(E-\mu)}{k_B T}}}{1 + e^{-\frac{(E-\mu)}{k_B T}}}\, dE$$

$$= -\frac{m k_B T}{\pi \hbar^2} \left\{ \ln\left(1 + e^{-\frac{(E-\mu)}{k_B T}}\right) \right\} \Big|_0^\infty$$

$$= + \frac{m k_B T}{\pi \hbar^2} \ln\left(1 + e^{\frac{\mu}{k_B T}}\right)$$

Solving for μ yields:

$$\frac{n \pi \hbar^2}{m k_B T} = \ln\left(1 + e^{\mu / k_B T}\right)$$

$$\Leftrightarrow \quad e^{\mu / k_B T} = e^{\frac{\hbar^2 n \pi}{m k_B T}} - 1$$

$$\Leftrightarrow \quad \mu = k_B T \ln\left(e^{\frac{\hbar^2 n \pi}{m k_B T}} - 1\right), \quad \hbar = \frac{h}{2\pi}$$

5. Fermi-Energy and Fermi-Temperature

$$E_F = \frac{\hbar^2}{2m} (3 \pi^2 n)^{2/3}, \quad T_F = \frac{E_F}{k_B}$$

a) $\rho = \frac{m}{V} = \frac{N \cdot m_{Au}}{V} \Leftrightarrow n = \frac{N}{V} = \frac{\rho}{m_{Au}}$

$$n = \frac{19\, g/cm^3}{197u} = \frac{19 \cdot 10^{-3} \frac{kg}{cm^3}}{3{,}271 \cdot 10^{-25} kg} = 5{,}81 \cdot 10^{22} \frac{1}{cm^3}$$

$$= 5{,}81 \cdot 10^{28} \frac{1}{m^3}$$

$\Rightarrow E_F =$

$8{,}764 \cdot 10^{-19} J = 5{,}5 eV$

$T_F =$ $63507{,}266\, K$

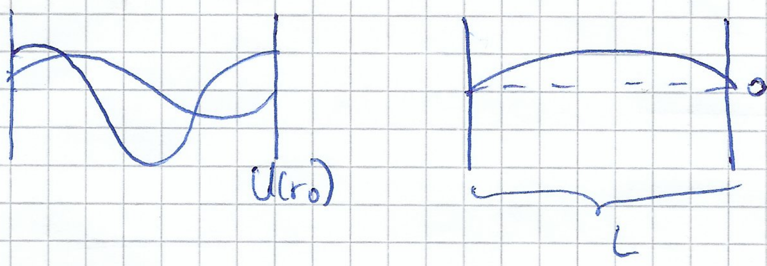
5) $n = \frac{\rho}{m_{He_3}} = \frac{0{,}081 \, g/cm^3}{3u} = 1{,}62 \cdot 10^{22} \, \frac{1}{cm^3} = 1{,}62 \cdot 10^{28} \, \frac{1}{m^3}$

$\Rightarrow \quad E_F = 4{,}2 \cdot 10^{-4} \, eV$

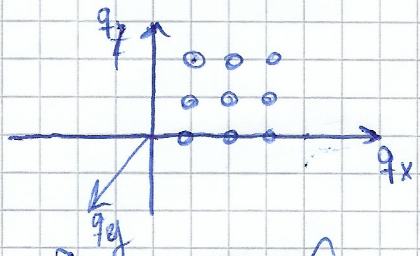
$T_F = 4{,}88 \, K$

Spin?

1. Density of States of Phonons



$V_c = L^3$



$$q_i = \frac{\pi}{L}, \frac{2\pi}{L}, \frac{3\pi}{L}, \dots$$

only positive

$$D(\omega) = \frac{V_c}{\pi^3}\int_{S^+(\omega)} \frac{dS_\omega}{|\nabla_q \omega(q)|} = \frac{1}{8}\frac{V_c}{\pi^3}\int_{S(\omega)} \frac{dS_\omega}{|\nabla_q \omega(q)|}$$

$$\frac{V_c}{(2\pi)^3}\int_{S(\omega)} \frac{dS_\omega}{|\nabla_q \omega(q)|}$$

Same result as for periodic boundary conditions

$$\frac{\partial f}{\partial E} = -\frac{e^{(E-\mu)/k_BT}\cdot\frac{1}{k_BT}}{\left(e^{(E-\mu)/k_BT}+1\right)^2} = -\frac{1}{k_BT}\frac{e^{(E+\mu)/k_BT}}{\left(e^{E/k_BT}+e^{\mu/k_BT}\right)^2}$$

3. Fermi-Dirac-Distribution

$$f(E) = \frac{1}{\exp[(E-\mu)/k_BT]+1}$$

$$f(E)|_\mu = f(\mu) + \frac{\partial f}{\partial E}\Big|_{E=\mu}(E-\mu)$$

$$= \frac{1}{2} - \frac{\exp((E+\mu)/k_BT)}{k_BT\left(\exp(\mu/k_BT)+\exp(E/k_BT)\right)^2}\Bigg|_{E=\mu}(E-\mu)$$

$$= \frac{1}{2} - \frac{\exp(2\mu/k_BT)}{k_BT\cdot 4\exp(2\mu/k_BT)}(E-\mu) = \frac{1}{2} - \frac{E-\mu}{4k_BT}$$

$f(E_1) = 1, \quad f(E_2) = 0$

$\frac{1}{2} = \frac{E_2-\mu}{4k_BT} \qquad \Delta E = 4k_BT$

$\Rightarrow E_2 = 2k_BT + \mu$

$-\frac{1}{2} = \frac{E_1-\mu}{4k_BT}$

$-2k_BT + \mu = E_1$

$$\frac{\Delta E}{E_F} \approx \frac{\Delta E}{\mu} = \frac{4k_BT}{\mu}$$