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.

20.04.16 **Condensed Matter Physics Ex. 1**

Van-der-Waals Interaction

1) $\hat{H}_{HO,1} = \frac{\hat{p}_1^2}{2m} + \frac{m\omega^2}{2}\hat{x}_1^2 \;,\; \hat{H}_{HO,2} = \frac{\hat{p}_2^2}{2m} + \frac{m\omega^2}{2}\hat{x}_2^2$

$$\hat{H}_{Coulomb} = \frac{e^2}{4\pi\epsilon_0}\left\{\frac{1}{R} - \frac{1}{R-x_1} - \frac{1}{R+x_2} + \underbrace{\frac{1}{R-x_1+x_2}}_{\frac{1}{R-(x_1-x_2)}}\right\} \quad (*)$$

Taylor Series Second order: $\frac{1}{1-x} = 1 + x + x^2 + \mathcal{O}(x^3)$

$$\frac{1}{1+x} = 1 - x + x^2 + \mathcal{O}(x^3)$$

$$\frac{1}{1-x_1+x_2} = 1 + (x_1-x_2) + (x_1-x_2)^2 + \mathcal{O}(x^3)$$

W.W. Potential

Elektron ~~vernachlässigt?~~

→ Included in harmonic osc.

$$(*) = \frac{e^2}{4\pi\epsilon_0 R}\left\{1 - \frac{1}{1-\frac{x_1}{R}} - \frac{1}{1+\frac{x_2}{R}} + \frac{1}{1-\frac{x_1}{R}+\frac{x_2}{R}}\right\}$$

$|x_1|, |x_2| \ll R$

$$\approx \frac{e^2}{4\pi\epsilon_0 R}\left\{1 - \left[1 + \frac{x_1}{R} + \left(\frac{x_1}{R}\right)^2\right] - \left[1 - \frac{x_2}{R} + \left(\frac{x_2}{R}\right)^2\right] + \left[1 + \left(\frac{x_1}{R} - \frac{x_2}{R}\right) + \left(\frac{x_1}{R} - \frac{x_2}{R}\right)^2\right]\right\}$$

$$= \frac{e^2}{4\pi\epsilon_0 R}\left\{-\left(\frac{x_1}{R}\right)^2 - \left(\frac{x_2}{R}\right)^2 + \left(\frac{x_1}{R} - \frac{x_2}{R}\right)^2\right\}$$

$$= \frac{e^2}{4\pi\epsilon_0 R}\left\{-2\frac{x_1 x_2}{R^2}\right\} = -\frac{e^2 x_1 x_2}{2\pi\epsilon_0 R^3}$$

$$\Rightarrow \hat{H} = \frac{\hat{p}_1^2}{2m} + \frac{m\omega^2}{2}\hat{x}_1^2 + \frac{\hat{p}_2^2}{2m} + \frac{m\omega^2}{2}\hat{x}_2^2 - \frac{e^2 x_1 x_2}{2\pi\epsilon_0 R^3}$$

$x_1 = \frac{1}{\sqrt{2}}(x_s + x_a) \;,\; x_2 = \frac{1}{\sqrt{2}}(x_s - x_a) \;\Big|\; \Leftrightarrow x_{s/a} = \frac{1}{\sqrt{2}}(x_1 \pm x_2)$

$$\Rightarrow p_{s/a} = -i\hbar\frac{\partial}{\partial x_{s/a}} = -i\hbar\left(\frac{\partial}{\partial x_1}\frac{\partial x_1}{\partial x_{s/a}} + \frac{\partial}{\partial x_2}\frac{\partial x_2}{\partial x_{s/a}}\right)$$

$$= \frac{-i\hbar}{\sqrt{2}}\left(\frac{\partial}{\partial x_1} \pm \frac{\partial}{\partial x_2}\right) = +\frac{1}{\sqrt{2}}(p_1 \pm p_2)$$

$$\Rightarrow p_1 = \frac{1}{\sqrt{2}}(p_s + p_a) \;,\; p_2 = \frac{1}{\sqrt{2}}(p_s - p_a)$$

$$\hat{H} = \frac{1}{2m}\left(\hat{p}_1^2 + \hat{p}_2^2\right) + \frac{m\omega^2}{2}\left(\hat{x}_1^2 + \hat{x}_2^2\right) - \frac{e^2 x_1 x_2}{2\pi\epsilon_0 R^3}$$

Substitute

$$= \frac{1}{2m}\left(\frac{1}{2}\left\{[p_s+p_a]^2 + [p_s-p_a]^2\right\}\right) + \frac{m\omega^2}{2}\left(\frac{1}{2}\left\{[x_s+x_a]^2 + [x_s-x_a]^2\right\}\right) - \frac{e^2 (x_s+x_a)(x_s-x_a)}{4\pi\epsilon_0 R^3}$$

$$\overset{*}{=} \frac{1}{2m}\left\{\hat{p}_s^2 + \hat{p}_a^2\right\} + \frac{m\omega^2}{2}\left\{\hat{x}_s^2 + \hat{x}_a^2\right\} - \frac{e^2(\hat{x}_s^2 - \hat{x}_a^2)}{4\pi\epsilon_0 R^3}$$

$$= \frac{\hat{p}_s^2}{2m} + \underbrace{\left(\frac{m\omega^2}{2} - \frac{e^2}{4\pi\epsilon_0 R^3}\right)}_{k_s = k - \frac{e^2}{2\pi\epsilon_0 R^3}}\hat{x}_s^2 + \frac{\hat{p}_a^2}{2m} + \underbrace{\left(\frac{m\omega^2}{2} + \frac{e^2}{4\pi\epsilon_0 R^3}\right)}_{k_a = k + \frac{e^2}{2\pi\epsilon_0 R^3}}\hat{x}_a^2$$

Rühren die 'neuen Systeme'

Hamiltonian decouples into 2 independent oscillators;

$$\omega_{s,a} = \sqrt{\frac{k_{s/a}}{m}} = \sqrt{\frac{k}{m} \mp \frac{e^2}{2\pi\epsilon_0 R^3 m}}$$

$$E = \frac{\hbar}{2}(\omega_s + \omega_a)$$

Only Ground state?

→ Superposition results in all states

$$\sqrt{\beta + x} \approx \sqrt{\beta} + \frac{1}{2\sqrt{\beta}}x - \frac{1}{8\beta^{3/2}}x^2 + \ldots$$

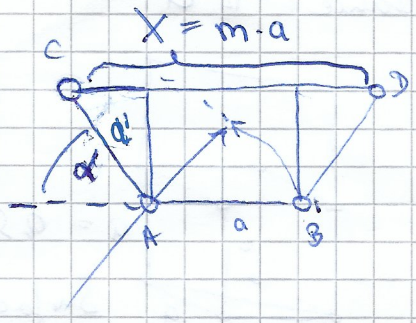
$$\frac{\hbar}{2}(\omega_s + \omega_a) - \frac{\hbar}{2}(\omega_0 + \omega_0) = \frac{1}{2}\hbar\left[\omega_0 + \omega_0 - \frac{e^4}{16\omega_0^3\pi^2\epsilon_0^2 m^2 R^6}\right] - \frac{1}{2}\hbar(\omega_0 + \omega_0)$$

$$= -\frac{e^2}{32\pi^2\epsilon_0^2 m^2\omega_0^3 R^6}$$

low interaction

2) Symmetries in Bravais Lattices

Was ist mit face-centered symmetrie etc.?



B is being rotated to the spot of C, by the axis through A, perpendicular to the plane of the sheet.

Warum beide Seiten gleich lang a? Zwangsweise so? Integer multiple of a?

Apparently, $\alpha = \alpha'$, and the rotation angle is $\pi - \alpha = \varphi \Leftrightarrow \alpha = \varphi + \pi$

Furthermore, $|CD| = X = m \cdot a$, because they both coincide with lattice points, which have a distance of a in our lattice, so they should be seperated by $m \cdot a$

Prove that there is a max. of 1, 2, 3, 4, 6 fold axis

Additionally, $m \cdot a = a + 2a\cos(\alpha) \Leftrightarrow m = 1 + 2\cos(\varphi + \pi)$

$$= 1 - 2\cos(\varphi)$$

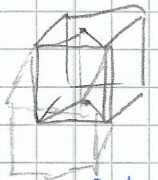
$$\Leftrightarrow \cos\varphi = \frac{1-m}{2} \quad , m \in \mathbb{Z}, \ \cos\varphi \in [-1;1]$$

$\cos\varphi = 1$ for $m = -1$

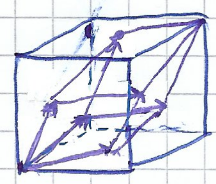
$\quad " \quad = -1$ for $m = 3$

$\Rightarrow m \in [-1;3] \subset \mathbb{Z}$ ~~[illegible]~~

m	$\frac{1-m}{2}$ ($\cos\varphi$)	φ	n
-1	1	0 (0)	1
0	1/2	60 ($\frac{\pi}{3}$)	6
1	0	90 ($\frac{\pi}{2}$)	4
2	-1/2	120 ($\frac{2}{3}\pi$)	3
3	-1	180 (π)	2



3) Simple Crystal Structures



why no base centered Cubic? Easier to cover in a different way

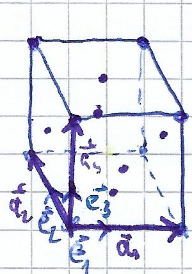
- Simple Cubic (sc) contains 1 atom
- Body centered Cubic (bcc) contains 2 atoms
- Face centered Cubic (fcc) contains 4 atoms

Conventional unit cell? just the one usual for simple cubic

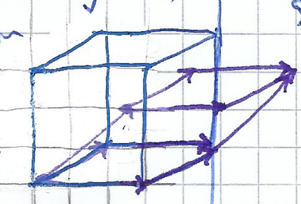
What are primitive if this set contains all lattice vectors?

SC: $\vec{a}_i = a\vec{e}_i$

$\vec{a}_1, \vec{a}_2, \vec{a}_3$ span the primitive unit cell



bcc:
$a\vec{e}_x$
$a\vec{e}_y$
$\frac{a}{2}(\vec{e}_x + \vec{e}_y + \vec{e}_z)$
span



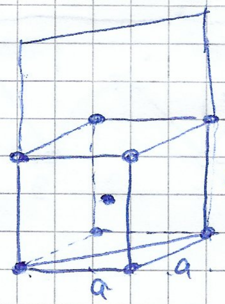
fcc:
$\frac{a}{2}(\vec{e}_x + \vec{e}_y)$
$\frac{a}{2}(\vec{e}_y + \vec{e}_z)$
$\frac{a}{2}(\vec{e}_x + \vec{e}_z)$

- SC: 6 nearest neighbours, distance a

  bcc: 8 nearest neighbours, distance $\frac{\sqrt{2}}{2}a$

  fcc: ~~4~~ 12 nearest neighbours, distance: $\frac{1}{\sqrt{2}}a$

for which atom nearest neighbours?



4) 1,5 atoms per plane

a = 0,5nm

Surface density

$$A = \sqrt{2}\,a \cdot a = \sqrt{2}\,a^2$$

$$\rho_s = \frac{1{,}5 \text{ atoms}}{\sqrt{2}\,a^2} = 4{,}243 \cdot 10^{18} \frac{\text{atoms}}{m^2} = 4{,}243 \frac{\text{atoms}}{nm^2}$$

5) 3 axes: angles: 90°, 180°, 270°, $\overbrace{(360°)}^{\text{trivial}}$

reflection: in 12 different planes

inversion: 1 time $r \mapsto -r$

What is point group?

→ point symmetries from the point group: octahedral group