Karlsruher Institut für Technologie

Institut für Theorie der Kondensierten Materie

Theorie der Kondensierten Materie I   WS 2018/19

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Blatt 1

Lösungsvorschlag

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1. Reziprokes Gitter:

(a) *das reziproke Gitter eines reziproken Gitters*

Bravais Gitter:

$$\boldsymbol{l} = l_1\boldsymbol{a}_1 + l_2\boldsymbol{a}_2 + l_3\boldsymbol{a}_3.$$

Periodizität:

$$f(\boldsymbol{r}+\boldsymbol{l}) = f(\boldsymbol{r}) \quad \Rightarrow \quad f(\boldsymbol{r}) = \sum_{\boldsymbol{g}} A_{\boldsymbol{g}} e^{i\boldsymbol{g}\cdot\boldsymbol{r}}.$$

Reziprokes Gitter

$$\boldsymbol{g} = g_1\boldsymbol{b}_1 + g_2\boldsymbol{b}_2 + g_3\boldsymbol{b}_3,$$

$$\boldsymbol{b}_1 = \frac{\boldsymbol{a}_2\times\boldsymbol{a}_3}{\boldsymbol{a}_1\cdot[\boldsymbol{a}_2\times\boldsymbol{a}_3]}, \qquad \boldsymbol{b}_2 = \frac{\boldsymbol{a}_3\times\boldsymbol{a}_1}{\boldsymbol{a}_1\cdot[\boldsymbol{a}_2\times\boldsymbol{a}_3]}, \qquad \boldsymbol{b}_3 = \frac{\boldsymbol{a}_1\times\boldsymbol{a}_2}{\boldsymbol{a}_1\cdot[\boldsymbol{a}_2\times\boldsymbol{a}_3]},$$

Volumen der Einheitszelle des reziproken Gitters

$$(2\pi)^3\boldsymbol{b}_1\cdot[\boldsymbol{b}_2\times\boldsymbol{b}_3] = \frac{(2\pi)^3}{\boldsymbol{a}_1\cdot[\boldsymbol{a}_2\times\boldsymbol{a}_3]}$$

Reziprokes Gitter eines reziproken Gitters

$$\frac{\boldsymbol{b}_2\times\boldsymbol{b}_3}{\boldsymbol{b}_1\cdot[\boldsymbol{b}_2\times\boldsymbol{b}_3]} = \boldsymbol{a}_1,$$

usw.

(b) *das reziproke Gitter des flächenzentrierten kubischen (fcc) Gitters*

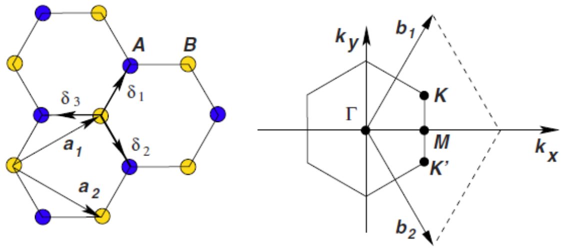
Einheitsvektoren eines FCC-Gitters

$$\boldsymbol{a}_1 = \frac{a}{2}(0,1,1), \qquad \boldsymbol{a}_2 = \frac{a}{2}(1,0,1), \qquad \boldsymbol{a}_3 = \frac{a}{2}(1,1,0).$$

Das reziproke Gitter des FCC-Gitters ist ein BCC-Gitter mit den Einheitsvektoren

$$\boldsymbol{b}_1 = \frac{2\pi}{a}(-1,1,1), \qquad \boldsymbol{b}_2 = \frac{2\pi}{a}(1,-1,1), \qquad \boldsymbol{b}_3 = \frac{2\pi}{a}(1,1,-1).$$

(c) *das reziproke Gitter des zwei-dimensionalen Honigwabengitters*



Einheitsvektoren (siehe Abbildung)

$$\boldsymbol{a}_1 = \frac{a}{2}(3, \sqrt{3}), \qquad \boldsymbol{a}_1 = \frac{a}{2}(3, -\sqrt{3}).$$

Reziprokes Gitter in Graphene

$$\boldsymbol{b}_2 \cdot \boldsymbol{a}_1 = 0, \qquad \boldsymbol{b}_2 \cdot \boldsymbol{a}_2 = 2\pi;$$
$$\boldsymbol{b}_1 \cdot \boldsymbol{a}_2 = 0, \qquad \boldsymbol{b}_1 \cdot \boldsymbol{a}_1 = 2\pi.$$

Davon finden wir

$$\boldsymbol{b}_1 = \frac{2\pi}{3a}(1, \sqrt{3}), \qquad \boldsymbol{b}_2 = \frac{2\pi}{3a}(1, -\sqrt{3}).$$

die erste Brillouin-Zone von Graphen

Siehe Abbildung.

2. Korrelationsfunktionen:

$$\frac{1}{V}\sum_{\mathbf{k}} \to \int \frac{d^d k}{(2\pi\hbar)^d},$$

$$\epsilon(\mathbf{k}) = \frac{k^2}{2m}.$$

(a) *Fermi-Impuls*

$$n(T=0) = \frac{2s+1}{V}\sum_{\lambda}\langle n_\lambda\rangle = (2s+1)\int\limits_{|k|<k_F} \frac{d^d k}{(2\pi\hbar)^d} \Rightarrow \int_0^{k_F} \frac{k^2 dk}{\pi^2\hbar^3} = \frac{k_F^3}{3\pi^2\hbar^3}.$$

Hier $s = 1/2$.

(b) *Anti-Vertauschungsrelationen*

$$\left\{\hat{\Psi}_\sigma(\boldsymbol{r}), \hat{\Psi}^\dagger_{\sigma'}(\boldsymbol{r}')\right\} = \frac{1}{V}\sum_{\boldsymbol{k},\boldsymbol{k}'} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}'} \left(\hat{a}_\sigma(\boldsymbol{k})\hat{a}^\dagger_{\sigma'}(\boldsymbol{k}') + \hat{a}^\dagger_{\sigma'}(\boldsymbol{k}')\hat{a}_\sigma(\boldsymbol{k})\right) =$$

$$= \frac{1}{V}\sum_{\boldsymbol{k},\boldsymbol{k}'} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}'} \delta_{\sigma\sigma'}\delta_{\boldsymbol{k}\boldsymbol{k}'} = \delta_{\sigma\sigma'}\delta(\boldsymbol{r}-\boldsymbol{r}').$$

(c) *Ein-Teilchen Korrelationsfunktion*

Der Grundzustand:

$$|GS\rangle = \prod_{|\mathbf{k}_a|\leqslant k_F,\sigma} \hat{a}^\dagger_{\mathbf{k}_a\sigma}|0\rangle.$$

Die Korrelationsfunktion:

$$G_\sigma(\boldsymbol{r}-\boldsymbol{r}') = \langle GS|\hat{\Psi}^\dagger_\sigma(\boldsymbol{r})\hat{\Psi}_\sigma(\boldsymbol{r}')|GS\rangle$$

$$= \frac{1}{V}\sum_{\boldsymbol{k},\boldsymbol{k}'} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}'} \langle GS|\hat{a}^\dagger_\sigma(\boldsymbol{k})\hat{a}_\sigma(\boldsymbol{k}')|GS\rangle = \begin{cases} 1, & \boldsymbol{k}=\boldsymbol{k}', |\boldsymbol{k}|\leqslant k_F \\ 0, & \textit{sonst} \end{cases}$$

$$= \frac{1}{V}\sum_{\boldsymbol{k}}^{k_F} e^{i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}')}$$

$$= \int_0^{k_F} k^2 dk \int_{-1}^{1} \frac{d\cos\theta}{(2\pi)^2} e^{ik|\boldsymbol{r}-\boldsymbol{r}'|\cos\theta} = \frac{1}{(2\pi)^2|\boldsymbol{r}-\boldsymbol{r}'|^3}\int_0^x z^2 dz \int_{-1}^{1} dy e^{iyz}$$

$$= \frac{3n(\sin x - x\cos x)}{2x^3}.$$

(d) *Zwei-Teilchen Korrelationsfuntion,* $\sigma_1 \neq \sigma_2$

$$g_{\sigma_1\sigma_2}(\boldsymbol{r}_1-\boldsymbol{r}_2) = \frac{4}{n^2}\langle GS|\hat{\Psi}^\dagger_{\sigma_1}(\boldsymbol{r}_1)\hat{\Psi}^\dagger_{\sigma_2}(\boldsymbol{r}_2)\hat{\Psi}_{\sigma_2}(\boldsymbol{r}_2)\hat{\Psi}_{\sigma_1}(\boldsymbol{r}_1)|GS\rangle$$

$$= \frac{1}{V^2}\sum_{\boldsymbol{k}_1,\boldsymbol{k}'_1} e^{i\boldsymbol{k}_1\cdot\boldsymbol{r}_1} e^{-i\boldsymbol{k}'_1\cdot\boldsymbol{r}_1} \sum_{\boldsymbol{k}_2,\boldsymbol{k}'_2} e^{i\boldsymbol{k}_2\cdot\boldsymbol{r}_2} e^{-i\boldsymbol{k}'_2\cdot\boldsymbol{r}_2} \langle GS|\hat{a}^\dagger_{\sigma_1}(\boldsymbol{k}_1)\hat{a}^\dagger_{\sigma_2}(\boldsymbol{k}_2)\hat{a}_{\sigma_2}(\boldsymbol{k}'_2)\hat{a}_{\sigma_1}(\boldsymbol{k}'_1)|GS\rangle$$

$$= \frac{1}{V^2}\sum_{\boldsymbol{k}_1,\boldsymbol{k}'_1} e^{i\boldsymbol{k}_1\cdot\boldsymbol{r}_1} e^{-i\boldsymbol{k}'_1\cdot\boldsymbol{r}_1} \sum_{\boldsymbol{k}_2,\boldsymbol{k}'_2} e^{i\boldsymbol{k}_2\cdot\boldsymbol{r}_2} e^{-i\boldsymbol{k}'_2\cdot\boldsymbol{r}_2} \delta_{\boldsymbol{k}_1\boldsymbol{k}'_1}\delta_{\boldsymbol{k}_2\boldsymbol{k}'_2} = 1.$$

(e) *Zwei-Teilchen Korrelationsfuntion,* $\sigma_1 = \sigma_2$

$$
\begin{aligned}
g_{\sigma\sigma}(\boldsymbol{r}_1 - \boldsymbol{r}_2) &= \frac{4}{n^2}\langle GS|\hat{\Psi}^\dagger_\sigma(\boldsymbol{r}_1)\hat{\Psi}^\dagger_\sigma(\boldsymbol{r}_2)\hat{\Psi}_\sigma(\boldsymbol{r}_2)\hat{\Psi}_\sigma(\boldsymbol{r}_1)|GS\rangle \\
&= \frac{4}{n^2V^2}\sum_{\boldsymbol{k}_1,\boldsymbol{k}'_1} e^{i\boldsymbol{k}_1\cdot\boldsymbol{r}_1}e^{-i\boldsymbol{k}'_1\cdot\boldsymbol{r}_1}\sum_{\boldsymbol{k}_2,\boldsymbol{k}'_2} e^{i\boldsymbol{k}_2\cdot\boldsymbol{r}_2}e^{-i\boldsymbol{k}'_2\cdot\boldsymbol{r}_2}\langle GS|\hat{a}^\dagger_\sigma(\boldsymbol{k}_1)\hat{a}^\dagger_\sigma(\boldsymbol{k}_2)\hat{a}_\sigma(\boldsymbol{k}'_2)\hat{a}_\sigma(\boldsymbol{k}'_1)|GS\rangle \\
&= \frac{4}{n^2V^2}\sum_{\boldsymbol{k}_1,\boldsymbol{k}'_1} e^{i\boldsymbol{k}_1\cdot\boldsymbol{r}_1}e^{-i\boldsymbol{k}'_1\cdot\boldsymbol{r}_1}\sum_{\boldsymbol{k}_2,\boldsymbol{k}'_2} e^{i\boldsymbol{k}_2\cdot\boldsymbol{r}_2}e^{-i\boldsymbol{k}'_2\cdot\boldsymbol{r}_2}\left[\delta_{\boldsymbol{k}_1\boldsymbol{k}'_1}\delta_{\boldsymbol{k}_2\boldsymbol{k}'_2} - \delta_{\boldsymbol{k}_2\boldsymbol{k}'_1}\delta_{\boldsymbol{k}_1\boldsymbol{k}'_2}\right] \\
&= 1 - \frac{4}{n^2}G^2_\sigma(\boldsymbol{r}_1 - \boldsymbol{r}_2).
\end{aligned}
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(f) *Pauli-Prinzip*

$$
\begin{aligned}
\frac{n}{2}\int d^3r\,[g_{\sigma\sigma}(r) - 1] &= -\frac{9n}{2}\int d^3r\frac{(\sin k_Fr - k_Fr\cos k_Fr)^2}{k_F^6r^6} \\
&= -\frac{18\pi n}{k_F^3}\int_0^\infty dx\frac{(\sin x - x\cos x)^2}{x^4} = -1.
\end{aligned}
$$