

Musterlösung: Quantisierung der Elektron-Phonon-WW (6. ÜB)

$$H_{e-i} = \sum_i \sum_j V_{e-i}(\underline{r}_i - \underline{R}_j)$$

↑
Elektronen
←
Ionen
←
 $\underline{R}_j^{(0)} + \underline{u}_j$ → Auslenkung um die Ruhelage

Taylor:

$$V_{e-i}(\underline{r}_i - \underline{R}_j) = V_{e-i}(\underline{r}_i - \underline{R}_j^{(0)}) - \sum_n \underline{u}_n \cdot \underline{\nabla}_{\underline{R}_n} V_{e-i}(\underline{r}_i - \underline{R}_j^{(0)}) + \dots$$

linearer Näherung
 betrachten nur harmonische Effekte (anharmonische Effekte in höheren Phonon-Phonon WW)

2. Quantisierung

$$H_{e-i} \rightarrow H = - \sum_{i,j} \sum_n \langle i | \underline{u}_n \cdot \left[\underline{\nabla}_{\underline{R}_n} V_{e-i}(\underline{r} - \underline{R}_n^{(0)}) \right] | j \rangle$$

$i, j = \{ \text{Elektronen} \}$

$$\stackrel{!}{=} - \sum_{i,j} \sum_n \int d^3r \varphi_i^*(\underline{r}) \underline{u}_n \cdot \underline{\nabla}_{\underline{R}_n} V_{e-i}(\underline{r} - \underline{R}_n^{(0)}) \varphi_i(\underline{r}) a_i^\dagger a_j$$

$$\left[\begin{aligned} \psi^*(\underline{r}, t) &\rightarrow \psi(\underline{r}, t) = \sum_i \varphi_i^*(\underline{r}) a_i^\dagger(t) \\ \varphi_i^*(\underline{r}) &= \frac{1}{\sqrt{V}} e^{i \underline{k} \cdot \underline{r}} \underline{u}_{\underline{k} i}(\underline{r}) \end{aligned} \right.$$

(Blockfaktor)

$$= -\sum_{ij} \sum_n \frac{1}{V} \int d^3 r \underbrace{u_{\underline{R}_i \underline{R}_j}^*(\underline{r})}_{\left(e^{-i(\underline{R}_i - \underline{R}_j) \cdot \underline{r}} a_{\underline{R}_i \underline{R}_j}^+ a_{\underline{R}_j \underline{R}_i} \right)} u_n \left[\nabla_{\underline{R}_i} V_{el} - i\omega_n(\underline{r} - \underline{R}_i^{(0)}) \right] u_{\underline{R}_j \underline{R}_i}(\underline{r})$$

WW-Potential Fouriersreihe

$$V_{el} - i(\underline{r} - \underline{R}_i^{(0)}) = \frac{1}{\Omega} \sum_{\underline{q}} V_{el} - i(\underline{q}) e^{i\underline{q} \cdot (\underline{r} - \underline{R}_i^{(0)})}$$

$$H_{el-ph} = -\sum_{ijl} \sum_n \sum_{\underline{q}} \frac{1}{\Omega V} \int d^3 r \{ \dots \}$$

$$\{ \dots \} = \underbrace{u_{\underline{R}_i \underline{R}_j}^*(\underline{r})}_{a_{\underline{R}_i \underline{R}_j}^+ a_{\underline{R}_j \underline{R}_i}} u_n - \underline{q} V_{\underline{q}} e^{i\underline{q} \cdot (\underline{r} - \underline{R}_i^{(0)})} u_{\underline{R}_j \underline{R}_i}(\underline{r})$$

einsetzen von u_n :

$$u_n := \sum_{\underline{q}'l} \sqrt{\frac{\hbar^2}{2m\omega_{\underline{q}}(\underline{q}')}} A_{\underline{q}}(\underline{q}') e^{i\underline{q}' \cdot \underline{R}_n} (\beta_{-\underline{q}'l}^+ + \beta_{\underline{q}'l})$$

$$= \sum_{ijl} \sum_n \sum_{\underline{q}'l'} \frac{1}{\Omega V} \sqrt{\frac{\hbar^2}{2m\omega_{\underline{q}}(\underline{q}')}} a_{\underline{R}_i \underline{R}_j}^+ a_{\underline{R}_j \underline{R}_i} (\beta_{-\underline{q}'l}^+ + \beta_{\underline{q}'l}) \underbrace{R_i = R_n^{(0)}}_{\int d^3 r \{ u_{\underline{R}_i}^*(\underline{r}) [A_{\underline{q}}(\underline{q}')] V_{\underline{q}'} e^{i\underline{q}' \cdot \underline{r} - i(\underline{q}' - \underline{q}) \cdot \underline{R}_n} u_{\underline{R}_j}(\underline{r}) e^{-i(\underline{R}_i - \underline{R}_j) \cdot \underline{r}} \}}$$

$$\left[\int d^3 r = \sum_{n'} \int_{\underline{V}_n} d^3 s \text{ mit } \underline{r} = \underline{R}_{n'} + \underline{s} \right]$$

$$= \sum_{ijl} \sum_{n'} \sum_{\underline{q}'l'} \frac{V_{\underline{q}'}}{\Omega V} \sqrt{\frac{\hbar^2}{2m\omega_{\underline{q}}(\underline{q}')}} \left[A_{\underline{q}}(\underline{q}') \cdot \underline{q}' \right] e^{-i(\underline{q}' - \underline{q}) \cdot \underline{R}_n} a_{\underline{R}_i \underline{R}_j} (\beta_{-\underline{q}'l}^+ + \beta_{\underline{q}'l})$$

$$\int_{\underline{V}_n} d^3 s \left\{ \underbrace{u_{\underline{R}_i}^*(\underline{s} + \underline{R}_{n'})}_{= u_{\underline{R}_i}^*(\underline{s})} \underbrace{u_{\underline{R}_j}(\underline{s} + \underline{R}_{n'})}_{= u_{\underline{R}_j}(\underline{s})} e^{i\underline{q}' \cdot (\underline{s} + \underline{R}_{n'}) - i(\underline{R}_i - \underline{R}_j) \cdot (\underline{s} + \underline{R}_{n'})} \right\}$$

$$\left[\sum_n e^{-i\underline{q}(\underline{q}' - \underline{q}) \cdot \underline{R}_n} = \Omega \delta_{\underline{q}\underline{q}'} \right]$$

$$= \frac{i}{\hbar} \sum_{ij} \sum_{\ell} \sum_{\mathbf{q}} \frac{V_{\mathbf{q}}}{V} \sqrt{\frac{\hbar^2}{2m\omega_{\mathbf{q}}}} A_{\ell}(\mathbf{q}) \cdot \mathbf{q} a_i^{\dagger} a_j (b_{-\mathbf{q}\ell}^{\dagger} + b_{\mathbf{q}\ell})$$

$$\int d^3s \left\{ u_i^*(\underline{s}) u_j(\underline{s}) e^{i[\mathbf{q} - (\mathbf{R}_i - \mathbf{R}_j)] \cdot \underline{s}} \frac{\hbar^2}{2m} e^{i[\mathbf{q} - (\mathbf{R}_i - \mathbf{R}_j)] \cdot \underline{s}} \right.$$

$$\left. \left[\sum_{\mathbf{u}} e^{i[\mathbf{q} - (\mathbf{R}_i - \mathbf{R}_j)] \cdot \underline{R}_{\mathbf{u}}} \right] = N \delta_{\mathbf{R}_i, \mathbf{R}_j + \mathbf{q}} \right.$$

$$= \frac{i}{\hbar} \sum_{\substack{\mathbf{R}_i \\ \mathbf{R}_j}} \sum_{\ell} \sum_{\mathbf{q}} \frac{N}{V} \frac{V_{\mathbf{q}}}{V} \sqrt{\frac{\hbar^2}{2m\omega_{\mathbf{q}}}} \left[A_{\ell}(\mathbf{q}) \cdot \mathbf{q} \right] a_{\mathbf{R}_i + \mathbf{q}\ell}^{\dagger} a_{\mathbf{R}_i \ell} (b_{-\mathbf{q}\ell}^{\dagger} + b_{\mathbf{q}\ell})$$

$$\int d^3s \left\{ u_{\mathbf{R}_i + \mathbf{q}\ell}^*(\underline{s}) u_{\mathbf{R}_i \ell}(\underline{s}) \right\}$$

$$\underbrace{\quad}_{|\mathbf{q}| \ll |\mathbf{R}_i|}$$

$$= V_{\mathbf{q}} \delta_{\mathbf{R}_i \ell} \quad (\text{Näherung, aber meist eine sehr gute})$$

Langwellennäherung

$$= \frac{i}{\hbar} \sum_{\mathbf{R}_i \ell} \sum_{\ell} \sum_{\mathbf{q}} \underbrace{\frac{N}{V} V_{\mathbf{q}}}_{=1} \frac{V_{\mathbf{q}} A_{\ell} \cdot \mathbf{q}}{\sqrt{2m\omega_{\mathbf{q}}}} a_{\mathbf{R}_i + \mathbf{q}\ell}^{\dagger} a_{\mathbf{R}_i \ell} (b_{-\mathbf{q}\ell}^{\dagger} + b_{\mathbf{q}\ell})$$

$$= \frac{i}{\hbar} \sum_{\mathbf{R}\ell} \sum_{\mathbf{q}\ell} a_{\mathbf{R} + \mathbf{q}\ell}^{\dagger} a_{\mathbf{R}\ell} (b_{-\mathbf{q}\ell}^{\dagger} + b_{\mathbf{q}\ell})$$

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Phononenarten (optische, akustische)

Phonon-Tripelübertrag

Elektronenimpuls

Bandstruktur