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

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

i: Elektronen, j: Ionen

$\underline{R}_j = \underline{R}_j^{(0)} + \underline{u}_j$ ← Auslenkung um die Ruhelage

Taylor:

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

lineare Näherung betrachten nur harmonische Effekte (anharmonische Effekte inkludieren Phonon-Phonon WW)

2. Quantisierung

$$H_{el-ph} = -\sum_{ij} \sum_n \langle i | \underline{u}_n \cdot [\nabla_{\underline{R}_n} V_{el-i}(\underline{r} - \underline{R}_n^{(0)})] | j \rangle$$

$i, j = \{\lambda, \underline{k}\}$

$$\stackrel{!}{=} -\sum_{ij} \sum_n \int d^3r\, \varphi_i^*(\underline{r})\, \underline{u}_n \cdot \nabla_{\underline{R}_n} V_{el-i}(\underline{r} - \underline{R}_n^{(0)})\, \varphi_j(\underline{r})\, a_i^+ a_j$$

$$\psi^*(\underline{r}, t) \rightarrow \psi^+(\underline{r}, t) = \sum_i \varphi_i^*(\underline{r})\, a_i^+(t)$$

$$\varphi_i^*(\underline{r}) = \frac{1}{\sqrt{V}} e^{-i \underline{k}_i \cdot \underline{r}}\, u_{k_i \lambda_i}(\underline{r})$$

Blochfaktor)

$$= -\sum_{ji}\sum_{n}\frac{1}{V}\int_V d^3r\, u^*_{k_i\lambda_i}(\underline{r})\,\underline{u}_n\left[D_{\underline{R}_n}V_{el-ion}(\underline{r}-\underline{R}_n^{(0)})\right]u_{k_j\lambda_j}(\underline{r})$$

$$\left(e^{-i(\underline{k}_i-\underline{k}_j)\cdot\underline{r}}\quad a^+_{k_i\lambda_i}\,a_{k_j\lambda_j}\right)$$

WW-Potential Fourierreihe

$$V_{el-i}(\underline{r}-\underline{R}_n^{(0)}) = \frac{1}{\sqrt{N}}\sum_{q} V_{el-i}(q)\,e^{i\underline{q}\cdot(\underline{r}-\underline{R}_n^{(0)})}$$

$$H_{el-ph} = -\sum_{ij}\sum_{n}\sum_{q}\frac{1}{\sqrt{N}}\frac{1}{V}\int d^3r\,\{\dots\}$$

$$\{\dots\} = i\,u^*_{k_i\lambda_i}(\underline{r})\,\underline{u}_n\cdot\underline{q}\,V_q\,e^{i\underline{q}\cdot(\underline{r}-\underline{R}_n^{(0)})}\,u_{k_j\lambda_j}(\underline{r})\,e^{-i(\underline{k}_i-\underline{k}_j)\cdot\underline{r}}\,a^+_i a_j$$

einsetzen von $\underline{u}_n$:

$$\underline{u}_n := \sum_{q'l}\sqrt{\frac{\hbar^2}{2mN\omega_l(q)}}\,\underline{A}_l(q)\,e^{i\underline{q}'\cdot\underline{R}_n}\left(b^+_{-q'l}+b_{q'l}\right)$$

$$= i\sum_{ijl}\sum_{n}\sum_{qq'}\frac{1}{NV}\sqrt{\frac{\hbar^2}{2m\omega_l(q)}}\,a^+_i a_j\left(b^+_{-ql}+b_{ql}\right)\qquad \underline{R}_n = \underline{R}_n^{(0)}$$

$$\int d^3r\left\{u^*_i(\underline{r})\left[\underline{A}_l\cdot\underline{q}'\right]V_{q'}\,e^{i\underline{q}\cdot\underline{r}-i(\underline{q}'-\underline{q})\cdot\underline{R}_n}\,u_j(\underline{r})\,e^{-i(\underline{k}_i-\underline{k}_j)\cdot\underline{r}}\right\}$$

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

$$= i\sum_{ijl}\sum_{nn'}\sum_{qq'}\frac{V_{q'}}{NV}\sqrt{\frac{\hbar^2}{2m\omega_l(q)}}\left[\underline{A}_l(q)\cdot\underline{q}'\right]e^{-i(\underline{q}'-\underline{q})\cdot\underline{R}_n}\,a^+_i a_j\left(b^+_{-ql}+b_{ql}\right)$$

$$\int_{V_{EZ}} d^3s\left\{\underbrace{u^*_i(\underline{s}+\underline{R}_{n'})}_{=u^*_i(\underline{s})}\,\underbrace{u_j(\underline{s}+\underline{R}_{n'})}_{=u_j(\underline{s})}\,e^{i\underline{q}\cdot(\underline{s}+\underline{R}_{n'})-i(\underline{k}_i-\underline{k}_j)\cdot(\underline{s}+\underline{R}_{n'})}\right\}$$

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

$$= i \sum_{ijl} \sum_{n'} \sum_{q} \frac{V_q}{V} \sqrt{\frac{\hbar^2}{2m\omega_l(q)}} \underline{A}_l(q) \cdot q \; a_i^+ a_j \left(b^+_{-ql} + b_{ql} \right)$$

$$\int_{V_{EZ}} d^3 s \left\{ u_i^*(\underline{s}) \, u_j(\underline{s}) \, e^{i[q - (k_i - k_j)] \cdot \underline{R}_{n'}} \, e^{i[q - (k_i - k_j)] \cdot \underline{s}} \right.$$

$$\left[\sum_{n'} e^{i[q - (k_i - k_j)] \cdot \underline{R}_{n'}} = N \, \delta_{k_i, k_j + q} \right.$$

$$= i \sum_{k_i \lambda_i \lambda_j} \sum_{l} \sum_{q} \frac{N}{V} V_q \sqrt{\frac{\hbar^2}{2m\omega_l(q)}} \left[\underline{A}_l(q) \cdot q \right] a^+_{k_i + q \lambda_i} a_{k_i \lambda_j} \left(b^+_{-ql} + b_{ql} \right)$$

$$\underbrace{\int_{V_{EZ}} d^3 s \left\{ u^*_{k_i + q \lambda_i}(\underline{s}) \, u_{k_i \lambda_j}(\underline{s}) \right\} \quad |q| << |k_i|}_{= V_{EZ} \, \delta_{\lambda_i \lambda_j}}$$

(Näherung, aber meist eine sehr gute)

Langwellennäherung

$$= i \sum_{k_i \lambda_i} \sum_{l} \sum_{q} \underbrace{\frac{N}{V} V_{EZ}}_{N V_{EZ} = 1} \hbar \frac{V_q \, \underline{A}_l \cdot q}{\sqrt{2m\omega_l(q)}} a^+_{k_i + q \lambda_i} a_{k_i \lambda_i} \left(b^+_{-ql} + b_{ql} \right)$$

$$= i \hbar \sum_{\lambda k} \sum_{ql} g_{ql} \, a^+_{k + q \lambda} a_{k \lambda} \left(b^+_{-ql} + b_{ql} \right)$$

- l — Phononensorten (optische, akustische)
- q — Phonon-Impulsübertrag
- k — Elektronenimpuls
- λ — Bandindex