# Theory of Phonon- Phonon Interaction in Semiconductor Crystals

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**Abstract:-** An equation of motion technique of quantum dynamics and Dyson equation approach have been used to obtain Fourier transformed electron Green`s function in presence of isotopic impurity and anharmonicity Hamiltonian has been taken as a sum of harmonic part , electron part , defect part , electron phonon interaction part , anharmonic part .The anharmonicity has been taken upto quartic terms . The response function has been obtained responsible for electron phonon linewidth . At high temperature, an expression of electron density of states (EDOS) has been obtained according to different fields present in semiconductor continuum. An EDOS has also been influenced by perturbed mode energy .The effect on intensity of peaks with respect to temperature and different excitations has been undertaken in this framework.

**Keywords:-** Electron , Phonon , Electron Green`s function , Anharmonic mode , Electron density of states .

## I. INTRODUCTION

Semiconductors are being widely used in computers and in electronic goods. Band gap engineering of crystal Materials: Band gap estimation of semiconductors via electronegativity [1] and performance estimation of silicon- based self-cooling device [2] are the recent advances in semiconductor technology. The theory based on non-interacting normal mode of vibrations is known as harmonic approximation. This can not explain the complete characteristics of properties like optical absorption, thermal conductivity, dielectric constant etc. It is essential to take cubic and quartic terms in Taylor series expansion of potential energy [3] to develop the theory. This results in a phonon phonon interaction to create anharmonic mode. The impurity inside the crystal breaks the symmetry and formation of localized mode takes place. Thus , semiconductor crystal can be consider as a container of harmonic field , localized field , cubic and quartic anharmonic field and electron . The double time temperature dependent electron Green`s function is taken to solve the present problem. The work has also been done on electron density of states in absence of phonon phonon interaction [4]. This paper is divided into sections namely formulation of the problem, evaluation of response function and electron phonon linewidth , electron density of states and conclusion of the present work at the end .

## II. FORMULATION OF THE PROBLEM

In present case of semiconductor crystals, density of states (DOS) in Lehman representation is taken as [5]

$$N_{qq`} = -\sum_{q} \text{Im}.G_{qq`}(\varepsilon) \tag{1}$$

In above eq.(1) , $\text{Im}.G_{qq`}(\varepsilon)$ represents imaginary part of electron Green`s function . So, the evaluation of electron Green`s function is the essential part of the problem .

## III. EVALUATION OF RESPONSE FUNCTION AND ELECTRON PHONON LINEWIDTH

Let us solve the present problem by taking the following electron Green`s function as [6]

$$G_{qq`}(t,t`) = \langle\langle b_q^*(t); b_{q`}(t`)\rangle\rangle \tag{2}$$

The Fourier transformation of above Green`s function $G_{qq`}(t,t`)$ can be obtained by developing many body system. An electron and phonon are the main source to develop this system. In presence of harmonic field, localized field and anharmonic field, an electron propagates through these fields. This can be done by taking

Hamiltonian $H$ as a sum of harmonic part $\left(H_{op}\right)$, electron part $\left(H_e\right)$, defect part $\left(H_D\right)$, electron-phonon interaction part $\left(H_{ep}\right)$ and anharmonic part $\left(H_A\right)$. This Hamiltonian $H$ is given by [7]-[17]

$$H = H_{op} + H_e + H_D + H_{ep} + H_A \tag{3}$$

Where,

$$H_{op} = \left(\frac{\hbar}{4}\right)\sum_k \varepsilon_k \left[A_k^* A_k + B_k^* B_k\right] \tag{4a}$$

$$H_e = \hbar \sum_q \varepsilon_q b_q^* b_q \tag{4b}$$

$$H_D = -\hbar \sum_{k_1,k_2}\left[C\left(\vec{k}_1,\vec{k}_2\right)B_{k_1}B_{k_2} - D\left(\vec{k}_1,\vec{k}_2\right)A_{k_1}A_{k_2}\right] \tag{4c}$$

$$H_{ep} = g\hbar \sum_{k,q} b_Q^* b_q B_k \tag{4d}$$

$$H_A = \hbar \sum_{s\geq 3}\ \sum_{k_1,k_2,\ldots,k_s} V^s\left(\vec{k}_1,\vec{k}_2,\ldots\vec{k}_s\right)A_{k_1}A_{k_3}..A_{k_s} \tag{4e}$$

Where,

$$A_k = a_k + a_{-k}^* = A_k^* \ ; \ B_k = a_k - a_{-k}^* = -B_{-k}^* \ ; \ \vec{Q} = \vec{k} + \vec{q} \tag{5}$$

The symbols $\varepsilon_k$, $\varepsilon_q$, $a_k^*\left(a_k\right)$, $b_q^*\left(b_q\right)$, $C\left(\vec{k}_1,\vec{k}_2\right)$, $D\left(\vec{k}_1,\vec{k}_2\right)$, $g$, $V^s\left(\vec{k}_1,\vec{k}_2,\vec{k}_3,\ldots\vec{k}_s\right)$ in eqs.(4a-4e,5) denote phonon frequency (in energy unit), electron band energy, creation (annihilation) operators of phonon, creation (annihilation) operators of electron, mass change parameter, force constant change parameter, electron phonon coupling constant and Fourier transform of atomic force constant [7]-[17]. An equation of motion technique of quantum dynamics via Hamiltonian described in eqs.(4a-4e) [6], [14], [15], [18], [19] and Dyson equation approach give the Fourier transformed electron Green`s function as

$$G_{qq'}\left(\varepsilon\right) = \frac{\delta_{qq'}\pi^{-1}}{\left[\left(\varepsilon - \tilde{\varepsilon}_q\right) + i\Gamma\left(kqQ,\varepsilon\right)\right]} \tag{6}$$

Where $\tilde{\varepsilon}_q$ is given by

$$\tilde{\varepsilon}_q = \varepsilon_q + \Delta\left(kqQ,\varepsilon\right) \tag{7}$$

The perturbed mode energy, electron phonon linewidth and electron phonon shift are given by the symbols $\tilde{\varepsilon}_q$, $\Gamma\left(kqQ,\varepsilon\right)$ and $\Delta\left(kqQ,\varepsilon\right)$ respectively in eqs.(6,7).

This method gives response function $P\left(kqQ,\varepsilon\right)$ as

$$P\left(kqQ,\varepsilon\right) = 8g^2\varepsilon_k N_Q\left(\varepsilon_k^2 - \varepsilon_q^2 + \varepsilon_q\varepsilon_k\right)\left(\varepsilon^2 - \varepsilon_k^2\right)^{-1}\left(\varepsilon - \varepsilon_q\right)^{-2} - 8g^2\varepsilon_k\varepsilon_q N_Q\left(\varepsilon - \varepsilon_k\right)^{-1}\left(\varepsilon - \varepsilon_q\right)^{-2}$$
$$+ \ \alpha g^2\left(\varepsilon + \varepsilon_Q\right)^{-1}\left(\varepsilon - \varepsilon_q\right)^{-2} + 32g^2 N_Q \sum_{k_1}\left|D\left(\vec{k}_1,-\vec{k}\right)\right|^2\varepsilon_{k_1}\left(\varepsilon^2 - \varepsilon_{k_1}^2\right)^{-1}\left(\varepsilon - \varepsilon_q\right)^{-2} + 72\pi^{-1}g^2 N_Q \sum_{k_1,k_2}$$
$$\left|V^3\left(\vec{k}_1,\vec{k}_2,-\vec{k}\right)\right|^2\eta_1\left[S_{+1}\varepsilon_{+\alpha}\left(\varepsilon - \varepsilon_q\right)^{-2}\left(\varepsilon^2 - \varepsilon_{+\alpha}^2\right)^{-1} + S_{-1}\varepsilon_{-\alpha}\left(\varepsilon - \varepsilon_q\right)^{-2}\left(\varepsilon^2 - \varepsilon_{-\alpha}^2\right)^{-1}\right] + 64\pi^{-1}g^2 N_Q$$
$$\sum_{k_1,k_2,k_3}\left|V^4\left(\vec{k}_1,\vec{k}_2,\vec{k}_3,-\vec{k}\right)\right|^2\eta_2\left[S_{+2}\varepsilon_{+\beta}\left(\varepsilon - \varepsilon_q\right)^{-2}\left(\varepsilon^2 - \varepsilon_{+\beta}^2\right)^{-1} + 3S_{-2}\varepsilon_{-\beta}\left(\varepsilon - \varepsilon_q\right)^{-2}\left(\varepsilon^2 - \varepsilon_{-\beta}^2\right)^{-1}\right] \tag{8}$$

Where,

$$N_Q = \left\langle b_Q^* b_Q\right\rangle \ ; \ n_k = \left\langle A_k^* A_k\right\rangle = \left(\frac{\tilde{\varepsilon}_k}{\varepsilon_k}\right)Coth\left(\frac{\beta\hbar\varepsilon_k}{2}\right) \ ; \ S_{\pm 1} = n_{k_2} \pm n_{k_1} \ \ ;$$

$$S_{\pm 2} = 1 \pm n_{k_1}n_{k_2} + n_{k_2}n_{k_3} \pm n_{k_3}n_{k_1} \tag{9a}$$

$$\alpha = 4\varepsilon_q{}^2\,\tilde{\tilde{n}}_k + 4\varepsilon_q\varepsilon_k\tilde{n}_k + \varepsilon_k{}^2 n_k \ , \ \text{where,} \ \tilde{n}_k = \langle A_k B_k \rangle \ ; \ \tilde{\tilde{n}}_k = \langle B_k{}^* B_k \rangle \tag{9b}$$

And,

$$\varepsilon_{\pm\alpha} = \tilde{\varepsilon}_{k_1} \pm \tilde{\varepsilon}_{k_2} \ ; \ \varepsilon_{\pm\beta} = \tilde{\varepsilon}_{k_1} \pm \tilde{\varepsilon}_{k_2} \pm \tilde{\varepsilon}_{k_3} \ ; \ \varepsilon_{\pm kq}{}^2 = \varepsilon_k{}^2 - \varepsilon_q{}^2 \pm \varepsilon_q\varepsilon_k \ ; \ \eta_{i-1} = \frac{\varepsilon_{k_1}\varepsilon_{k_2}...\varepsilon_{k_i}}{\tilde{\varepsilon}_{k_1}\tilde{\varepsilon}_{k_2}...\tilde{\varepsilon}_{k_i}} \tag{9c}$$

The response function $P(kqQ,\varepsilon)$ is related to electron phonon linewidth $\Gamma(kqQ,\varepsilon)$ and electron phonon shift $\Delta(kqQ,\varepsilon)$ as

$$P(kqQ,\varepsilon + i\omega) = \Delta(kqQ,\varepsilon) - i\Gamma(kqQ,\varepsilon) \ , \ \omega \to 0^+ \tag{10}$$

The phonon linewidth $\Gamma(kqQ,\varepsilon)$ of above eq.(10) is given by

$$\Gamma(kqQ,\varepsilon) = \Gamma_{oep}(kqQ,\varepsilon) + \Gamma_e(kqQ,\varepsilon) + \Gamma_D(kqQ,\varepsilon) + \Gamma_{De}(kqQ,\varepsilon) + \Gamma_{3A}(kqQ,\varepsilon) + \Gamma_{3Ae}(kqQ,\varepsilon) +$$
$$\Gamma_{4A}(kqQ,\varepsilon) + \Gamma_{4Ae}(kqQ,\varepsilon) \tag{11}$$

The various terms of eq.(11) are given by

$$\Gamma_{oep}(kqQ,\varepsilon) = 4\pi g^2 N_Q \{ \ \varepsilon_{+kq}{}^2 Y_{kq}{}^2(+)\delta(\varepsilon + \varepsilon_k) - \varepsilon_{-kq}{}^2 Y_{kq}{}^2(-)\delta(\varepsilon - \varepsilon_k) + 2\varepsilon_k\varepsilon_q(\varepsilon_k{}^2 - 3\varepsilon_q{}^2)$$
$$(Y_{kq}{}^2)^2 \delta(\varepsilon - \varepsilon_q) \ \} \tag{12a}$$

$$\Gamma_e(kqQ,\varepsilon) = \pi\alpha g^2 (\varepsilon_q + \varepsilon_Q)^{-2} [\delta(\varepsilon - \varepsilon_q) - \delta(\varepsilon + \varepsilon_Q)] \tag{12b}$$

$$\Gamma_D(kqQ,\varepsilon) = 16\pi g^2 N_Q \sum_{k_1} |D(\vec{k}_1,-\vec{k})|^2 [Y_{k_1 q}{}^2(-)\delta(\varepsilon + \varepsilon_{k_1}) - Y_{k_1 q}{}^2(+)\delta(\varepsilon - \varepsilon_{k_1})] \tag{12c}$$

$$\Gamma_{De}(kqQ,\varepsilon) = 64\pi g^2 N_Q \varepsilon_q \sum_{k_1} |D(\vec{k}_1,-\vec{k})|^2 \varepsilon_{k_1} (Y_{k_1 q}{}^2)^2 \delta(\varepsilon - \varepsilon_q) \tag{12d}$$

$$\Gamma_{3A}(kqQ,\varepsilon) = 36 g^2 N_Q \sum_{k_1,k_2} |V^3(\vec{k}_1,\vec{k}_2,-\vec{k})|^2 \eta_1 [ \ S_{+1}\{Y_{+\alpha q}{}^2(+)\delta(\varepsilon + \varepsilon_{+\alpha}) - Y_{+\alpha q}{}^2(-)\delta(\varepsilon - \varepsilon_{+\alpha})\} +$$
$$S_{-1}\{Y_{-\alpha q}{}^2(+)\delta(\varepsilon + \varepsilon_{-\alpha}) - Y_{-\alpha q}{}^2(-)\delta(\varepsilon - \varepsilon_{-\alpha})\} \ ] \tag{12e}$$

$$\Gamma_{3Ae}(kqQ,\varepsilon) = 144 g^2 \varepsilon_q N_Q \sum_{k_1,k_2} |V^3(\vec{k}_1,\vec{k}_2,-\vec{k})|^2 \eta_1 (S_{+1}\varepsilon_{+\alpha} Y_{+\alpha q}{}^2 + S_{-1}\varepsilon_{-\alpha} Y_{-\alpha q}{}^2)\delta(\varepsilon - \varepsilon_q) \tag{12f}$$

$$\Gamma_{4A}(kqQ,\varepsilon) = 32 g^2 N_Q \sum_{k_1,k_2,k_3} |V^4(\vec{k}_1,\vec{k}_2,\vec{k}_3,-\vec{k})|^2 \eta_2 [ \ S_{+2}\{Y_{+\beta q}{}^2(+)\delta(\varepsilon + \varepsilon_{+\beta}) - Y_{+\beta q}{}^2(-)\delta(\varepsilon - \varepsilon_{+\beta})\} -$$
$$3S_{-2}\{Y_{-\beta q}{}^2(+)\delta(\varepsilon + \varepsilon_{-\beta}) - Y_{-\beta q}{}^2(-)\delta(\varepsilon - \varepsilon_{-\beta})\} \ ] \tag{12g}$$

$$\Gamma_{4Ae}(kqQ,\varepsilon) = 128 g^2 \varepsilon_q N_Q \sum_{k_1,k_2,k_3} |V^4(\vec{k}_1,\vec{k}_2,\vec{k}_3,-\vec{k})|^2 \eta_2 (S_{+2}\varepsilon_{+\beta}Y_{+\beta q}{}^2 + 3S_{-2}\varepsilon_{-\beta}Y_{-\beta q}{}^2)\delta(\varepsilon - \varepsilon_q) \tag{12h}$$

Where,

$$Y_{ij}{}^2(\pm) = (\varepsilon_i \pm \varepsilon_j)^{-2} \ ; \ Y_{ij}{}^2 = (\varepsilon_i{}^2 - \varepsilon_j{}^2)^{-1} \ ; \ i = k, k_1, q, \pm\alpha, \pm\beta \ ; \ j = q \tag{13}$$

## IV. ELECTRON DENSITY OF STATES

An electron density of states $N(kqQ,\varepsilon)$ is evaluated by substituting eq.(6) into eq.(1) as

$$N(kqQ,\varepsilon) = \pi^{-1} \sum_q \Gamma(kqQ,\varepsilon) [(\varepsilon - \tilde{\varepsilon}_q)^2 + \Gamma^2(kqQ,\varepsilon)]^{-1} \tag{14}$$

If linewidth is very small , then in the Breit - Wigner expansion , EDOS tends to a delta- shape distribution . Eq.(14) can be written as

$$N(kqQ,\varepsilon) = \pi^{-1} \sum_q \Gamma(kqQ,\varepsilon)(\varepsilon - \tilde{\varepsilon}_q)^{-2} \tag{15}$$

In view of eqs.(12a-12h) , eq.(15) may be taken as[17] - [19]

$$N(kqQ,\varepsilon) = N_{op}(kqQ,\varepsilon) + N_e(kqQ,\varepsilon) + N_D(kqQ,\varepsilon) + N_{De}(kqQ,\varepsilon) + N_{3A}(kqQ,\varepsilon) +$$

$$N_{3Ae}(kqQ,\varepsilon) + N_{4A}(kqQ,\varepsilon) + N_{4Ae}(kqQ,\varepsilon) \tag{16}$$

Where ,

$$N_{oep}(kqQ,\varepsilon) = 32 g^6 k_B{}^2 T^3 (\varepsilon_q + \varepsilon_Q)^{-4} (\varepsilon_q{}^2 + \varepsilon_Q)(\varepsilon_Q - \tilde{\varepsilon}_Q)^{-2} \{ \varepsilon_{+kq}{}^2 Y_{kq}{}^2 (+)(\varepsilon_k + \tilde{\varepsilon}_q)^{-2} - \varepsilon_{-kq}{}^2 Y_{kq}{}^2 (-)$$
$$(\varepsilon_k - \tilde{\varepsilon}_q)^{-2} + 2\varepsilon_k \varepsilon_q (\varepsilon_k{}^2 - 3\varepsilon_q{}^2)(Y_{kq}{}^2)^2 (\varepsilon_q - \tilde{\varepsilon}_q)^{-2} \} \tag{17a}$$

$$N_e(kqQ,\varepsilon) = 2 g^2 k_B T (\varepsilon_q + \varepsilon_Q)^{-2} \{ g^2 T \varepsilon_k (\varepsilon_q + \varepsilon_Q)^{-2} (1 + 4\varepsilon_k) + \hbar^{-1} \tilde{\varepsilon}_q \} [(\varepsilon_q - \tilde{\varepsilon}_q)^{-2} - (\varepsilon_Q + \tilde{\varepsilon}_q)^{-2}] \tag{17b}$$

$$N_D(kqQ,\varepsilon) = 128 g^6 k_B{}^2 T^3 (\varepsilon_q + \varepsilon_Q)^{-4} (\varepsilon_q{}^2 + \varepsilon_Q)(\varepsilon_Q - \tilde{\varepsilon}_Q)^{-2} \sum_{k_1} \left| D(\vec{k}_1, -\vec{k}) \right|^2 [ Y_{k_1 q}{}^2 (-)(\varepsilon_{k_1} + \tilde{\varepsilon}_q)^{-2}$$
$$- Y_{k_1 q}{}^2 (+)(\varepsilon_{k_1} - \tilde{\varepsilon}_q)^{-2} ] \tag{17c}$$

$$N_{De}(kqQ,\varepsilon) = 512 g^6 k_B{}^2 T^3 \varepsilon_q (\varepsilon_q + \varepsilon_Q)^{-4} (\varepsilon_q{}^2 + \varepsilon_Q)(\varepsilon_Q - \tilde{\varepsilon}_Q)^{-2} \sum_{k_1} \left| D(\vec{k}_1, -\vec{k}) \right|^2 \varepsilon_{k_1} (Y_{k_1 q}{}^2)(\varepsilon_q - \tilde{\varepsilon}_q)^{-2} \tag{17d}$$

$$N_{3A}(kqQ,\varepsilon) \cong 1152 \hbar^{-1} g^6 k_B{}^3 T^4 (\varepsilon_q + \varepsilon_Q)^{-4} (\varepsilon_q{}^2 + \varepsilon_Q)(\varepsilon_Q - \tilde{\varepsilon}_Q)^{-2} \tilde{\varepsilon}_k{}^{-1} \sum_{k_1,k_2} \left| V^3(\vec{k}_1, \vec{k}_2, -\vec{k}) \right|^2 \eta_1 \{ Y_{+\alpha q}{}^2 (+)(\varepsilon_{+\alpha} + \tilde{\varepsilon}_q)^{-2}$$
$$- Y_{+\alpha q}{}^2 (-)(\varepsilon_{+\alpha} - \tilde{\varepsilon}_q)^{-2} \} \tag{17e}$$

$$N_{3Ae}(kqQ,\varepsilon) \cong 4608 \hbar^{-1} g^6 k_B{}^3 T^4 \varepsilon_q (\varepsilon_q + \varepsilon_Q)^{-4} (\varepsilon_q{}^2 + \varepsilon_Q)(\varepsilon_Q - \tilde{\varepsilon}_Q)^{-2} \tilde{\varepsilon}_k{}^{-1} \sum_{k_1,k_2} \left| V^3(\vec{k}_1, \vec{k}_2, -\vec{k}) \right|^2 \eta_1 \varepsilon_{+\alpha}$$
$$Y_{+\alpha q}{}^2 (\varepsilon_q - \tilde{\varepsilon}_q)^{-2} \tag{17f}$$

$$N_{4A}(kqQ,\varepsilon) \cong 3072 \hbar^{-2} g^6 k_B{}^4 T^5 (\varepsilon_q + \varepsilon_Q)^{-4} (\varepsilon_q{}^2 + \varepsilon_Q)(\varepsilon_Q - \tilde{\varepsilon}_Q)^{-2} \tilde{\varepsilon}_k{}^{-2} \sum_{k_1,k_2,k_3} \left| V^4(\vec{k}_1, \vec{k}_2, \vec{k}_3, -\vec{k}) \right|^2 \eta_2$$
$$\{ Y_{+\beta q}{}^2 (+)(\varepsilon_{+\beta} + \tilde{\varepsilon}_q)^{-2} - Y_{+\beta q}{}^2 (-)(\varepsilon_{+\beta} - \tilde{\varepsilon}_q)^{-2} \} \tag{17g}$$

$$N_{4Ae}(kqQ,\varepsilon) \cong 12288 \hbar^{-2} g^6 k_B{}^4 T^5 \varepsilon_q (\varepsilon_q + \varepsilon_Q)^{-4} (\varepsilon_q{}^2 + \varepsilon_Q)(\varepsilon_Q - \tilde{\varepsilon}_Q)^{-2} \tilde{\varepsilon}_k{}^{-2} \sum_{k_1,k_2,k_3} \left| V^4(\vec{k}_1, \vec{k}_2, \vec{k}_3, -\vec{k}) \right|^2 \eta_2$$
$$\varepsilon_{+\beta} Y_{+\beta q}{}^2 (\varepsilon_q - \tilde{\varepsilon}_q)^{-2} \tag{17h}$$

## V. CONCLUSIONS

The theory based on interaction of electron in harmonic field , localized field and anharmonic field gives some essential features regarding electron density of states (EDOS) . Fourier transformed electron Green`s function gives electron phonon linewidth which has harmonic part , electron part , defect part , cubic and quartic anharmonic part affected by electron interaction . It is clear from this many body approach that EDOS depends as $g^6$ on electron phonon coupling constant in every interaction fields except as $g^2$ and $g^4$ dependence in electron electron field . It is found from this work that EDOS is most probable in sixfold exciton excitations in comparison to other non-degenerate states such as harmonic state , localized state , two and three phonon renormalized state . This EDOS is affected by perturbed mode energy through electron phonon shift . It is also seen that at high temperature limit not only cubic and quartic anharmonic field but also harmonic field, localized field, electron- electron field give their contribution through different excitations. This many body approach interpret that the intensity of peaks depend as $T^3$ , ($T$ , $T^2$) , $T^3$ , $T^4$, and $T^5$ on temperature in harmonic field , electron electron field , localized field , cubic and quartic anharmonic field respectively . The excitations produced in semiconductor crystal in the form of harmonic state $\varepsilon_k$ , localized state $\varepsilon_{k_1}$ , two and three phonon renormalized states $\varepsilon_{\pm\alpha}$ , $\varepsilon_{\pm\beta}$ and exciton state $\varepsilon_q$ give their asymptotic behaviour when they become identical with perturbed mode energy . In harmonic field , localized field , anharmonic field in the condition of $\varepsilon_q = -\varepsilon_Q$ , $\varepsilon_Q = \tilde{\varepsilon}_Q$ and in electron electron interaction field in the condition $\varepsilon_q = -\varepsilon_Q$ , the peaks show tremendous increase their values . It is also found that an EDOS is affected by non-linearly on force constant change parameter, cubic and quartic atomic force constants.

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