On the Interatomic Correlations and Mean Square Relative Atomic Displacements in an Anharmonic BCC Crystal

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Using the correlative method of unsymmetrized self-consistent field we study equilibrium atomic properties of anharmonic crystals. Here we calculate dynamical characteristics of a weakly anharmonic crystal with the body-centered cubic lattice, namely, the quadratic correlation moments between atomic displacements and the mean square relative atomic displacements. Taking into account the nearest neighbour interactions in this lattice, the second order of the method enables one to calculate the correlations between the nearest, second, third and fifth neighbours. An influence of more distant interactions is discussed. Results are also correlated with those calculated early for the simple and face-centered cubic lattices.

I. Introduction

The main characteristics describing the correlations between two physical quantities are the second- order correlation moments, or quadratic correlations, see, e.g. Terletsky.[1]

In crystals such features are the quadratic correlation moments of atomic positions (QCM) or those of their displacements from the lattice points $\overline{q_i q_j}$.[2] Here i and j express the atomic positions (lattice points). It is also well known that one of the most important characteristics of the lattice dynamics expressing the effective amplitude of the atomic vibrations are the mean square relative displacements (MSRD) between any two atoms in a crystal $\overline{(q_i q_j)^2}$. The considerable importance of such investigations depends, in particular, upon the fact that some melting laws are formulated on a basis of the mean square atomic displacements[2,3]. Note also that correlations are closely allied to fluctuations in a system, for instance, to fluctuations of density in which it has been regenerated interest in recent years, see, e.g. Yukalov.[4]

In the harmonic approximation, the quadratic correlation moments and the mean square relative displacements have been calculated using the dynamical theory of crystal lattices[2]. But this approximation is valid only at very low temperatures[5]. In this theory, the inclusion of anharmonicity into QCM and MSRD involves difficults.

To investigate an influence of anharmonic effects on the QCM and MSRD in crystals one can utilize the correlative method of unsymmetrized self-consistent field (CUSF)[6-12]. It is based on the density matrix or phase-space probability density which is unsymmetrical with respect to the interchange of coordinates between identical atoms. The possibility of wave functions without permutation symmetry for a system of identical particles had been noted by Messiah[13]. Unsymmetrical density matrices have been used, for instance, in Refs. 11, 14. Here we keep within the limits of the classical approach.

When there is no permutation symmetry, even in the mean-field approximation which is the zeroth-order one for CUSF, one takes into account the static correlations in crystals (long-range order) and the short-range dynamical correlations eliminating the unlimited approach of atoms to each other. Such an approximation also includes the main anharmonic terms of the power-series expansion of the potential energy. The statistical

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perturbation theory makes more accurate the contribution of the anharmonicity to thermodynamic functions of crystals, taking into consideration the influence of the dynamical interatomic correlations at intermediate and long distances. Just because of this, CUSF provides a good fit to experimental data for thermodynamic properties of the simple Van der Waals crystals, alkali halides, some metals and fullerites up to the melting temperatures, see Refs. 9, 15-19.

From the above discussion it follows that the correlations of the atomic displacements themselves are of interest as well. CUSF enables one to calculate such correlations and the mean square relative atomic displacements in anharmonic crystals, including strongly anharmonic ones. Recently it has been made for the linear chain[20, 21], and also for weakly anharmonic crystals with the simple and face-centered cubic lattices[22, 23] . Here we use the CUSF for working out QCM and MSRD in an weakly anharmonic crystal with the body-centered cubic lattice. This research is important because some metals have the BCC structure.

II. General Relations

One can calculate equilibrium statistical averages of arbitrary functions of atomic coordinates in a crystal using the spatial probability density particles represented in the form:

$$W(\vec{r}_1, ...\vec{r}_N) = Ce^{-U^0/\Theta} W^0(\vec{r}_1, ...\vec{r}_N) \tag{1}$$

where the zeroth approximation of CUSF

$$W^0(\vec{r}_1, ...\vec{r}_N) = \frac{e^{-U^0/\Theta}}{\int e^{-U^0/\Theta} d\vec{r}_1, ...d\vec{r}_N}, \tag{2}$$

depends on the sum of the self-consistent potentials U^0 of atoms performing anharmonic vibrations near their lattice points[8]. In (1), the perturbing potential $U' = U - U^0$ where U the potential energy of a crystal, and C is the normalization constant. Here we consider a perfect lattice with pairwise central interactions

$$U(\vec{r}_1, ...\vec{r}_N) = \frac{1}{2} \sum_{i \neq j} \Phi(|\vec{r}_i, ...\vec{r}_j|) \ . \tag{3}$$

In CUSF, the mean square relative displacements of two atoms can be expressed as

$$D_{aa}(ij) = \overline{(q_{ia} - q_{ja})^2} = \overline{q_{ia}} + \overline{q_{ja}} - 2C_{aa}(ij) \ ,$$

$$q = r_i - \hat{A} \cdot n_i \ , \tag{4}$$

where $\hat{A}$ is the lattice matrix, n_i are the integer-components vectors, a denotes the Cartesian components of atomic displacements and

$$C_{aa}(ij) = \overline{q_{ia} q_{ja}}, \tag{5}$$

are the quadratic correlation moments. Note that strictly speaking, the variances of atomic positions $\overline{q^2_{ia}}$ should be computed with fixed centre of mass of a crystal. CUSF provides just such computations.

Retaining the anharmonic terms up to fourth order in U', and after some manipulations, one can obtain the variances of the atomic positions in the second order perturbation theory given by [21]

$$\begin{aligned}
\overline{q^2_{ia}} \;=\;& \overline{q^2_{ia}}^0 + \frac{1}{2\Theta^2} \sum_k \Big\{ \Phi_{\alpha\beta}(ik) \Phi_{\gamma\delta}(ik) \overline{\beta_k \delta_k}^0 \left(\overline{a_i^2 \gamma_i \delta_i}^0 \overline{-a_i^2}^0 \overline{a_i^2}^0 \overline{\alpha_i \gamma_i}^0 \right) \\
+\;& \frac{1}{4} \Phi_{\alpha\beta\gamma}(ik) \Phi_{\delta\epsilon\chi}(ik) \Big[\overline{\gamma_k \chi_k}^0 \left(\overline{a_i \alpha_i \beta_i \delta_i \epsilon_i}^0 \overline{-a_i^2}^0 \overline{\alpha_i \beta_i \delta_i \epsilon_i}^0 \right) \\
-\;& 2\overline{\delta_i \epsilon_i}^0 \overline{\gamma_i \chi_i}^0 \left(\overline{a_i^2 \alpha_i \beta_i}^0 \overline{-a_i^2}^0 \overline{-a_i \beta_i}^0 \right) \\
+\;& \left(\overline{a_i^2 \alpha_i \delta_i}^0 - \overline{-a_i^2}^0 \overline{\alpha_i \delta_i}^0 \right) \left(\overline{\beta_k \gamma_k \epsilon_k \chi_k}^0 - \overline{\beta_k \gamma_k}^0 \overline{\epsilon_k \chi_k}^0 \right) \Big] \\
+\;& \frac{1}{3} \Phi_{\alpha\beta}(ik) \Phi_{\gamma\delta\epsilon\chi}(ik) \Big[\overline{\beta_k \chi_k}^0 \left(\overline{a_i^2 \alpha_i \gamma_i \delta_i \epsilon_i}^0 - \overline{a_i^2}^0 \overline{\alpha_i \gamma_i \delta_i \epsilon_i}^0 \right) \\
+\;& \overline{\beta_k \delta_k \epsilon_k \chi_k}^0 \left(\overline{a_i^2 \alpha_i \gamma_i}^0 \overline{-a_i^2} \overline{\alpha_i \gamma_i}^0 \right) \Big] \Big\}
\end{aligned} \tag{6}$$

were,

$$\Phi_{\alpha\beta\ldots}(ij) = \frac{\partial\ldots(\Phi(|\vec{r}|)}{\partial x_\alpha \partial x_{\beta\ldots}}\Big|_{r=\hat{A}(n_i-n_k)} , \tag{7}$$

are the derivatives of the interatomic potential. For shortness, we consider

$$\overline{a_i^2\alpha_i\beta_{i\ldots}} \equiv \overline{q_{a_i}^2 q_{\alpha_q} q_{\beta_i}\ldots}^{0} = \int a_{a_i}^2 a_{\alpha_i} q_{\beta_i}\ldots W^0(\vec{r}_1\ldots\vec{r}_N)d\vec{r}_1\ldots d\vec{r}_N \ , \tag{8}$$

where the zeroth attached to the bar denotes avering over the undisturbed moments, i.e., over that with the sum of the self-consistent potentials.

In a similar way, for the quadratic correlation moments we have [20]

$$\begin{aligned}
C_{ab} \ &= \ \frac{1}{\Theta}\Phi_{\alpha\beta}(ij)\overline{a_i\alpha_i}^{0}\overline{b_j\beta_j}^{0} + \frac{1}{6\Theta}\Phi_{\alpha\beta\gamma\delta}(ij)\left\{\overline{a_i\alpha_i\gamma_i\delta_i}^{0}\overline{b_j\beta_j}^{0} + \overline{a_i\alpha_i}^{0}\overline{a_j\alpha_j\gamma_j\delta_j}^{0}\right) \\
&+ \ \frac{1}{4\Theta^2}\left(\Phi_{\alpha\beta\gamma}(ij)\Phi_{\delta\epsilon\chi} + \Phi_{\alpha\beta}\Phi_{\gamma\delta\epsilon\chi}(ij)\right)\overline{\alpha_i\alpha_i\gamma_i\delta_i}^{0}\overline{b_j\beta_j\epsilon_j\chi_j}^{0} \\
&+ \ \frac{1}{4\Theta^2}\sum_k\Big\{4\Phi_{\alpha\gamma}(ik)\Phi_{\beta\delta}(jk)\overline{\alpha_i\alpha_i}^{0}\overline{b_j\beta_j}^{0}\overline{\gamma_k\delta_k}^{0} \\
&+ \ \Phi_{\alpha\beta\gamma}(ik)\Phi_{\delta\epsilon\chi}(jk)\overline{a_i\alpha_i}^{0}\overline{b_j\beta_j}^{0}\left(\overline{\beta_k\gamma_k\epsilon_k\chi_k}^{0} - \overline{\beta_k\gamma_k}^{0}\overline{\epsilon_k\chi_k}^{0}\right) \\
&+ \ \Phi_{\alpha\beta\gamma}(ij)\left(\Phi_{\delta\epsilon\chi}(jk)\overline{a_i\alpha_i}^{0}\overline{b_j\beta_j\gamma_j\delta_j}^{0} - \Phi_{\delta\epsilon\chi}(ik)\overline{a_i\alpha_i\gamma_i\delta_i}^{0}\overline{b_j\beta_j}^{0}\right)\overline{\epsilon_k\chi_k}^{0}\Big\} \\
&+ \ \frac{1}{6\Theta^2}\sum_k\Big\{\Phi_{\alpha\gamma}(ik)\Phi_{\beta\delta\epsilon\chi}(jk)\overline{a_i\alpha_i}^{0}\left(\overline{b_j\beta_j}^{0}\overline{\gamma_k\delta_k\epsilon_k\chi_k}^{0} + \overline{b_j\beta_j\delta_j\epsilon_j}^{0}\overline{\gamma_k\chi_k}^{0}\right) \\
&+ \ \Phi_{\beta\gamma}(jk)\Phi_{\alpha\delta\epsilon\chi}(ik)\overline{b_j\beta_j}^{0}\left(\overline{a_i\alpha_i}^{0}\overline{\gamma_k\delta_k\epsilon_k\chi_k}^{0} + \overline{a_i\alpha_i\delta_i\epsilon_i}^{0} + \overline{\gamma_k\chi_k}^{0}\right)\Big\} \ ,
\end{aligned} \tag{9}$$

Formulas (6) and (9) are valid for any Bravais lattice of arbitrary dimensionality.

III. A weakly anharmonic BCC crystal

We consider a crystal with the BCC lattice (Fig. 1) in the approximation of a weak anharmonicity, that is valid at not high temperatures. First we shall take into account only the nearest neighbour interactions. Then, in the lowest orders of anharmonicity, the interatomic distance at low pressures ($P \to 0$), is [12]

$$a \approx r_0 - \frac{3\Theta}{8f^2}\left(g + \frac{2f}{r_0}\right) \ . \tag{10}$$

In this case, the moments contained in (9) take the form

$$\begin{aligned}
\overline{q_\alpha^2}^{0} \ &\approx \ \frac{3\Theta}{8f}\left[1 + \frac{3\Theta}{8f^2}\left(\frac{g^2}{f} - h + \frac{4f}{r_0^2}\right)\right] \\
\overline{q_\alpha^4}^{0} \ &\approx \ \frac{27\Theta^2}{64f^2}\left[1 + \frac{\Theta}{4f^2}\left(\frac{3g^2}{f} - \frac{19h}{6} - \frac{2g}{r_0} + \frac{14f}{r_0^2}\right)\right] \\
\overline{q_\alpha^2 q_\beta^2}^{0} \ &\approx \ \frac{9\Theta^2}{64f^2}\left[1 + \frac{\Theta}{4f^2}\left(\frac{3g^2}{f} - \frac{7h}{2} + \frac{9f}{r_0^2}\right)\right] \ , \ \alpha \neq \beta \\
\overline{q_\alpha^6}^{0} \ &\approx \ 15\Theta^3\left(\frac{3}{8f}\right)^3
\end{aligned} \tag{11}$$

where r_0 is the minimum point of the interatomic potential and

$$f = \Theta^{II}(r_0), \ g = \Theta^{III}(r_0), \ h = \Phi^{IV}(r_0),$$

are the second, third and fifth derivatives in this point. To simplify calculations one can use a diagram technique [20, 21].

IV. Correlation moments and mean square relative displacements

After some manipulations, the variances of the atomic positions (6) in a weakly anharmonic BBC crystal become

$$\overline{q_\alpha^2} \approx \frac{33\Theta}{64f}\left[1+\frac{\Theta}{264f^2}\left(\frac{1457g^2}{9f}-\frac{173h}{2}-\frac{10g}{3r_0}+\frac{1654f}{3r_0^2}\right)\right] . \tag{12}$$

In this case, the first-order perturbation theory enables one to calculate QCM only between the nearest neighbours, while the second-order theory does also between the second, third and fifth ones. The corresponding interatomic distances are a, $2a/\sqrt{3}$, $4a/\sqrt{6}$, and $2a$. For any atomic pair we use in which the X-axis runs through their centres, see Fig. 1a.

For the nearest and fifth neighbours, it points in the [111] crystallographic direction while the orientations of the Y- and Z-axes are shown in Fig. 1b. We find

$$\begin{aligned} C_{xx}(1) &= \frac{9\Theta}{64f}\left[1+\frac{9\Theta}{768f^2}\left(59h\frac{23g^2}{f}+\frac{24g}{r_0}-\frac{68f}{r_0^2}\right)\right]; \\ C_{yy}(1) &= C_{zz}(1)-\frac{81g\Theta}{4096r_0f^3} \end{aligned} \tag{13}$$

$$\begin{aligned} C_{xx}(5) &= \frac{27\Theta}{512f}\left[1-\frac{3\Theta}{8f^2}\left(h-\frac{g^2}{2f}-\frac{3f}{r_0^2}\right)\right]; \\ C_{yy}(5) &= C_{zz}(5)-\left(\frac{9\Theta}{64fr_0}\right)^2 . \end{aligned} \tag{14}$$

For the second neighbours, it is natural to use the crystallographic coordinate system and we get

$$C_{xx}(2)=-C_{yy}(2)=-C_{zz}(2)=-\frac{3\Theta}{128f}\left[1+\frac{\Theta}{32f^2}\left(\frac{14g^2}{f}-12h+\frac{156f}{r_0^2}\right)\right] . \tag{15}$$

Finally, under a rotation of $\pi/4$ around the crystallographic Z-axis, we obtain for the third neighbours

$$\begin{aligned} C_{xx}(3) &= \frac{3\Theta}{128f}\left[1-\frac{\Theta}{128f^2}\left(12h-\frac{10g^2}{f}-\frac{24g}{r_0}-\frac{54f}{r_0^2}\right)\right]; \\ C_{yy}(3) &= -\frac{3}{2}\left(\frac{3\Theta}{32fr_0}\right)^2; \\ C_{zz}(3) &= -\frac{3\Theta}{256f}\left[1-\frac{\Theta}{16f^2}\left(6h-\frac{5g^2}{f}+\frac{30f}{r_0^2}\right)\right]; \end{aligned} \tag{16}$$

Note that because of the symmetry of the coordinate systems, the both components of transversal correlations between the nearest, second and fifth neighbours are the same: $C_{yy}(n) = C_{zz}(n), n = 1, 3, 5$. In general, the transversal correlation moments are much smaller than the longitudinal ones, however for the second neighbours they are equal in their absolute values but opposite in sign.

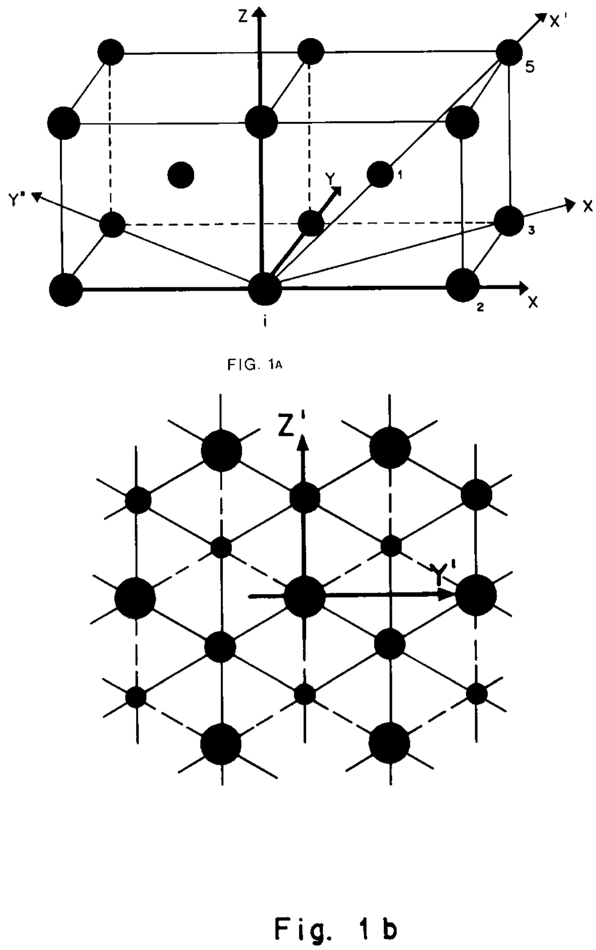

Figure 1. The arrangement of the neighbours of an atom in the BCC lattice. a) the spatial fragment of this lattice; b) its (111) section with the Y- and Z- coordinates for the nearest and fifth neighbours.

Inserting (12)-(16) into (4) we find the mean square relative displacements of the nearest, second, third and fifth neighbours. In this approximation, the MSRD of more distant atoms are equal to,

$$D_{\alpha\alpha}(n)=2\overline{q_\alpha^2}\ ,\quad n\geq 5\ . \tag{17}$$

In the numerical calculations we have utilized two typical for short-range potentials. The first one is the Morse potential

$$\Phi_M(r)=\epsilon[e^{-2\alpha(r-r_0)}-2e^{-\alpha(r-r_0)}]\ ,\alpha=6/r_0, \tag{18}$$

for which

$$f=72\epsilon/r_0^2,\quad g=-1296\epsilon/r_0^3,\quad h=18144\epsilon/r_0^4.$$

The second one is the Lennard-Jones potential

$$\Phi_{LJ}(r)=\epsilon\left[\left(\frac{r_0}{r}\right)^{12}-2\left(\frac{r_0}{r}\right)^6\right]\ , \tag{19}$$

in this case

$$f=72\epsilon/r_0^2,\quad g=-1512\epsilon/r_0^3,\quad h=26712\epsilon/r_0^4.$$

The latter is more anharmonic and decreases with increasing interatomic distance somewhat slower than former.

Both potentials give very close values except for $C_{xx}(1)$ and $C_{xx}(5)$ which are shown in Fig. 2 in relation to the dimensionless temperature kT/ϵ. A considarable difference of results decreasing with temperature (especially for the nearest neighbours) testifies that at high temperatures anharmonic effects are strong and formulae (10) and (11) used in calculations of correlation moments become invalid.

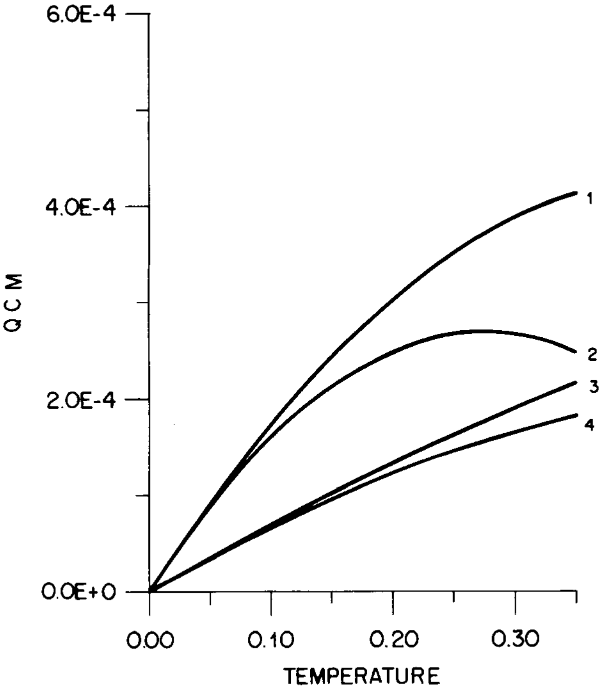

Figure 2. Longitudinal correlation moments C_{xx} between the nearest (1, 2) and fifth (3, 4) neighbours calculated using the Morse (1, 3) and Lenard-Jones (2, 4) potentials.

Fig. 3 demonstrates longitudinal and transversal correlation moments calulated using the Morse potential (18). Some moments are negative. This implies that corresponding atoms oscillate at such a direction for the most part opposite in phase. One can see also that the transversal correlation moments $C_{\alpha\alpha}(1)$ and $C_{\alpha\alpha}(5)$ $(\alpha = y, z)$ are very small, as well as $C_{yy}(3)$ which is not shown here. The negative sign of the longitudinal correlation moment in the second-order perturbation theory results from the obtuse angle between them and each of their common nearest neighbour. When this angle is acute, such a correlation is positive [23] and in the case of the straight angle, it is very small being proportional to the temperature squared.[22, 23]

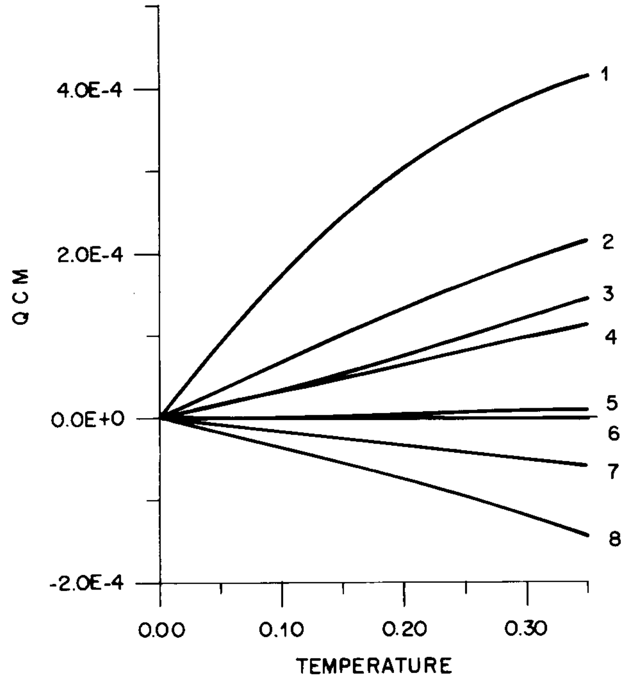

Figure 3. Correlation moments in the BCC lattice calculated using the Morse potential: $C_{xx}(1)$, 2 - $C_{xx}(5)$, 3 - $C_{yy}(2)$, 4 - $C_{xx}(3)$, 5 - $C_{yy}(1)$, 6 - $C_{yy}(5)$, 7 - $C_{zz}(3)$, 8 - $C_{xx}(2)$.

The mean square relative atomic displacements are shown in Fig. 4. The harmonic approximation for the nearest neighbours is given as well. One can see once more an importat role of anharmonic effects at high temperatures.

Note that in the BCC crystals, the interactions between more distant atoms play an important role. In particular, just such interactions provide the thermodynamic stability of this lattice.[24, 17] Consequently, it is appropriate here to estimate their influence on the interatomic correlations.

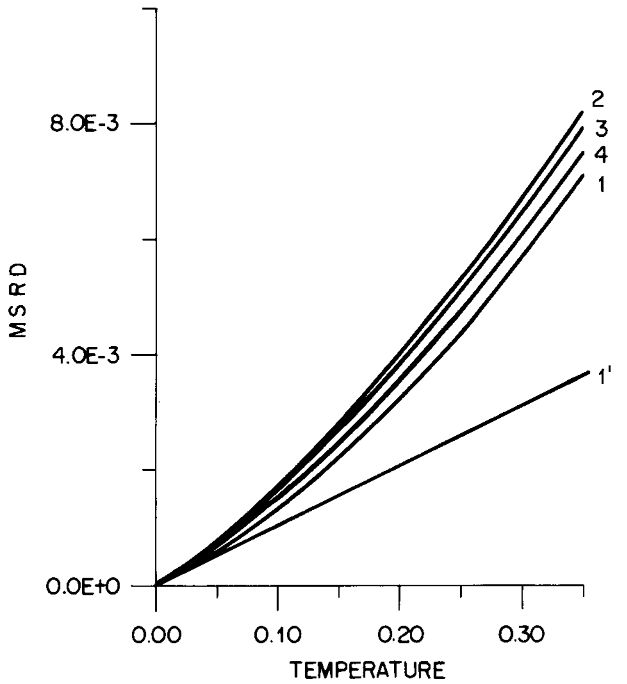

Figure 4. Longitudinal mean square relative displacements: 1- $D_{xx}(1)$, 2- $D_{xx}(2)$, 3- $D_{xx} \cong D_{xx}(n)$, $n \geq 6$; 4- $D_{xx}(5)$, 1'- $D_{xx}(1)$ in the harmonic approximation.

V. An influence of the more distant interactions

We shall study such an influence using the first-order perturbation theory. In this case, the interatomic distance is

$$a \approx r_0 - \frac{1}{Z_1 f} \sum_{l \geq 2} Z_l \nu_l e_l - \frac{3\Theta}{8f^2}\left(g + \frac{2f}{r_0}\right), (20)$$

instead of (10). Here ν_l are the dimensionless coefficients defining the coordinaton radii in a lattice $R_l = \nu_l a$, Z_l the coordination numbers, i.e. numbers of neighbours of a given atom which are situated at distances R_l, and $e_l = \Phi'(\nu_l r_0)$. (Clearly $\nu_1 = 1$ and $e_1 = 0$). In the case of the BCC lattice, $Z_1 = 8$, $Z_2 = 6$, $Z_3 = 12$, $Z_4 = 24$, $Z_5 = 8$, ... and $\nu_2 = 2/\sqrt{3} \approx 1.155$, $\nu_3 = 4a/\sqrt{6} \approx 1.633$, $\nu_4 = \sqrt{(11/3)} \approx 1.915$, $\nu_5 = 2, \ldots$. In this lattice, the difference between the nearest- and second-neighbour distances is about 15.5 %, while that between the second- and third-neighbour ones is more than 40 %. Hence, we shall include only the second-neighbour interactions. For the Morse and Lennard-Jones potentials, and $e_2 \approx 2.927\epsilon/r_0$, $f_2 \approx -7.673\epsilon/r_0^2$, respectively. In this case we obtain (21) As is seen from

Fig. 5, the second-neighbour interactions in the Morse or Lennard-Jones form decrease correlations between them. Contributions from the second-neighbour interactions to other correlation moments appearing in the second order of the perturbation theory are significally less.

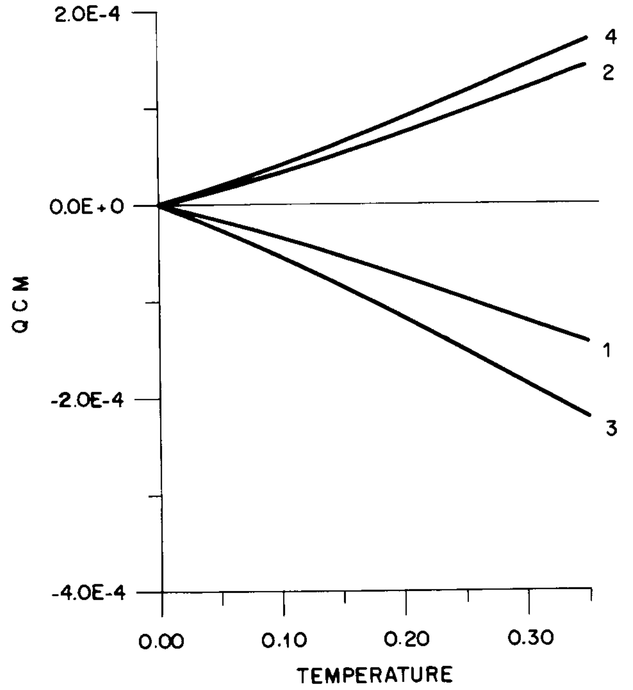

Figure 5. Longitudinal $C_{xx}(2)$ (1, 3) and transversal $C_{yy}(2)$ (2, 4) correlation moments without (1, 2) and with the second-neighbour interactions (3, 4).

VI. Discussion

So, we have calculate the interatomic correlation moments and mean square relative atomic displacements in a model of the anharmonic BCC crystal with pairwise interactions. For the most part, They are less than those in a simple cubic lattice [22] and more than in a face-centered cubic crystal [23]. It results from the fact that its packing is intermediate between those of SC and FCC lattices. The difference between results obtained with the Morse and Lennard-Jones potentials are due to anharmonic effects.

In conclusion note that the weakly anharmonic approximation used here provides good quantitative results at temperatures below about a half of the melting point (for thermodynamic properties see Refs. 7, 8, and for interatomic forrelations Ref. 21). For the BCC lattice, it corresponds to $kT/\epsilon \approx 0.175$. At higher temperature the strong anharmonicity must be taken into account. It is appropriate also to use more realistic potential for the BCC crystal, for instance the Schiff potential.[25] We intend to do this in the future.

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