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THE METHOD OF THE DEFORMATION OPERATOR IN QUANTUM ACOUSTICS — A FORMULATION OF PERTURBATION CALCULUS

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This paper gives a formulation of perturbation calculus which is useful for the description of coherent states related to the propagation of ultrasonic waves in crystals. This formulation is based on the results of the theory of coherent states, particularly on the properties of the deformation operator. The method of the construction of the initial state, which is used in perturbation calculus, is verified through comparison with the results of the method of the quasi-equilibrium density matrix based on the use of information theory in statistical physics. The method of perturbation calculus which is presented in this paper describes the time dependence of the mean value of any physical quantity for a crystal which undergoes dynamic deformation. This method makes it possible to grasp the dependence of phenomena observed on the phase and amplitude of the initially excited acoustic wave.

1. Introduction

This investigation used the properties of the deformation operator which is known from the theory of coherent states [1, 3, 6, 7, 9] to formulate perturbation calculus which describes effects related to the propagation of travelling ultrasonic waves in crystals. The method of the construction of the initial state, to be used in perturbation calculus, was verified through comparison with the results of the method of the quasi-equilibrium density matrix [2]. It was found that both methods lead to similar results, with the results being the same in the case of harmonic crystals. The difference which occurs in the general case is related to the fact that the method of the deformation operator does not account for the irreversible processes which occur in the dynamic deformation of crystals. An essential advantage of the method of the deformation operator is that it leads directly to a formulation of perturbation calculus.

The considerations given in this paper concern an infinite continuous medium; they can, however, be naturally extended to the case of a continuous medium.

2. Method of the deformation operator

The method of the deformation operator consists in the description of medium deformation by means of a unitary operator,

$$D(\{\alpha_{\boldsymbol{q},p}\}) = \exp\Big[\sum_{\boldsymbol{q},p}(\alpha_{\boldsymbol{q},p}\hat{a}^{+}_{\boldsymbol{q},p} - \bar{\alpha}_{\boldsymbol{q},p}\hat{a}_{\boldsymbol{q},p})\Big], \tag{1}$$

where $\boldsymbol{q}$ and p are wave vectors and phonon vibration branches [4, 5], $\hat{a}_{\boldsymbol{q},p}$ and $\hat{a}^{+}_{\boldsymbol{q},p}$ are the operators of phonon annihilation and creation [4, 5], $\alpha_{\boldsymbol{q},p}$ are complex numbers, and the dash over the variable denotes its complex conjugate.

As a result of crystal deformation, the wave function ψ which describes the state of the crystal before deformation passes into the function $\hat{D}(\{\alpha_{\boldsymbol{q},p}\})\psi$; thus, the deformation of the crystal described by the density matrix $\hat{\varrho}$ corresponds to the transformation of the density matrix

$$\hat{\varrho} \rightarrow \hat{D}(\{\alpha_{\boldsymbol{q},p}\})\hat{\varrho}\hat{D}^{-1}(\{\alpha_{\boldsymbol{q},p}\}). \tag{2}$$

Paper [3] gave a deformation operator which corresponds to static deformation; the considerations in [3] lead to the determination of the value of the coefficients $\alpha_{\boldsymbol{q},p}$,

$$\alpha_{\boldsymbol{q},p} = -\sum_{\boldsymbol{b},\boldsymbol{l},j} u\begin{pmatrix}\boldsymbol{l}\\ \boldsymbol{b}\end{pmatrix}_j i\sqrt{\frac{m_{\boldsymbol{b}}\,\omega(\boldsymbol{q},p)}{2NV\hbar}}\;\bar{e}\begin{pmatrix}\boldsymbol{q}\\ \boldsymbol{b}\end{pmatrix}_{j,p}\exp(-i\boldsymbol{q}\boldsymbol{l}), \tag{3}$$

where N is the number of elementary cells in unit volume, V is the volume of the crystal, $\boldsymbol{l}$ is a vector which defines the elementary cell [4, 5], i is imaginary unity (i.e. $i = \sqrt{-1}$), $m_{\boldsymbol{b}}$ is the mass of the atom which occupies the place in the elementary cell defined by the vector $\boldsymbol{b}$ [4, 5], $u\begin{pmatrix}\boldsymbol{l}\\ \boldsymbol{b}\end{pmatrix}_j$ is the jth component of the displacement of the corresponding atom, related to the deformation of the crystal, $e\begin{pmatrix}\boldsymbol{q}\\ \boldsymbol{b}\end{pmatrix}_{j,p}$ is a complex polarisation vector of the vibration mode corresponding to the wave vector $\boldsymbol{q}$ and the vibration branch p [4, 5], $\omega(\boldsymbol{q}, p)$ is the vibration frequency in the particular mode, and $\hbar$ is the Planck constant divided by 2π.

From the point of view of acoustics, the deformation operator with parameters defined by formula (3) has nevertheless a serious disadvantage. The initial stage which it serves to derive is useless in describing travelling waves.

This can be shown in the case of a harmonic crystal which is in a state of termodynamic equilibrium before deformation. Let $\hat{\varrho}$ be a density matrix which describes the crystal in a state of termodynamic equilibrium. The dependence of the deformation field on time can be found in the case when at $t = 0$ the crystal undergoes deformation which is represented by the deformation operator with parameters determined by formula (3).

The use of formula (2), the representation of the deformation field operator by the operators of phonon creation and annihilation [4, 5],

$$\hat{R}\binom{\boldsymbol{l}}{\boldsymbol{b}}_j = \sum_{\boldsymbol{q},p} \bar{e}\binom{\boldsymbol{q}}{\boldsymbol{b}}_{j,p} i\sqrt{\frac{\hbar}{2NVm_{\boldsymbol{b}}\,\omega(\boldsymbol{q},p)}}\,(\hat{a}_{-\boldsymbol{q},p} - \hat{a}^{+}_{\boldsymbol{q},p})\exp(-i\boldsymbol{q}\boldsymbol{i}), \tag{4}$$

where the notation is as in (3), the invariance of the trace with respect to the cyclic representation of the operators and formulae which follow from the commutation rules [6],

$$\begin{aligned} \hat{D}^{-1}(\{\alpha_{\boldsymbol{q},p}\})\,\hat{a}_{\boldsymbol{k},g}\,\hat{D}(\{\alpha_{\boldsymbol{q},p}\}) &= \hat{a}_{\boldsymbol{k},g} + \alpha_{\boldsymbol{k},g}; \\ \hat{D}^{-1}(\{\alpha_{\boldsymbol{q},p}\})\,\hat{a}^{+}_{\boldsymbol{k},g}\,\hat{D}(\{\alpha_{\boldsymbol{q},p}\}) &= \hat{a}_{\boldsymbol{k},g} + \bar{\alpha}_{\boldsymbol{k},g}; \end{aligned} \tag{5}$$

give

$$\begin{aligned} \left\langle\!\!\left\langle \hat{R}\binom{\boldsymbol{l}}{\boldsymbol{b}}_j(t) \right\rangle\!\!\right\rangle &= \mathrm{Tr}\left\{\hat{D}(\{\alpha_{\boldsymbol{q},p}\})\,\hat{\varrho}\,\hat{D}^{-1}(\{\alpha_{\boldsymbol{q},p}\})\,\hat{R}\binom{\boldsymbol{l}}{\boldsymbol{b}}_j(t)\right\} \\ &= \mathrm{Tr}\left\{\hat{\varrho}\,\hat{D}^{-1}(\{\alpha_{\boldsymbol{q},p}\})\,\hat{R}\binom{\boldsymbol{l}}{\boldsymbol{b}}_j(t)\,\hat{D}(\{\alpha_{\boldsymbol{q},p}\})\right\} \\ &= \sum_{\boldsymbol{q},p} \bar{e}\binom{\boldsymbol{q}}{\boldsymbol{b}}_{j,p} i\sqrt{\frac{\hbar}{2NVm_{\boldsymbol{b}}\,\omega(\boldsymbol{q},p)}}\,\{\alpha_{-\boldsymbol{q},p}\exp[-i\omega(-\boldsymbol{q},p)t] - \\ &\qquad - \bar{\alpha}_{\boldsymbol{q},p}\exp[i\omega(\boldsymbol{q},p)t]\exp(-i\boldsymbol{q}\boldsymbol{l}), \end{aligned} \tag{6}$$

where $\langle\!\langle \hat{A} \rangle\!\rangle$ is the mean value of the operator $\hat{A}$ and $\mathrm{Tr}\{\hat{A}\}$ is the trace of this operator.

When Q denotes such a set of wave vectors that out of each pair $\{\boldsymbol{q}, -\boldsymbol{q}\}$ strictly one vector belongs to Q, the mean (6) can be written in the form

$$\begin{aligned} \left\langle\!\!\left\langle \hat{R}\binom{\boldsymbol{l}}{\boldsymbol{b}}_j(t) \right\rangle\!\!\right\rangle &= \sum_{p,\boldsymbol{q}\in Q} i\sqrt{\frac{\hbar}{2NVm_{\boldsymbol{b}}\,\omega(\boldsymbol{q},p)}}\left\{\bar{e}\binom{\boldsymbol{q}}{\boldsymbol{b}}_{j,p}\alpha_{-\boldsymbol{q},p}\exp[-i\omega(-\boldsymbol{q},p)t]\times\right. \\ &\times\exp(-i\boldsymbol{q}\boldsymbol{l}) - \bar{e}\binom{\boldsymbol{q}}{\boldsymbol{b}}_{j,p}\bar{\alpha}_{\boldsymbol{q},p}\exp[i\omega(\boldsymbol{q},p)t]\exp(-i\boldsymbol{q}\boldsymbol{l}) + \\ &+ \bar{e}\binom{\boldsymbol{q}}{\boldsymbol{b}_{j,p}}\alpha_{\boldsymbol{q},p}\exp[-i\omega(\boldsymbol{q},p)t]\exp(i\boldsymbol{q}\boldsymbol{l}) - \bar{e}\binom{-\boldsymbol{q}}{\boldsymbol{b}}_{j,p}\bar{\alpha}_{-\boldsymbol{q},p}\exp[i\omega(-\boldsymbol{q},p)t]\times \\ &\left.\times\exp(i\boldsymbol{q}\boldsymbol{l})\right\}. \end{aligned} \tag{7}$$

Taking into account the identities [4, 5]

$$\omega(-\boldsymbol{q}, p) = \omega(\boldsymbol{q}, p); \qquad \bar{e}\begin{pmatrix} -\boldsymbol{q} \\ \boldsymbol{b} \end{pmatrix}_{j,p} = e\begin{pmatrix} \boldsymbol{q} \\ \boldsymbol{b} \end{pmatrix}_{j,p} \tag{8}$$

and the following relation which results from (3)

$$\bar{a}_{\boldsymbol{q},p} = -a_{-\boldsymbol{q},p}, \tag{9}$$

gives

$$\left\langle\left\langle \hat{R}\begin{pmatrix} \boldsymbol{l} \\ \boldsymbol{b} \end{pmatrix}_j (t) \right\rangle\right\rangle = \sum_{p,\boldsymbol{q}\in Q} - \sqrt{\frac{{}^{0}_{0}\hbar}{NVm_{\boldsymbol{b}}\,\omega(\boldsymbol{q}\ ,p)}}\ \mathrm{Im}\left\{ e\begin{pmatrix} \boldsymbol{q} \\ \boldsymbol{b} \end{pmatrix}_{j,p} a_{\boldsymbol{q},p} \exp(i\boldsymbol{q}\boldsymbol{l}) \right\} \cos\omega(\boldsymbol{q}, p)t, \tag{10}$$

where Im is the imaginary part of the complex number.

In expression (10) no more than one standing wave corresponds to each vibration mode and to each pair $\{\boldsymbol{q}, -\boldsymbol{q}\}$. It thus follows that the initial state which leads to the formation of a single travelling wave in the crystal cannot be derived with deformation represented by the deformation operator with the parameters $a_{\boldsymbol{q},p}$ defined by formula (3).

An attempt can now be made to modify the present procedure so that it may also be used in the case of the travelling wave. The analogy to quantum optics where arbitrary complex numbers can become parametres which occur in the deformation operator may be used for this purpose [7, 8].

Let $R'\begin{pmatrix} \boldsymbol{l} \\ \boldsymbol{b} \end{pmatrix}_j$ and $P'\begin{pmatrix} \boldsymbol{l} \\ \boldsymbol{b} \end{pmatrix}_j$ denote predetermined values of displacement and momentum of atoms, let $\hat{D}(\{a_{\boldsymbol{q},p}\})$ be a deformation operator with arbitrary complex coefficients (particularly those which do not necessarily satisfy relation (9)) and let $\hat{\varrho}$ denote some density matrix which describes the crystal. The mean values of position and momentum of the atoms in the state $\hat{\varrho}$ will be represented by $r\begin{pmatrix} \boldsymbol{l} \\ \boldsymbol{b} \end{pmatrix}_j$ and $p\begin{pmatrix} \boldsymbol{l} \\ \boldsymbol{b} \end{pmatrix}_j$.

The parameters of the deformation operator can be determined so that the operation

$$\hat{\varrho} \to \hat{D}(\{a_{\boldsymbol{q},p}\})\hat{\varrho}\,\hat{D}^{-1}(\{a_{\boldsymbol{q},p}\})$$

leads to a change in the mean values of the position of the atoms from $r\begin{pmatrix} \boldsymbol{l} \\ \boldsymbol{b} \end{pmatrix}_j$ to $r\begin{pmatrix} \boldsymbol{l} \\ \boldsymbol{b} \end{pmatrix}_j + R'\begin{pmatrix} \boldsymbol{l} \\ \boldsymbol{b} \end{pmatrix}_j$ and a change in the mean momentum values from $p\begin{pmatrix} \boldsymbol{l} \\ \boldsymbol{b} \end{pmatrix}_j$ to $p\begin{pmatrix} \boldsymbol{l} \\ \boldsymbol{b} \end{pmatrix}_j + P'\begin{pmatrix} \boldsymbol{l} \\ \boldsymbol{b} \end{pmatrix}_j$. The use of formulae (5) and (8) and the representation of the momentum operators by the operators of phonon creation and annihilation [4, 5]

$$\hat{P}\begin{pmatrix}\boldsymbol{l}\\ \boldsymbol{b}\end{pmatrix}_j = \sum_{\boldsymbol{q},p} \sqrt{\frac{m_b\hbar\omega(\boldsymbol{q},p)}{2NV}} \left\{ e\begin{pmatrix}\boldsymbol{q}\\ \boldsymbol{b}\end{pmatrix}_{j,p} \hat{a}_{\boldsymbol{q},p}\exp(i\boldsymbol{q}\boldsymbol{l}) + \bar{e}\begin{pmatrix}\boldsymbol{q}\\ \boldsymbol{b}\end{pmatrix}_{j,p} \hat{a}^{+}_{q,p}\exp(-i\boldsymbol{q}\boldsymbol{l}) \right\}, \tag{11}$$

give

$$\left\langle\left\langle \hat{R}\begin{pmatrix}\boldsymbol{l}\\ \boldsymbol{b}\end{pmatrix}_j \right\rangle\right\rangle = \mathrm{Tr}\left\{\hat{D}(\{\alpha_{\boldsymbol{q},p}\})\hat{\varrho}\hat{D}^{-1}(\{\alpha_{\boldsymbol{q},p}\})\hat{R}\begin{pmatrix}\boldsymbol{l}\\ \boldsymbol{b}\end{pmatrix}_j\right\}$$

$$= \mathrm{Tr}\{\hat{\varrho}\hat{D}^{-1}(\{\alpha_{\boldsymbol{q},p}\})\hat{R}\begin{pmatrix}\boldsymbol{l}\\ \boldsymbol{b}\end{pmatrix}_j \hat{D}(\{\alpha_{\boldsymbol{q},p}\})$$

$$= r\begin{pmatrix}\boldsymbol{l}\\ \boldsymbol{b}\end{pmatrix}_j + \sum_{\boldsymbol{q},p} \bar{e}\begin{pmatrix}\boldsymbol{q}\\ \boldsymbol{b}\end{pmatrix}_{j,p} i\sqrt{\frac{\hbar}{2NVm_{\boldsymbol{b}}\omega(\boldsymbol{q},p)}}(\alpha_{-\boldsymbol{q},p}-\bar{\alpha}_{\boldsymbol{q},p})\exp(-i\boldsymbol{q}\boldsymbol{l});$$

$$\left\langle\left\langle \hat{P}\begin{pmatrix}\boldsymbol{l}\\ \boldsymbol{b}\end{pmatrix}_j \right\rangle\right\rangle = \mathrm{Tr}\left\{\hat{D}(\{\alpha_{\boldsymbol{q},p}\})\hat{\varrho}\hat{D}^{-1}(\{\alpha_{\boldsymbol{q},p}\})\hat{P}\begin{pmatrix}\boldsymbol{l}\\ \boldsymbol{b}\end{pmatrix}_j\right\} = \mathrm{Tr}\{\hat{\varrho}\hat{D}^{-1}(\{\alpha_{\boldsymbol{q},p}\}) \times$$

$$\times \hat{P}\begin{pmatrix}\boldsymbol{l}\\ \boldsymbol{b}\end{pmatrix}_j \hat{D}(\{\alpha_{\boldsymbol{q},p}\})\}$$

$$= p\begin{pmatrix}\boldsymbol{l}\\ \boldsymbol{b}\end{pmatrix}_j + \sum_{\boldsymbol{q},p}\sqrt{\frac{m_b\hbar\omega(\boldsymbol{q},p)}{2NV}}\, e\begin{pmatrix}\boldsymbol{q}\\ \boldsymbol{b}\end{pmatrix}_{j,p}(\alpha_{\boldsymbol{q},p}+\bar{\alpha}_{-\boldsymbol{q},p})\exp(i\boldsymbol{q}\boldsymbol{l}). \tag{12}$$

From the system of equations

$$\sum_{\boldsymbol{q},p} \bar{e}\begin{pmatrix}\boldsymbol{q}\\ \boldsymbol{b}\end{pmatrix}_{j,p} i\sqrt{\frac{\hbar}{2NVm_{\boldsymbol{b}}\omega(\boldsymbol{q},p)}}(\alpha_{\boldsymbol{q},p}-\bar{\alpha}_{\boldsymbol{q},p})\exp(-i\boldsymbol{q}\boldsymbol{l}) = R'\begin{pmatrix}\boldsymbol{l}\\ \boldsymbol{b}\end{pmatrix}_j;$$

$$\sum_{\boldsymbol{q},p} e\begin{pmatrix}\boldsymbol{q}\\ \boldsymbol{b}\end{pmatrix}_{j,p} \sqrt{\frac{\hbar}{2NVm_{\boldsymbol{b}}\omega(\boldsymbol{q},p)}}(\alpha_{\boldsymbol{q},p}+\bar{\alpha}_{-\boldsymbol{q},p})\exp(i\boldsymbol{q}\boldsymbol{l}) = P'\begin{pmatrix}\boldsymbol{l}\\ \boldsymbol{b}\end{pmatrix}_j; \tag{13}$$

the following formula can be obtained

$$\alpha_{\boldsymbol{q},p} = \sum_{\boldsymbol{l},\boldsymbol{b},j}\left\{\sqrt{\frac{1}{2NVm_{\boldsymbol{b}}\hbar\omega(\boldsymbol{q},p)}}\,P'\begin{pmatrix}\boldsymbol{l}\\ \boldsymbol{b}\end{pmatrix}_j - i\sqrt{\frac{m_b\omega(\boldsymbol{q},p)}{2NV\hbar}}\,R'\begin{pmatrix}\boldsymbol{l}\\ \boldsymbol{b}\end{pmatrix}_j\right\}\bar{e}\begin{pmatrix}\boldsymbol{q}\\ \boldsymbol{b}\end{pmatrix}_{j,p} \times$$

$$\times\exp(-i\boldsymbol{q}\boldsymbol{l}). \tag{14}$$

It can be seen that in a specific case of static deformation when $P'\begin{pmatrix}\boldsymbol{l}\\ \boldsymbol{b}\end{pmatrix}_j = 0$ formula (14) can be reduced to (3). In a general case $P'\begin{pmatrix}\boldsymbol{l}\\ \boldsymbol{b}\end{pmatrix}_j \neq 0$ and the parameters $\alpha_{\boldsymbol{q},p}$ defined by formula (4) can take any complex values. It can readily be shown that the deformation operator with its parameters defined by (14) can describe perturbations which lead to the formation of travelling waves in the crystal. The assumption of a harmonic crystal and the repetition of the train of thought which previously gave formula (10) now give

$$\left\langle\!\left\langle \hat{R}\begin{pmatrix} \boldsymbol{l} \\ \boldsymbol{b} \end{pmatrix}_j (t) \right\rangle\!\right\rangle$$
$$= -\sum_{\boldsymbol{q},p} \sqrt{\frac{2\hbar}{NVm_{\boldsymbol{b}}\omega(\boldsymbol{q},p)}}\ \mathrm{Im}\left\{\alpha_{\boldsymbol{q},p} e\begin{pmatrix} \boldsymbol{q} \\ \boldsymbol{b} \end{pmatrix}_{j,p} \exp\{-i[\omega(\boldsymbol{q},p)t - \boldsymbol{q}\boldsymbol{l}]\}\right\}. \tag{15}$$

In particular, the choice of $\alpha_{\boldsymbol{q},p} = \delta_{\boldsymbol{q},\boldsymbol{d}}\delta_{p,s}(\delta_{\boldsymbol{q},\boldsymbol{d}}$ and $\delta_{p,s}$ denote particular Kronecker deltas) leads to an evolution of the deformation field which corresponds to the propagation of a single S-type travelling wave with the wave vector $\boldsymbol{d}$. It can thus be seen that in effect the present procedure of the "imposition" on the crystal of arbitrary fields of the displacements $R'\begin{pmatrix} \boldsymbol{l} \\ \boldsymbol{b} \end{pmatrix}_j$ and velocities $P'\begin{pmatrix} \boldsymbol{l} \\ \boldsymbol{b} \end{pmatrix}_j / m_{\boldsymbol{b}}$ of the atoms permits the construction of initial states which are useful for describing travelling waves.

This approach is extremely convenient, since it will be seen that it leads in a natural way to the formulation of perturbation calculus.

Let the crystal in a state described by the density matrix undergo at a time $t = 0$ dynamic deformation represented by the deformation operator $\hat{D}(\{\alpha_{\boldsymbol{q},p}\})$, where the parameters $\alpha_{\boldsymbol{q},p}$ are defined by predetermined fields of displacement and momentum of atoms according to formula (14). After deformation the crystal is therefore described by the density matrix $\hat{D}(\{\alpha_{\boldsymbol{q},p}\})\hat{\varrho}\hat{D}^{-1}(\{\alpha_{\boldsymbol{q},p}\})$ and thus the mean value of the arbitrary operator $\hat{A}$ at a time t, $t > 0$, is

$$\langle\!\langle \hat{A}(t) \rangle\!\rangle = \frac{\mathrm{Tr}\{\hat{D}(\{\alpha_{\boldsymbol{q},p}\})\hat{\varrho}D^{-1}(\{\alpha_{\boldsymbol{q},p}\})\hat{A}(t)\}}{\mathrm{Tr}\{\hat{D}(\{\alpha_{\boldsymbol{q},p}\})\hat{\varrho}\hat{D}^{-1}(\{\alpha_{\boldsymbol{q},p}\})}$$
$$= \frac{\mathrm{Tr}\left\{\hat{D}(\{\alpha_{\boldsymbol{q},p}\})\hat{\varrho}\hat{D}^{-1}(\{\alpha_{\boldsymbol{q},p}\})\exp\left(\frac{i}{\hbar}Ht\right)A\exp\left(-\frac{i}{\hbar}Ht\right)\right\}}{\mathrm{Tr}\{\hat{D}\{(\alpha_{\boldsymbol{q},p}\})\hat{\varrho}\hat{D}^{-1}(\{\alpha_{\boldsymbol{q},p}\})\}}. \tag{16}$$

Cyclic transpositions under the trace sign and the use of the unitariness of the deformation operator give

$$\langle\!\langle A(t) \rangle\!\rangle = \frac{\mathrm{Tr}\left\{\hat{D}(\{\alpha_{\boldsymbol{q},p}\})\hat{\varrho}\hat{D}^{-1}(\{\alpha_{\boldsymbol{q},p}\})\exp\left(\frac{i}{\hbar}Ht\right)A\exp\left(-\frac{i}{\hbar}Ht\right)\right\}}{\mathrm{Tr}\{\hat{D}(\{\alpha_{\boldsymbol{q},p}\})\hat{\varrho}\hat{D}^{-1}(\alpha\{_{\boldsymbol{q},p}\})\}}$$
$$= \mathrm{Tr}\left\{\hat{\varrho}\hat{D}^{-1}(\{\alpha_{\boldsymbol{q},p}\})\exp\left(\frac{i}{\hbar}\hat{H}t\right)\hat{D}(\{\alpha_{\boldsymbol{q},p}\})\hat{D}^{-1}(\{\alpha_{\boldsymbol{q},p}\})\hat{A}\hat{D}(\{\alpha_{\boldsymbol{q},p}\})\hat{D}^{-1}(\{\alpha_{\boldsymbol{q},p}\}) \times \right.$$
$$\left. \times\exp\left(-\frac{i}{\hbar}Ht\right)\hat{D}(\{\alpha_{\boldsymbol{q},p}\})\right\}$$

$$= \operatorname{Tr}\left\{\hat{\varrho}\exp\left[\frac{i}{\hbar}\hat{D}^{-1}(\{a_{\boldsymbol{q},p}\})\hat{H}\hat{D}(\{a_{\boldsymbol{q},p}\})t\right]\hat{D}^{-1}(\{a_{\boldsymbol{q},p}\})\hat{A}\hat{D}(\{a_{\boldsymbol{q},p}\})\times\right. \tag{17}$$
$$\left.\times\exp\left[-\frac{i}{\hbar}\hat{D}^{-1}(\{a_{\boldsymbol{q},p}\})\hat{H}\hat{D}(\{a_{\boldsymbol{q},p}\})t\right]\right\}.$$

It can be seen that formally expression (17) can be interpreted as the mean value of the operator $\hat{D}^{-1}(\{a_{\boldsymbol{q},p}\})\hat{A}\hat{D}(\{a_{\boldsymbol{q},p}\})$ at a time $t, t > 0$, when the time dependence of the operator $\hat{D}^{-1}(\{a_{\boldsymbol{q},p}\})\hat{A}\hat{D}(\{a_{\boldsymbol{q},p}\})$ is defined by Heisenberg representation corresponding to the "hamiltonian" $\hat{D}^{-1}(\{a_{\boldsymbol{q},p}\})\hat{H}\hat{D}(\{a_{\boldsymbol{q},p}\})$ and the state of the crystal is described by the density matrix $\hat{\varrho}$.

All hamiltonians which occur in quantum acoustics are, in terms of the operators of phonon creation and annihilation, polynomials of finite order. In this case, it follows from formulae (5) that the "new" hamiltonian $\hat{D}^{-1}(\{a_{\boldsymbol{q},p}\})\hat{H}\hat{D}(\{a_{\boldsymbol{q},p}\})$ consists of the "old" hamiltonian $\hat{H}$ and the "remainder" $\hat{D}^{-1}(\{a_{\boldsymbol{q},p}\})\hat{H}\hat{D}(\{a_{\boldsymbol{q},p}\})-\hat{H}$. The remainder is the sum of terms each of which, in terms of the numbers $a_{\boldsymbol{q},p}$ and $\bar{a}_{\boldsymbol{q},p}$, is a polynomial of at least the first order.

In the case when

$$\hat{H}' = \hat{D}^{-1}(\{a_{\boldsymbol{q},p}\})\hat{H}\hat{D}(\{a_{\boldsymbol{q},p}\})-\hat{H} \tag{18}$$

is much smaller than $\hat{H}$, it is possible, treating $\hat{H}'$ as perturbation and $\hat{H}$ as unperturbed hamiltonian, to represent the mean value of the operator $\hat{A}$ for $t > 0$ by the response of the system to the sudden introduction of the perturbation $\hat{H}'$ at a time $t = 0$ [2],

$$\langle\!\langle \hat{A}(t)\rangle\!\rangle = \operatorname{Tr}\left\{\hat{\varrho}\exp\left(\frac{i}{\hbar}\hat{H}t\right)\hat{D}^{-1}(\{a_{\boldsymbol{q},p}\})\hat{A}\hat{D}(\{a_{\boldsymbol{q},p}\})\exp\left(-\frac{i}{\hbar}\hat{H}t\right)\right\}+$$
$$+\sum_{n=1}^{\infty}\left(\frac{1}{i\hbar}\right)^{n}\int_{0}^{t}\int_{0}^{t_1}\ldots\int_{0}^{t_{n-1}}dt_1\ldots dt_n\operatorname{Tr}\left\{\left(\hat{D}^{-1}(\{a_{\boldsymbol{q},p}\})\hat{A}\hat{D}(\{a_{\boldsymbol{q},p}\})\right)t\times\right.$$
$$\left.\times\left[\hat{H}'_{t_1}\left[\ldots\left[\hat{H}'_{t_n},\hat{\varrho}\right]\ldots\right]\right\}. \tag{19}$$

(The time dependence of the operators which occur in the subintegral function is defined by Heisenberg representation corresponding to the hamiltonian $\hat{H}$.)

3. Method of the quasi-equilibrium density matrix

The method of the quasi-equilibrium density matrix [2] can serve to determine the statistical quantum state representing a crystal with predetermined mean values of the displacement and velocity fields and with predetermined mean energy. In terms of information theory it can be stated that the task is to eliminate "excess" information (related to the description of the microscopic state of the system) from the density matrix describing the crystal and at the same time to retain that information which corresponds to the given mean values of the predetermined physical quantities.

The solution results from the taking into account of the fact that in practice the crystal is never fully isolated from the environment which plays the role of the thermostat. The interaction between the crystal and the thermostat is random and leads to part of the information contained in the density matrix being "forgotten" [2]. (In classical statistical physics this process involves a "fuzziness" of the trajectories describing the evolution of the system in the phase space, which leads to a smoothing of the distribution function).

The information which corresponds to the predetermined mean values of displacement and momentum of atoms and the predetermined mean energy of the crystal is imposed by the generator exciting ultrasonic waves and the temperature of the thermostat, and therefore it is not "forgotten". It can thus be seen that the density matrix of interest can be determined by the variational method, seeking such a statistical state to which there corresponds the maximum value of information entropy [2]

$$S = -\mathrm{Tr}\{\hat{\varrho}\ln\hat{\varrho}\}, \tag{20}$$

under the condition of a definite mean value of the total energy of the crystal

$$\langle\!\langle \hat{H} \rangle\!\rangle = E, \tag{21}$$

the conditions corresponding to the predetermined mean values of the displacement of the atoms from the equilibrium positions

$$\left\langle\!\!\left\langle \hat{R}\begin{pmatrix} \boldsymbol{l} \\ \boldsymbol{b} \end{pmatrix}_j \right\rangle\!\!\right\rangle = R\begin{pmatrix} \boldsymbol{l} \\ \boldsymbol{b} \end{pmatrix}_j, \tag{22}$$

the conditions corresponding to the predetermined mean values of the momentum of the atoms

$$\left\langle\!\!\left\langle \hat{P}\begin{pmatrix} \boldsymbol{l} \\ \boldsymbol{b} \end{pmatrix}_j \right\rangle\!\!\right\rangle = P\begin{pmatrix} \boldsymbol{l} \\ \boldsymbol{b} \end{pmatrix}_j \tag{23}$$

and the condition of normalisation of the density matrix

$$\langle\!\langle \hat{\varrho} \rangle\!\rangle = 1. \tag{24}$$

The solution of the present variational problem is the density matrix [2]

$$\hat{\varrho} = \exp\left[-\Phi - \beta\hat{H} - \sum_{\boldsymbol{l},\boldsymbol{b},j} f\begin{pmatrix} \boldsymbol{l} \\ \boldsymbol{b} \end{pmatrix}_j \hat{R}\begin{pmatrix} \boldsymbol{l} \\ \boldsymbol{b} \end{pmatrix}_j - \sum_{\boldsymbol{l},\boldsymbol{b},j} h\begin{pmatrix} \boldsymbol{l} \\ \boldsymbol{b} \end{pmatrix}_j \hat{P}\begin{pmatrix} \boldsymbol{l} \\ \boldsymbol{b} \end{pmatrix}_j\right], \tag{25}$$

where $f\begin{pmatrix} \boldsymbol{l} \\ \boldsymbol{b} \end{pmatrix}_j$ are Lagrange multipliers corresponding to the conditions of the predetermined mean values of the displacement of atoms, $h\begin{pmatrix} \boldsymbol{l} \\ \boldsymbol{b} \end{pmatrix}_j$ are Lagrange multipliers corresponding to the conditions of the predetermined mean values of the momentum of atoms, β is a Lagrange multiplier corresponding to the condition of the predetermined mean energy of the crystal and with interpretation $1/kT$ (k being a Boltzmann constant and T the absolute temperature of the crystal), and $\Phi - 1$ is a Lagrange multiplier corresponding to the condition of normalisation of the density matrix.

It can readily be shown that differentiation of $-\Phi$ with respect to β, $h\begin{pmatrix}\boldsymbol{l}\\ \boldsymbol{b}\end{pmatrix}_j$ and $f\begin{pmatrix}\boldsymbol{l}\\ \boldsymbol{b}\end{pmatrix}_j$ gives respectively the mean value of the total energy of the crystal, the mean values of the momentum of atoms and the mean values of the displacement of atoms from the equilibrium positions. It can be seen that in a specific case when the predetermined mean values of the momentum of atoms and the mean values of the displacement of atoms from the equilibrium positions are zero, the Lagrange factors $h\begin{pmatrix}\boldsymbol{l}\\ \boldsymbol{b}\end{pmatrix}_j$ and $f\begin{pmatrix}\boldsymbol{l}\\ \boldsymbol{b}\end{pmatrix}_j$ are also zero and the density matrix (25) describes the state of thermodynamic equilibrium (corresponding to the canonical distribution).

4. Comparison of the results of the two methods

The results obtained by the method of the deformation operator and by the method of the quasi-equilibrium density matrix can first be compared for the case of a harmonic crystal. The method of the deformation operator can serve to find a density matrix which describes a dynamically deformed harmonic crystal which before deformation was in the state of thermodynamic equilibrium described by the canonical distribution.

Consideration of formulae (2) and (5) and the identity, which results from definition (1),

$$\hat{D}(\{a_{\boldsymbol{q},p}\}) = \hat{D}^{-1}(\{-a_{\boldsymbol{q},p}\}), \tag{26}$$

gives

$$\begin{aligned}\hat{\varrho} &= \hat{D}(\{a_{\boldsymbol{q},p}\})\exp\Big[-\Phi-\beta\sum_{\boldsymbol{k},g}\hbar\omega(\boldsymbol{k},g)\,\hat{a}^{+}_{\boldsymbol{k},g}\hat{a}_{\boldsymbol{k},g}\Big]\hat{D}^{-1}(\{a_{\boldsymbol{q},p}\})\\ &= \hat{D}^{-1}(\{-a_{\boldsymbol{q},p}\})\exp\Big[-\Phi-\beta\sum_{\boldsymbol{k},g}\hbar\omega(\boldsymbol{k},g)\,\hat{a}^{+}_{\boldsymbol{k},g}\hat{a}_{\boldsymbol{k},g}\Big]\hat{D}(\{-a_{\boldsymbol{q},p}\})\\ &= \frac{\exp\big[-\beta\sum\limits_{\boldsymbol{k},g}\hbar\omega(\boldsymbol{k},g)\,\hat{a}^{+}_{\boldsymbol{k},g}\hat{a}_{\boldsymbol{k},g}+\beta\sum\limits_{\boldsymbol{k},g}a_{\boldsymbol{k},g}\hat{a}^{+}_{\boldsymbol{k},g}+\beta\sum\limits_{\boldsymbol{k},g}\bar{a}_{\boldsymbol{k},g}\hat{a}_{\boldsymbol{k},g}\big]}{\mathrm{Tr}\big\{\exp\big[-\beta\sum\limits_{\boldsymbol{k},g}\hbar\omega(\boldsymbol{k},g)\,\hat{a}^{+}_{\boldsymbol{k},g}\hat{a}_{\boldsymbol{k},g}+\beta\sum\limits_{\boldsymbol{k},g}a_{\boldsymbol{k},g}\hat{a}^{+}_{\boldsymbol{k},g}+\beta\sum\limits_{\boldsymbol{k},g}\bar{a}_{\boldsymbol{k},g}\hat{a}_{\boldsymbol{k},g}\big]\big\}},\end{aligned} \tag{27}$$

(the values of the parameters $a_{\boldsymbol{q},p}$ in (27) are defined by formulae (14) and the other notation remains as above).

Using formula (4) and (11) the quasi-equilibrium density matrix which describes a dynamically deformed harmonic crystal can be expressed by the operators of phonon creation and annihilation

$$\hat{\varrho} = \exp\Big[-\Phi' - \beta' \sum_{\boldsymbol{k},g} \hbar\omega(\boldsymbol{k}, g)\, \hat{a}^{+}_{\boldsymbol{k},g} \hat{a}_{\boldsymbol{k},g} - \sum_{\boldsymbol{k},g} f\binom{\boldsymbol{l}}{\boldsymbol{b}}_j \hat{R}\binom{\boldsymbol{l}}{\boldsymbol{b}}_j - \sum_{\boldsymbol{k},g} h\binom{\boldsymbol{l}}{\boldsymbol{b}}_j \hat{P}\binom{\boldsymbol{l}}{\boldsymbol{b}}_j$$

$$= \frac{\exp\big[-\beta' \sum\limits_{\boldsymbol{k},g} \hbar\omega(\boldsymbol{k}, g)\, \hat{a}^{+}_{\boldsymbol{k},g} \hat{a}_{\boldsymbol{k},g} - \sum\limits_{\boldsymbol{k},g} \bar{\gamma}_{\boldsymbol{k},g} \hat{a}_{\boldsymbol{k},g} - \sum\limits_{\boldsymbol{k},g} \gamma_{\boldsymbol{k},g} \hat{a}^{+}_{\boldsymbol{k},g}\big]}{\mathrm{Tr}\big\{\exp\big[-\beta' \sum\limits_{\boldsymbol{k},g} \hbar\omega(\boldsymbol{k}, g)\, \hat{a}^{+}_{\boldsymbol{k},g} \hat{a}_{\boldsymbol{k},g} - \sum\limits_{\boldsymbol{k},g} \bar{\gamma}_{\boldsymbol{k},g} \hat{a}_{\boldsymbol{k},g} - \sum\limits_{\boldsymbol{k},g} \gamma_{k,g} \hat{a}^{+}_{k,g}\big]\big\}}, \tag{28}$$

where

$$\gamma_{\boldsymbol{k},g} = \sum_{\boldsymbol{b},\boldsymbol{l},j} \Bigg(-f\binom{\boldsymbol{l}}{\boldsymbol{b}}_j i \sqrt{\frac{\hbar}{2NVm_{\boldsymbol{b}}\omega(\boldsymbol{k}, g)}} + h\binom{\boldsymbol{l}}{\boldsymbol{b}}_j \sqrt{\frac{m_{\boldsymbol{b}}\hbar\omega(\boldsymbol{k}, g)}{2NV}}\; \bar{e}\binom{\boldsymbol{k}}{\boldsymbol{b}}_{j,g} \times \times \exp(-i\boldsymbol{k}\boldsymbol{l}). \tag{29}$$

It can be seen that the density matrices (27) and (28) have the same form and differ only in terms of parameters which occur in them. The imposition of the condition of equal mean values of the total energy of the crystal, of the position and momentum of the atoms will permit equation of particular parameters and, as a result, determination of the values of the Lagrange factors which occur in (28).

Let us calculate the mean value of the total energy of the crystal in the state described by the density matrix (27)

$$\langle\!\langle \hat{H} \rangle\!\rangle = \mathrm{Tr}\Big\{\Big[\sum_{\boldsymbol{k},g} \hbar\omega(\boldsymbol{k}, g)\, \hat{a}^{+}_{\boldsymbol{k},g} \hat{a}_{\boldsymbol{k},g}\Big] \hat{D}(\{\alpha_{\boldsymbol{q},p}\}) \exp\Big[-\Phi - \beta \sum_{\boldsymbol{k},g} \hbar\omega(\boldsymbol{k}, g) \times \times \hat{a}^{+}_{\boldsymbol{k},g} \hat{a}_{\boldsymbol{k},g}\Big] \hat{D}^{-1}(\{\alpha_{\boldsymbol{q},p}\})\Big\}$$

$$= \mathrm{Tr}\Big\{\hat{D}^{-1}(\{\alpha_{\boldsymbol{q},p}\}) \Big[\sum_{\boldsymbol{k},g} \hbar\omega(\boldsymbol{k}, g)\, \hat{a}^{+}_{\boldsymbol{k},g} \hat{a}_{\boldsymbol{k},g}\Big] \hat{D}(\{\alpha_{\boldsymbol{q},p}\}) \exp\Big[-\Phi - \beta \times$$

$$\times \sum_{\boldsymbol{k},g} \hbar\omega(\boldsymbol{k}, g)\, \hat{a}^{+}_{\boldsymbol{k},g} \hat{a}_{\boldsymbol{k},g}\Big]\Big\} = \sum_{\boldsymbol{k},g} \frac{\hbar\omega(\boldsymbol{k}, g)}{\exp[\beta\hbar\omega(\boldsymbol{k}, g)] - 1} + \sum_{\boldsymbol{k},g} \hbar\omega(\boldsymbol{k}, g)\, \bar{\alpha}_{\boldsymbol{k},g} \alpha_{\boldsymbol{k},g}. \tag{30}$$

Using formulae (14) and taking into account the relations serving to "diagonalize" the hamiltonian of a harmonic crystal [4, 5], the second term of expression (30) can be expressed by the changes in the mean values of the displacement and momentum of atoms caused by dynamic deformation

$$\sum_{\boldsymbol{k},g} \hbar\omega(\boldsymbol{k}, g)\, \bar{\alpha}_{k,g} \alpha_{k,g} = \sum_{\boldsymbol{k},g} \frac{P^{2'}\binom{\boldsymbol{l}}{\boldsymbol{b}}_j}{2m_{\boldsymbol{b}}} + \sum_{\boldsymbol{l},\boldsymbol{b},j} \frac{\partial^2 W}{\partial R\binom{\boldsymbol{l}}{\boldsymbol{b}}_j \partial R\binom{\boldsymbol{l}'}{\boldsymbol{b}'}_{j'}} R'\binom{\boldsymbol{l}}{\boldsymbol{b}}_j R'\binom{\boldsymbol{l}'}{\boldsymbol{b}'}_{j'}, \tag{31}$$

where W is the potential energy of a crystal described in adiabatic approximation [4, 5], $R'\binom{\boldsymbol{l}}{\boldsymbol{b}}_j$ and $R'\binom{\boldsymbol{l}'}{\boldsymbol{b}'}_j$ are atom displacements from the equilibrium positions (understood "classically", i.e. in the sense corresponding to the description of a crystal "before quantization"), and the partial derivatives are assumed for zero displacements.

It can be seen that expression (31) can be interpreted as deformation energy and that the value of the expression $\beta = 1/kT$ in formula (27) corresponds to such temperature of the crystal at which the mean energy in the state of thermodynamic equilibrium is equal to the difference between the predetermined total energy and the deformation energy. This determines $\beta = \beta'$ as a function of the mean energy of the crystal, the mean positions and momenta of the atoms. From the equation

$$\beta\hbar\omega(\boldsymbol{k}, g)\, a_{\boldsymbol{k},g} = -\gamma_{\boldsymbol{k},g} \tag{32}$$

it is possible to determine

$$\begin{aligned} h\begin{pmatrix}\boldsymbol{l}\\ \boldsymbol{b}\end{pmatrix}_j &= -\sum_{\boldsymbol{k},g} \beta \sqrt{\frac{\hbar\omega(\boldsymbol{k}, g)}{2NVm_{\boldsymbol{b}}}}\,(\bar{a}_{\boldsymbol{k},g} + a_{-\boldsymbol{k},g})\,\bar{e}\begin{pmatrix}\boldsymbol{k}\\ \boldsymbol{b}\end{pmatrix}_{j,g} \exp(-i\boldsymbol{kl});\\ f\begin{pmatrix}\boldsymbol{l}\\ \boldsymbol{b}\end{pmatrix}_j &= \sum_{\boldsymbol{k},g} i\beta \sqrt{\frac{m_{\boldsymbol{b}}\hbar\omega^3(\boldsymbol{k}, g)}{2NV}}\,(\bar{a}_{\boldsymbol{k},g} - a_{-\boldsymbol{k},g})\,\bar{e}\begin{pmatrix}\boldsymbol{k}\\ \boldsymbol{b}\end{pmatrix}_{j,g} \exp(-i\boldsymbol{kl}). \end{aligned} \tag{33}$$

Consideration of formula (14) leads to an explicit form of the Lagrange multipliers which occur in (28),

$$\begin{aligned} h\begin{pmatrix}\boldsymbol{l}\\ \boldsymbol{b}\end{pmatrix}_j &= -\frac{\beta}{m_{\boldsymbol{b}}} P'\begin{pmatrix}\boldsymbol{l}\\ \boldsymbol{b}\end{pmatrix}_j,\\ f\begin{pmatrix}\boldsymbol{l}\\ \boldsymbol{b}\end{pmatrix}_j &= -\beta \sum_{\boldsymbol{b},\boldsymbol{l},j} \frac{\partial^2 W}{\partial R\begin{pmatrix}\boldsymbol{l}\\ \boldsymbol{b}\end{pmatrix}_j \partial R\begin{pmatrix}\boldsymbol{l'}\\ \boldsymbol{b'}\end{pmatrix}_{j'}} R'\begin{pmatrix}\boldsymbol{l'}\\ \boldsymbol{b'}\end{pmatrix}_{j'}. \end{aligned} \tag{34}$$

(with notation as in (31) and previous formulae).

Thus, it can be seen that in the case of a harmonic crystal the two methods lead to the same results.

In a general case when the hamiltonian of the crystal is not a square function of the operators of phonon creation and annihilation, the results of the two methods are slightly different. E.g. for the hamiltonian of the form [4, 5]

$$\begin{aligned} \hat{H} &= \sum_{\boldsymbol{k},g} \hbar\omega(\boldsymbol{k}, g)\,\hat{a}^+_{\boldsymbol{k},g}\hat{a}_{\boldsymbol{k},g} + \\ &+ \sum_{\substack{\boldsymbol{q}_1,\boldsymbol{q}_2,\boldsymbol{q}_3,\\ p_1,p_2,p_3,}} V\begin{pmatrix}\boldsymbol{q}_1\boldsymbol{q}_2\boldsymbol{q}_3\\ p_1p_2p_3\end{pmatrix} (\hat{a}^+_{\boldsymbol{q}_1,p_1} - \hat{a}_{-\boldsymbol{q}_1,p_1})(\hat{a}^+_{\boldsymbol{q}_2,p_2} - \hat{a}_{-\boldsymbol{q}_2,p_2})(\hat{a}^+_{\boldsymbol{q}_3,p_3} - \hat{a}_{-\boldsymbol{q}_3,p_3}) \end{aligned} \tag{35}$$

the density matrix of the deformed crystal obtained by the method of the deformation operator will have the form

$$\hat{\varrho} = \hat{D}(\{\alpha_{\boldsymbol{q},p}\})\exp[-\Phi-\beta\hat{H}]\hat{D}^{-1}(\{\alpha_{\boldsymbol{q},p}\}) =$$
$$=\exp\Big\{-\Phi-\beta\sum_{\boldsymbol{k},g}\hbar\omega(\boldsymbol{k},g)\hat{a}^{+}_{\boldsymbol{k},g}\hat{a}_{\boldsymbol{k},g}+\beta\sum_{\boldsymbol{k},g}\hbar\omega(\boldsymbol{k},g)\bar{\alpha}_{\boldsymbol{k},g}\hat{a}_{\boldsymbol{k},g}+\beta\sum_{\boldsymbol{k},g}\hbar\omega(\boldsymbol{k},g)\alpha_{\boldsymbol{k},g}\hat{a}^{+}_{\boldsymbol{k},g}-$$
$$-\beta\sum_{\boldsymbol{k},g}\hbar\omega(\boldsymbol{k},g)\bar{\alpha}_{\boldsymbol{k},g}\alpha_{\boldsymbol{k},g}-\beta\sum_{\substack{\boldsymbol{q}_1,\boldsymbol{q}_2,\boldsymbol{q}_3\\ p_1,p_2,p_3}}V\begin{pmatrix}\boldsymbol{q}_1,\boldsymbol{q}_2,\boldsymbol{q}_3\\ p_1,p_2 p_3\end{pmatrix}(\hat{a}^{+}_{\boldsymbol{q}_1,p_1}-\bar{\alpha}_{\boldsymbol{q}_1,p_1}\hat{a}_{-\boldsymbol{q}_1,p_1}+$$
$$+\alpha_{-\boldsymbol{q}_1 p_1})(\hat{a}^{+}_{\boldsymbol{q}_2,p_2}-\bar{\alpha}_{\boldsymbol{q}_2,p_2}-\hat{a}_{-\boldsymbol{q}_2,p_2}+\alpha_{-\boldsymbol{q}_2,p_2})(\hat{a}^{+}_{\boldsymbol{q}_3,p_3}-\bar{\alpha}_{\boldsymbol{q}_3 p_3}-\hat{a}_{-\boldsymbol{q}_3,p_3}+\alpha_{-\boldsymbol{q}_3,p_3})\Big\} \tag{36}$$

(the assumption being that before deformation the crystal was in the state of thermodynamic equilibrium, described by the canonical distribution).

The method of the quasi-equilibrium density matrix leads to the result

$$\hat{\varrho} = \exp\Big\{-\Phi'-\beta'\sum_{\boldsymbol{k},g}\hbar\omega(\boldsymbol{k},g)\hat{a}^{+}_{\boldsymbol{k},g}\hat{a}_{\boldsymbol{k},g}-\sum_{\boldsymbol{k},g}\bar{\gamma}_{\boldsymbol{k},g}\hat{a}_{\boldsymbol{k},g}-\sum_{\boldsymbol{k},g}\gamma_{\boldsymbol{k},g}\hat{a}^{+}_{\boldsymbol{k},g}-$$
$$-\beta'\sum_{\substack{\boldsymbol{q}_1,\boldsymbol{q}_2,\boldsymbol{q}_3\\ p_1,p_2,p_3}}V\begin{pmatrix}\boldsymbol{q}_1\boldsymbol{q}_2\boldsymbol{q}_3\\ p_1 p_2 p_3\end{pmatrix}(\hat{a}^{+}_{\boldsymbol{q}_1,p_1}-\hat{a}_{-\boldsymbol{q}_1,p_1})(\hat{a}^{+}_{\boldsymbol{q}_2,p_2}-\hat{a}_{-\boldsymbol{q}_2,p_2})(\hat{a}^{+}_{\boldsymbol{q}_2,p_3}-\hat{a}_{-\boldsymbol{q}_3,p_3})\Big\} \tag{37}$$

($\boldsymbol{k}, g$ are defined as in (29)).

It can be seen that the density matrices (36) and (37) are different even when they lead to the same mean values of the total energy of the crystal, the positions and momenta of the atoms.

The description of dynamic deformation by means of the deformation operator was based on the assumption that the deformation of the crystal involves the following transformation of the density matrix which describes the crystal

$$\hat{\varrho}\rightarrow\hat{D}(\{\alpha_{\boldsymbol{q},p}\})\,\hat{\varrho}\,\hat{D}^{-1}(\{\alpha_{\boldsymbol{q},p}\}),$$

where $\hat{D}(\{\alpha_{\boldsymbol{q},p}\})$ is a unitary operator defined from formula (1).

This assumption made it possible to find a relation between the values of the changes in the mean values of the positions and momenta of the atoms and the values of the parameters $\alpha_{\boldsymbol{q},p}$ which occur in the deformation operator. The physical sense of the above assumption is particularly conspicuous in the case of static deformation i.e. such that leads to changes in the mean values of the positions of the atoms, without simultaneously changing, however, the mean values of the momenta of the atoms.

It follows from the considerations in paper [3] that the description of static deformation by the deformation operator involves the assumption that deformation of each wave function describing the crystal can be reduced to the subtraction of the corresponding displacement vectors from the arguments of the wave function. It can be said, though not very precisely, that with deformation of this type the information is related to the form of the wave functions describing the crystal remains. The mathematical counterpart of this is the fact that no deformation represented by the deformation operator changes the value of information entropy (this can readily be shown when $\hat{\varrho}' = \hat{D}(\{a_{q,p}\}) \hat{\varrho}\, \hat{D}^{-1}(\{a_{q,p}\})$ is inserted into (20) and the operators which occur under the trace sign are cyclically rearranged).

The case is different with the method of the quasi-equilibrium density matrix. This method accounts indirectly for the processes which are related to the interaction between the crystal and the environment and lead to the destruction of information contained in the density matrix. It can thus be expected that the results obtained by the method of the quasi-equilibrium density matrix are closer to reality than those of the method of the deformation operator An essential advantage of the method of the deformation operator, however, is that it leads directly to the formulation of perturbation calculus.

References

[1] R. J. GLAUBER, *Coherent and incoherent states of the radiation field*, Phys. rev., **131**, 6, 2766 (1963).

[2] N. D. ZUBAREV, *Neravnovesnaya staticheskaya termodynamika*, Nauka, Moscow 1971.

[3] K. SZUMILIN, *The theory of externally deformed crystals at low temperatures*, Bull. Ac. Pol. Sc., sc. tec., **20**, 12, 509 (1972).

[4] M. BORN, K. HUANG, *Dynamical theory of crystal lattices*, Clarendon Press, Oxford 1954.

[5] J. M. ZIMAN, *Electrons and phonons*, Clarendon Press, Oxford 1960.

[6] J. PERINA, *Coherence of light*, Nostrand, London 1972.

[7] J. R. KLAUDER, E. C. G. SUDARSHAN, *Fundamentals of quantum optics*, Benjamin, New York 1968.

[8] W. H. LOUISELL, *Quantum statistical properties of radiation*, J. Wiley, New York 1973.

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