Influence of Pendellosung effect on the degree of optical modulation of an electron beam diffracted in a crystal

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(Submitted 2 August 1979)
Zh. Eksp. Teor. Fiz. **78**, 782–787 (February 1980)

We consider the singularities of the modulation mechanism based on stimulated Pendellosung absorption of photons by electrons in the course of diffraction in a single-crystal plate illuminated by a laser beam. It is shown that on account of the Pendellosung effect, for electrons in a state with $s = 0$ (s is the number of absorbed photons) in contrast to the previously considered cases, the depth of modulation in one of the electron beams, direct or diffracted, having a minimal intensity at the exit from the crystal, can greatly exceed the amplitude of the stimulated emission of the photon and reach an estimated value of ~20%.

PACS numbers: 61.80.Fe, 78.45. + h

1. The quantum theory of modulation of an electron beam passing through a dielectric plate along which an electromagnetic wave propagates was developed by Varshalovich and D'yankonov.[1,2] It is shown that the modulation in the region of the optical frequencies is essentially a quantum effect and is due to the interference between states with different energies, produced as a result of stimulated absorption of s quanta $\hbar\omega(s = 0, \pm1, \pm2...)$ by the electron. In Refs. 1 and 2 they considered a case when absorption or emission of a photon by an electron becomes possible because of the jump in the dielectric constant near the plate boundaries (the transition-radiation mechanism).

A more effective modulation mechanism, based on the Cerenkov effect, was proposed by D'yakonov and Varshalovich[3] and by Van Zandt and Meyer. It makes possible a higher degree of modulation by increasing the thickness of the plate, since the photon absorption takes place in the entire volume of the dielectric.

Zaretskiĭ and Lomonosov[5] developed a theory of diffraction of electrons in a single-crystal plate placed in the field of a circularly polarized electromagnetic wave directed perpendicular to the plate boundary. It is shown that additional Bragg maxima appear, with intensities that depend on the amplitude of the applied field, and can in certain cases be modulated by its frequency.

The depth of modulation of the electron current in the foregoing cases[1-5] is determined by the amplitude $a_{\pm\omega}$ of the stimulated absorption (emission) of the photon, and turns out to be ≤ 0.1 at realistically attainable field intensities in the dielectric.

2. The present paper discusses the distinguishing features of the previously proposed[6] modulation mechanism based on stimulated Pendellosung absorption (emission) of photons,[7,8] when electrons are diffracted in a single crystal in accordance with the Laue scheme. It is shown that the depth of modulation in one of the electron beams passing through the crystal (direct or diffracted), in contrast to the results of other workers[1-5], can exceed considerably the value[1)] $|a_{\pm\omega}|$. This result is the consequence of the Pendellosung effect for electrons in a state with $s = 0$, and is due to the character of the Pendellosung radiation, inasmuch as the Pendellosung effect does not exist for electrons in states with $s = \pm1$. By decreasing the amplitude of the direct or diffracted electron wave in the state with $s = 0$ via the Pendellosung effect (with suitable choice of the crystal thickness) it is possible to attain a modulation depth ~0.2 at stimulated Pendellosung emissions $|a_{\pm\omega}| \leq 0.01$.

3. We consider electrons of energy $E_0 = \hbar\omega_0$ and momentum $\mathbf{p}_0 = \hbar\mathbf{k}_0$ incident on a crystal at the Bragg angle θ_B and reflected by the planes as shown in the figure. In the two-beam approximation of the dynamic theory of diffraction, the wave function of the electron inside the crystal in the absence of interaction with the magnetic field is of the form[2)] (see, e.g., Ref. 9)

$$\psi_c = 2^{-1/2}[\psi^{(1)}(\mathbf{k}_0^{(1)}, \mathbf{r}) + \psi^{(2)}(\mathbf{k}_0^{(2)}, \mathbf{r})]\exp(-i\omega_0 t), \quad (1)$$

where

$$\psi^{(1,2)}(\mathbf{k}, \mathbf{r}) = 2^{-1/2}(e^{i\mathbf{k}\mathbf{r}} \mp e^{i(\mathbf{k}+\mathbf{g})\mathbf{r}}), \quad (2)$$

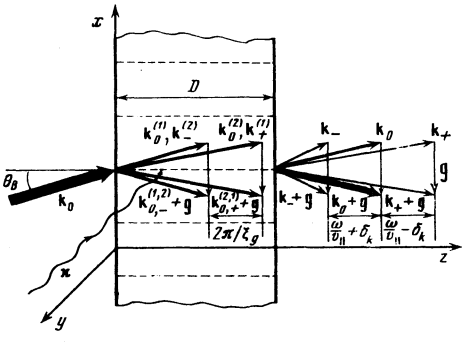

FIG. 1. Incidence of electrons with momentum $\hbar\mathbf{k}_0$ at the Bragg angle on reflecting planes (dashed lines) parallel to the yz plane. The thicknesses of the arrows are proportional to the intensities of the corresponding plane waves (in the state with $s = 0$). The vectors $\mathbf{k}_0$, $\mathbf{k}_0^{(\alpha)}$, $\mathbf{g}$ lie in the xz plane. The wave vector $\varkappa$ of the photon (wavy line) is perpendicular to the xz plane. In the presented case the intensity of the beam passing through the crystal is concentrated predominantly in the diffracted wave. The direct beam is then maximally modulated. The vectors $\mathbf{k}_\pm^{(\alpha)}$, $\mathbf{k}_\pm$ are shown projected on the xz plane.

 0038-5646/80/020394-04$02.40

$\mathbf{g}$ is the reciprocal-lattice vector, $\mathbf{g} = 2\pi/d$, d is the distance between the planes, the indices (1) and (2) number the branches of the dispersion surface E_0 of the electron in the crystal. Its equation, when the Bragg condition is exactly satisfied, takes the form[9]

$$k_0^{(1,2)^2} = K_0^2 \mp U_g. \tag{3}$$

Here $K_0^2 = 2m(E_0 + V_0)/\hbar^2$, $U_g = 2mV_g/\hbar^2$; V_0, V_g are the amplitudes of the corresponding harmonics of the periodic potential of the lattice.

Assume that a plane-parallel electromagnetic wave with frequency ω and wave vector $\varkappa$, directed parallel to the y axis (see the figure) propagates through the crystal,[3)] so that the stimulated absorption or emission of the photon by the electron does not violate the Bragg condition. We consider the case of resonance, when the frequency ω of the modulating wave coincides with the frequency of the "oscillations" of the electron upon diffraction (see "Pendellosung emission"[6-8]), i.e.,

$$\omega = 2V_g/\hbar = 2\pi v_\parallel/\xi_g. \tag{4}$$

Here $v_\parallel = \hbar K_0 \cos\theta_B/m$ and ξ_g is the extinction length characterizing the spatial period of the beats produced in the crystal by the electron waves pertaining to different branches of the dispersion surface ($2\pi/\xi_g = k_{0g}^2 - k_{0g}^1$). Emission of a photon $\hbar\omega$ by an electron is the result of the transition $(1)_{E0} - (2)_{E-}$, while absorption is the result of transition $(2)_{E0} - (1)_{E+}$,[6-8] where $E_\pm = E_0 \pm \hbar\omega$, $(\alpha)_E$ denotes the branch α of the dispersion surface E.

Thus, assuming $|a_{\pm\omega}| \ll 1$ and neglecting the change of the amplitude of the state ψ_0, we can write for the wave function of an electron in a crystal placed in the field of an electromagnetic wave the following expression:

$$\psi(\mathbf{r}, t) = 2^{-1/2}[\psi^{(1)}(\mathbf{k}_0^{(1)}, \mathbf{r}) + \psi^{(2)}(\mathbf{k}_0^{(2)}, \mathbf{r})]\exp(-i\omega_0 t)$$
$$+ a_{+\omega}\psi^{(1)}(\mathbf{k}_+^{(1)}, \mathbf{r})\exp[-i(\omega_0+\omega)t] + a_{-\omega}\psi^{(2)}(\mathbf{k}_-^{(2)}, \mathbf{r})\exp[-i(\omega_0-\omega)t], \tag{5}$$

here $\mathbf{k}_+^{(1)} = \mathbf{k}_0^{(2)} + \varkappa$; $\mathbf{k}_-^{(2)} = \mathbf{k}_0^{(1)} - \varkappa$; the functions $\psi^{(1)}(\mathbf{k}_+^{(1)}, \mathbf{r})\psi^{(2)}(\mathbf{k}_-^{(2)}, \mathbf{r})$ take the form (2), since the Bragg condition is not violated ($\varkappa\mathbf{g} = 0$). The vectors $\mathbf{k}_\pm^{(1,2)}$ belong to the dispersion surfaces $E_\pm$, whose equations take the form (3).

The amplitudes $a_{\pm\omega}$ of stimulated absorption or emission of a photon $\hbar\omega$ are, in first-order perturbation theory,

$$a_{\pm\omega} = -\frac{i}{\hbar}\int_0^{z/v_\parallel} 2^{-1/2}\langle\psi_\pm^{(1,2)}|w|\psi_0^{(2,1)}\rangle dt,$$
$$w = \frac{e}{mc}\mathbf{A}i\hbar\nabla, \qquad \mathbf{A} = A\mathbf{u}\cos(\varkappa\mathbf{r} - \omega t), \tag{6}$$

$\mathbf{A}$ is the vector potential of the modulating field and $\mathbf{u}$ is a unit polarization vector.

Calculation of the matrix element in (6) yields the following result:

$$\langle\psi_\pm^{(1,2)}|w|\psi_0^{(2,1)}\rangle = \frac{e\mathscr{E}_\perp v_\perp}{2\omega}, \tag{7}$$

where $\xi_\perp$ is the electric-field amplitude component in the direction of x (i.e., in the direction of the oscillations of the electron in the crystal), $\mathscr{E}_\perp = \mathscr{E}\mathbf{u}g/|\mathbf{u}||g|$; $\mathscr{E} = \omega A/c$; $v_\perp = \hbar g/2m = \pi\hbar/md$ is the electron velocity corresponding to the transverse momentum $\hbar g/2$.

Introducing the notation $a_{\pm\omega} = -2^{-1/2}ia_\omega$, we get

$$a_\omega = \frac{e\mathscr{E}_\perp z \operatorname{tg}\theta_B}{2\hbar\omega}, \qquad \operatorname{tg}\theta_B = \frac{v_\perp}{v_\parallel}. \tag{8}$$

4. The function wave ψ_f of the electron passing through a crystal of thickness D is determined in the region behind the crystal ($z > D$) by the boundary conditions on the exit face of the crystal; these, if we neglect the waves reflected from the boundary, reduce to the condition of continuity of the wave function.[9] As a result, writing ψ_f in the form

$$\psi_f = \psi_f^0 + \psi_f^g, \tag{9}$$

where ψ_f^0 describes the forward electron beam and ψ_f^g the diffracted beam, we have

$$\psi_f^0 = \cos\frac{\pi D}{\xi_g}\exp(i\mathbf{k}_0\mathbf{r} - i\omega_0 t) - \frac{ia_\omega(D)}{2}$$
$$\times[\exp(i\mathbf{k}_+\mathbf{r} - i(\omega_0+\omega)t) + \exp(i\mathbf{k}_-\mathbf{r} - i(\omega_0-\omega)t)], \tag{10}$$
$$\psi_f^g = i\sin\frac{\pi D}{\xi_g}\exp(i(\mathbf{k}_0+\mathbf{g})\mathbf{r} - i\omega_0 t) + \frac{ia_\omega(D)}{2}$$
$$\times[\exp(i(\mathbf{k}_+ + \mathbf{g})\mathbf{r} - i(\omega_0+\omega)t) - \exp(i(\mathbf{k}_- + \mathbf{g})\mathbf{r} - i(\omega_0-\omega)t)]. \tag{11}$$

Here $\mathbf{k}_0$ and $\mathbf{k}_\pm$ are wave vectors with the following components: $\mathbf{k}_0 = (-g/2;\ 0,\ k_{0z})$, $\hbar^2 k_0^2/2m = E_0$; $\mathbf{k}_\pm = (-g/2,\ \mp\varkappa,\ k_{\pm z})$. The quantities $k_{\pm z}$ are obtained from the condition $\hbar^2 k_\pm^2/2m = \hbar(\omega_0 \pm \omega)$ and are equal to

$$\hbar k_{\pm z} = (\hbar^2 k_{0z}^2 \pm 2m\hbar\omega - \hbar^2\varkappa^2)^{1/2}. \tag{12}$$

The periodic dependence of the amplitudes of the states with wave vectors $\mathbf{k}_0$ and $\mathbf{k}_0 + \mathbf{g}$ on D is the result of beats between electron waves belonging to different branches of the dispersion surface E_0 in the crystal (the Pendellosung effect[9]).

Confining ourselves to two terms of the expansion in the small quantity $\hbar\omega/E_{0\parallel}(E_{0\parallel} = \hbar^2 k_{0z}^2/2m)$ in analogy with Refs. 1 and 2, we obtain for $k_{\pm z}$ from (12)

$$k_{\pm z} = k_{0z} \pm \omega/v_{0\parallel} - \delta_k, \tag{13}$$

where

$$\delta_k = \frac{1}{4}\frac{\omega}{v_{0\parallel}}\frac{\hbar\omega}{E_{0\parallel}}. \tag{14}$$

As a result, the density of the electron current per electron in the direct and diffracted beams is determined by the following expressions ($\mathbf{j}_{0,g} \approx e\mathbf{v}_{0,g}|\psi_f^{0,g}|^2$):

$$\mathbf{j}_0(\mathbf{r}, t) = e\mathbf{v}_0\cos^2\frac{\pi D}{\xi_g}\left[1 - \frac{2a_\omega(D)\sin\delta_k z}{\cos(\pi D/\xi_g)}\cos\omega\tau\right], \tag{15}$$
$$\tau = \frac{z}{v_{0\parallel}} - \frac{y}{c_{\text{ph}}} - t,$$
$$\mathbf{j}_g(\mathbf{r}, t) = e\mathbf{v}_g\sin^2\frac{\pi D}{\xi_g}\left[1 + \frac{2a_\omega(D)\sin\delta_k z}{\sin(\pi D/\xi_g)}\sin\omega\tau\right] \tag{16}$$

accurate to terms $\sim a_\omega^2$. Here $c_{\text{ph}} = c/n$ is the phase velocity of the photons in the crystal, v_0 and v_g are the velocities of the electrons in the forward and diffracted beams, and with $|\mathbf{v}_0| = |\mathbf{v}_g|$.

We note that at the width L of the electron beam the forward and diffracted beams diverge in space by a distance $z_0 \sim L/2\tan\theta_B$ behind the plate; for example, at $L \sim 10^{-3}$ and $E_0 \sim 50$ keV ($\theta_B \sim 0.03$) we have $z_0 \sim 0.2$ mm. The corresponding overlap regions for the states with $s = 0$ and ± 1 in each of these beams were (15) and (16) are valid are 10^3—10^4 times larger in the optical frequency band.

A substantial quantum periodicity of the depth of modulation of the electron current as a function of z, with a spatial period $l = \pi/\delta_k$, was first noted by Varshalovich and D'yakonov[1] and discussed by them in detail.[1,2] On the other hand, the dependence on the ratio D/ξ_g, which is the consequence of the Pendellosung effect for the electrons diffracted in the crystal, has not yet been considered. As a result, as follows from (15) and (16), the depth of modulation in one of the electron beams passing through the absorbind crystal can be arbitrary, up to unity. We note that the increase of the depth of modulation is due to the increase of the relative contribution of the states with $s = \pm 1$ with decreasing intensity in one of the beams (in this case the intensity increases in the other beam, and the degree of modulation decreases correspondingly). In particular, a modulation depth of 100% is reached at zero beam intensity (in this case the degree of modulation in the second beam is minimal and equal to $2a_\omega$). However, elastic scattering of the electrons leads to a different damping of the waves 1 and 2 in the crystal, owing to the different symmetry of these waves (effect of anomalous absorption[9]). Therefore the intensities in the forward and diffracted beams in the state with $s = 0$ never vanish and are always finite, thereby strongly limiting the maximum possible depth of modulation.

5. The effects of damping of the Bloch waves in a crystal are described phenomenologically by introducing an imaginary potential $iV'(\mathbf{r})$, and it is usually assumed that $V'(\mathbf{r})$ does not depend on the coordinate, just as the real lattice potential $V(\mathbf{r})$, but is 10–30 times smaller than the latter.[9] The electron wave functions corresponding to different branches of the dispersion surface then acquire the form

$$\Phi^{(1,2)}(\mathbf{k}^{(1,2)}, \mathbf{r}) = \psi^{(1,2)}(\mathbf{k}^{(1,2)}, \mathbf{r}) \exp\left[-\pi\left(\frac{1}{\xi_0'} \mp \frac{1}{\xi_g'}\right) z\right]. \qquad (17)$$

Here $\Phi^{(1,2)}$ are the wave functions with allowance for the absorption, $\psi^{(1,2)}$ are defined by (2), ξ_0', ξ_g' are the damping lengths connected with the corresponding harmonics of the potential $V'(\mathbf{r})$, and $\xi_{0,g}' = \pi\hbar v_\parallel / V_{0,g}'$.

In the case when $D \ll \xi_0'$ and $D \ll \xi_g'$, confining ourselves to the first terms of the expansion in $\pi D/\xi_g'$, we obtain from (17) for the amplitude $a_0^{(0)}$ of the $s = 0$ direct wave, passing through the crystal,

$$a_0^{(0)} = \left(\cos\frac{\pi D}{\xi_g} - i\frac{\pi D}{\xi_g'}\sin\frac{\pi D}{\xi_g}\right)\exp\left(-\frac{\pi D}{\xi_0'}\right) \equiv a_0 \exp(i\rho_0), \qquad (18)$$

where a_0 and ρ_0 are respectively the modulus and the phase of the complex quantity $a_0^{(0)}$,

$$a_0 = \left[\cos^2\frac{\pi D}{\xi_g}\left(1 - \frac{\pi^2 D^2}{\xi_g'^2}\right) + \frac{\pi^2 D^2}{\xi_g'^2}\right]^{1/2} \exp\left(-\frac{\pi D}{\xi_0'}\right). \qquad (19)$$

It follows directly from (19) that the minimal amplitude of the direct wave, accurate to terms of higher order in $\pi D/\xi_{0,g}$, is equal to $a_0^{\min} = \pi D/\xi_g'$. As a result we obtain for the maximum depth of modulation reached in the direct beam

$$\gamma_0^{\max} \approx \frac{2a_\omega(D)\xi_g'}{\pi D} = \frac{e\mathscr{E}_\perp \xi_g' \operatorname{tg}\theta_B}{\pi\hbar\omega}. \qquad (20)$$

In the diffracted beam the quantity $\gamma_g^{\max}$ coincides with $\gamma_0^{\max}$. The presence of $\exp(i\rho_0)$ in expression (18) leads to a phase shift by an amount ρ_0 in the periodic dependence of the depth of modulation on z.[4)]

In the optical region, for example, at $\hbar\omega = 2$eV, which at $E_0 = 50$ keV ($\beta = 0.41$; $\operatorname{tg}\theta_B \approx 2.7 \cdot 10^{-2}$) corresponds to $\xi_g \approx 2540$ Å, an estimate by means of (20) yields for $\mathscr{E}_\perp = 6 \cdot 10^4$ V/cm and $\xi_g' \approx 30\xi_g$, a value $\gamma_0^{\max} \approx 19.5\%$, which is approximately 10 times the value of $2a_\omega$ (at $D \sim \xi_g$), for the depth of modulation of a beam passing with maximum intensity through the crystal. In the case described in Refs. 1 and 2, the maximum depth of modulation is reached when the polarization vector is parallel to the z axis, and depends on $(n^2 - 1)/n^2$, and at $n \approx 1.3$ and for the same values of $\hbar\omega$, E_0, $\mathscr{E}$ it amounts to ~12.4%.

It must be emphasized that the influence of the Pendellosung effect in a state with $s = 0$ on the depth of modulation of the electron beam is due to the character of the Pendellosung radiation, wherein, as a result of absorption or emission of the photon, only one of the branches (E_+ or E_-) of the dispersion surface of the electron is excited, so that in states with $s = +1$ there is no Pendellosung effect. A similar enhancement of the modulation effect is possible also for another mechanism, if in the stimulated absorption of the photon the branches of the dispersion surface of the electron in the crystal are excited with substantially different amplitudes.

In conclusion the author is deeply grateful to D. A. Varshalovich, K. E. Kir'yanov, A. S. Ryl'nikov, A. I. Smirnov, and O. I. Sumbeav for helpful discussions.

[1)] The behavior of electrons in the region behind a crystal was not considered in Ref. 6.

[2)] The effects connected with the damping of the electron waves in a crystal are discussed in Sec. 6 below.

[3)] It is assumed that the crystal constitutes for the photons a homogeneous medium with a refractive index n, so that $\varkappa = \omega n/c$.

[4)] In next order in the expansion in $\pi D/\xi_g'$, the difference between the damping of the waves in the states with $s = \pm 1$ comes into play, and leads in the direct-beam current to a modulation wave of the form

$$\sim \sin(\delta_k z + \rho_0)\cos\omega\tau - (\pi D/\xi_g')\cos(\delta_k z + \rho_0)\sin\omega\tau.$$

As a result not only the amplitude but also the phase of the modulation wave has a periodic dependence on z.

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Translated by J. G. Adashko

Soliton motion in a one-dimensional molecular lattice with account taken of thermal oscillations

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(Submitted 3 August 1979)
Zh. Eksp. Teor. Fiz. **78**, 789–796 (February 1980)

We study the effect of thermal oscillations of molecules in a one-dimensional molecular lattice on soliton properties. We show that with increasing temperature the soliton size increases and its properties come ever closer to those of an exciton. We also investigate the dependence of the soliton parameters on its velocity.

PACS numbers: 61.50. – f

1. INTRODUCTION

It was shown in Refs. 1 to 5 that in soft one-dimensional molecular lattices the collective states corresponding to intra-molecular excitations with a transition dipole moment directed along the lattice are solitons propagating with a constant velocity which does not exceed the velocity of the longitudinal sound waves. The exceptionally large stability of the solitons allows one to expect that they may play a large role in the energy transfer along quasi-one-dimensional molecular chains.[2,4,5]

In all papers mentioned above it is assumed that the lattice is at zero absolute temperature. It is of interest to study the effect of the thermal oscillations of the molecules in a one-dimensional lattice on the soliton properties. The present paper is devoted to an elucidation of that problem.

2. HAMILTONIAN OF COLLECTIVE EXCITATIONS

One can consider the solitons to be bound states of an exciton and a local lattice deformation. In a one-dimensional molecular lattice consisting of N ($\gg 1$) neutral molecules occupying the sites $z_n = an$ ($n = 1, 2, \ldots, N$) the solitons are described by the Hamiltonian

$$H = H_{ex} + H_{ph} + H_{int}, \tag{2.1}$$

where effective mass (m) approximation for the exciton its energy operator has the form[1)]

$$H_{ex} = \sum_n \left[\left(\mathscr{E}_0 + \frac{\hbar^2}{ma^2} \right) A_n^+ A_n - \frac{\hbar^2}{2ma^2} (A_n^+ A_{n-1} + A_n^+ A_{n+1}) \right]. \tag{2.2}$$

Here $\mathscr{E}_0$ is the energy of the bottom of the exciton band, A_n^+ and A_n are operators corresponding to the presence and absence of intra-molecular excitations of the molecule n. The summation in (2.2) and in all further expressions is over all N molecules.

The operator of the oscillations of the molecules relative to the equilibrium positions z_n in the harmonic approximation, i.e., the acoustic phonon operator, is given by the expression

$$H_{ph} = \sum_q \hbar \Omega_q b_q^+ b_q, \tag{2.3}$$

where b_q^+, b_q are the creation and annihilation operators of phonons with wave number q and frequency

$$\Omega_q = (\varkappa/M)^{1/2} |\sin(aq/2)| \approx |q| V_a, \tag{2.4}$$

where M is the mass of a molecule, $\varkappa$ the elasticity coefficient, and $V_a = a(\varkappa/M)^{1/2}$ the longitudinal sound velocity. In (2.3) and in all further sums the summation over q is over all N values which are uniformly distributed over the interval

$$-\pi/a < q \leqslant \pi/a.$$

The operator of the local interaction of an exciton with the displacements ξ_n of the molecules from their equilibrium positions takes in the approximation linear in the displacements the form[2)]

$$H_{int} = \chi \sum_n A_n^+ A_n (\xi_{n+1} - \xi_{n-1}). \tag{2.5}$$

For an analysis of the role of the thermal motions it is convenient to express the displacements in terms of the phonon creation and annihilation operators[6]:

$$\xi_n = \sum_q \left(\frac{\hbar}{2MN\Omega_q} \right)^{1/2} (b_q + b_{-q}^+) \exp(iqna). \tag{2.6}$$

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