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

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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.

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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 $z_n = an$ ($n = 1, 2, \dots, N$) the solitons are described by the Hamiltonian

$$H = H_{ex} + H_{ph} + H_{int}, \quad (2.1)$$

where effective mass (m) approximation for the exciton its energy operator has the form¹⁾

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

Here \mathcal{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

$$H_{ph} = \sum_q \hbar \Omega_q b_q^+ b_q, \quad (2.3)$$

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

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

where M is the mass of a molecule, κ the elasticity coefficient, and $V_a = a(\kappa/M)^{1/2}$ 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

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

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 form²⁾

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

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 operators⁶⁾:

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

The operator (2.5) then takes the form

$$H_{in} = \frac{1}{N^{1/2}} \sum_{n,q} F(q) A_n^+ A_n (b_q + b_{-q}^+) \exp(iqna), \quad (2.7)$$

where

$$F(q) = 2i\chi(\hbar/2M\Omega_q)^{1/2} \sin qa \\ \approx i\alpha(\hbar|q|/2MV_a)^{1/2} q/|q|, \quad \sigma = 2\alpha\chi. \quad (2.7a)$$

The collective states of the lattice corresponding to an/intra-molecular excitation and to displacements of the molecules from their equilibrium positions, and the phonon ensemble $\{\nu_q\} = \dots \nu_q \dots$ are determined by the wave function

$$\Psi_\nu(t) = \sum_n \varphi_n(t) A_n^+ |0\rangle U_n(t) |\nu\rangle, \quad (2.8)$$

where the phonon function is

$$|\nu\rangle = |\{\nu_q\}\rangle = \prod_q |\nu_q\rangle, \quad |\nu_q\rangle = (\nu_q!)^{-1/2} (b_q^+)^{\nu_q} |0\rangle.$$

The $U_n(t)$ are unitary operators of the displacements of the molecules from their equilibrium positions

$$U_n(t) = \exp \left\{ \sum_q [\tilde{\beta}_{qn}^*(t) b_q - \tilde{\beta}_{qn}(t) b_q^+] \right\}. \quad (2.9)$$

The functions $\tilde{\beta}_{qn}(t)$ are chosen in the form of modulated plane waves:

$$\tilde{\beta}_{qn}(t) = \beta_{qn}(t) \exp(-iqna). \quad (2.10)$$

The squares of the moduli of the functions $\varphi_n(t)$ satisfy the normalization condition

$$\sum_n |\varphi_n(t)|^2 = 1 \quad (2.11)$$

and determine the probability for the excitation of the molecules n .

The functions $\tilde{\beta}_{qn}(t)$ in (2.9) characterize the average displacements of the equilibrium positions of the molecules in the state $U_n(t) |\nu\rangle$. Indeed,

$$\langle \nu | U_n^+(t) b_q U_n(t) | \nu \rangle = -\tilde{\beta}_{qn}(t).$$

3. THE HAMILTON FUNCTION OF A SYSTEM IN THERMAL EQUILIBRIUM WITH A THERMOSTAT

We turn to the evaluation of the unknown functions $\varphi_n(t)$ and $\tilde{\beta}_{qn}(t)$ which determine the collective excitations in a one-dimensional lattice in thermal equilibrium with a thermostat which has a temperature T . In that case we must go over to a statistical description of the quantum states of the system.

We define the Hamilton function of the system by the expression

$$\mathcal{H} = \sum_\nu \rho_\nu H_{\nu\nu}, \quad (3.1)$$

where

$$H_{\nu\nu} = \langle \Psi_\nu(t) | H_{ex} + H_{in} | \Psi_\nu(t) \rangle + \sum_n \langle \nu | U_n^+ H_{ph} U_n | \nu \rangle \quad (3.2)$$

are the diagonal matrix elements of the energy operator of the system;

$$\rho_\nu = \frac{\langle \nu | \exp(-H_{ph}/\Theta) | \nu \rangle}{\sum_\nu \langle \nu | \exp(-H_{ph}/\Theta) | \nu \rangle} \quad (3.3)$$

are the diagonal elements of the density matrix of the phonon states, $\Theta = kT$.

The following matrix elements occur in Eq. (3.2)

$$\langle \nu | U_n^+ b_q^+ b_q U_n | \nu \rangle = \nu_q + |\beta_{qn}|^2, \quad (3.4a)$$

$$\langle \Psi_\nu | b_q | \Psi_\nu \rangle = - \sum_n |\varphi_n(t)|^2 \tilde{\beta}_{qn}(t), \quad (3.4b)$$

$$\langle \Psi_\nu | b_q^+ | \Psi_\nu \rangle = - \sum_n |\varphi_n(t)|^2 \tilde{\beta}_{qn}^*(t), \quad (3.4c)$$

$$\langle \Psi_\nu | A_n^+ A_{n-1} | \Psi_\nu \rangle = \varphi_n^* \varphi_{n-1} \exp(-W_n), \quad (3.4d)$$

where

$$\exp(-W_n) = \langle \nu | U_n^+ U_{n-1} | \nu \rangle. \quad (3.5)$$

Using the explicit form of the unitary operators (2.9) and the identity

$$\langle \nu_q | \exp(\alpha b_q^+ - \alpha^* b_q) \exp(\gamma^* b_q - \gamma b_q^+) | \nu_q \rangle \\ = \exp \{ (\nu_q + 1) \alpha \gamma^* + \nu_q \alpha^* \gamma - (\nu_q + 1/2) (|\alpha|^2 + |\gamma|^2) \},$$

we get

$$W_n = \sum_q \left[(\nu_q + 1) \beta_{qn} \beta_{q,n-1}^* e^{iqa} + \nu_q \beta_{qn}^* \beta_{q,n-1} e^{-iqa} \right. \\ \left. - \left(\frac{1}{2} + \nu_q \right) (|\beta_{qn}|^2 + |\beta_{q,n-1}|^2) \right]. \quad (3.6)$$

We are interested in those states of the system in which the displacements of the equilibrium positions of neighboring molecules differ little from one another. In that case we can write

$$W_n = 2 \sum_q |\beta_{qn}|^2 (2\nu_q + 1) \sin^2 \left(\frac{aq}{2} \right) \approx \frac{1}{2} a^2 \sum_q (2\nu_q + 1) q^2 |\beta_{qn}|^2. \quad (3.7)$$

Using the values of the matrix elements (3.4) we change Eq. (3.2) to the form

$$H_{\nu\nu} = \sum_n \left\{ \left(\mathcal{E}_0 + \frac{\hbar}{ma^2} \right) \varphi_n^* \varphi_n - \frac{\hbar^2 \exp(-W_n)}{2ma^2} (\varphi_n^* \varphi_{n-1} + \varphi_n^* \varphi_{n+1}) \right. \\ \left. - \frac{1}{N^{1/2}} \sum_q F(q) |\varphi_n|^2 (\beta_{qn} + \beta_{-q,n}^*) + \sum_q \hbar \Omega_q (\nu_q + |\beta_{qn}|^2) \right\}. \quad (3.8)$$

The statistical averaging of (3.1) reduces to replacing in Eq. (3.8) the quantum numbers ν_q by their averages

$$\bar{\nu}_q = [\exp(\hbar \Omega_q / \Theta) - 1]^{-1}. \quad (3.9)$$

Thus the Hamilton function, which depends on $\varphi_n(t)$, $\beta_{qn}(t)$, and the generalized momenta $i\hbar \dot{\beta}_{qn}^*$ and $i\hbar \dot{\beta}_{qn}$ which are canonically conjugate to them, is given by the expression

$$\mathcal{H} = \sum_n \left[\left(\mathcal{E}_0 - \frac{\hbar^2}{ma^2} \right) \varphi_n^* \varphi_n - \frac{\hbar^2 \exp(-W_n)}{2ma^2} (\varphi_n^* \varphi_{n-1} + \varphi_n^* \varphi_{n+1}) \right. \\ \left. - \frac{1}{N^{1/2}} \sum_q F(q) |\varphi_n|^2 (\beta_{qn} + \beta_{-q,n}^*) + \sum_q \hbar \Omega_q (\bar{\nu}_q + |\beta_{qn}|^2) \right]. \quad (3.10)$$

where \bar{W} is equal to (3.7) with ν_q replaced by $\bar{\nu}_q$.

Using the function \mathcal{H} we find the Hamilton equations

$$i\hbar \frac{\partial \varphi_n}{\partial t} = \frac{\partial \mathcal{H}}{\partial \varphi_n} = \left(\mathcal{E}_0 + \frac{\hbar}{ma^2} \right) \varphi_n - \frac{\hbar^2 \exp(-\bar{W}_n)}{2ma^2} (\varphi_{n-1} + \varphi_{n+1}) - \frac{1}{N^{1/2}} \sum_q F(q) (\beta_{qn} - \beta_{-q,n}^*) \varphi_n, \quad (3.11)$$

$$i\hbar \frac{\partial \beta_{qn}}{\partial t} = \frac{\partial \mathcal{H}}{\partial \beta_{qn}} = \hbar \Omega_q \beta_{qn} + \frac{1}{N^{1/2}} F(q) |\varphi_n|^2 + \frac{\hbar^2}{4m} \exp(-W_n) q^2 \beta_{qn} (\varphi_n^* \varphi_{n-1} + \varphi_n^* \varphi_{n+1}). \quad (3.12)$$

Usually the following inequality holds³⁾

$$V_a \gg \hbar |q| |\varphi_n|^2 / 4m, \quad (3.13)$$

so that we can replace Eq. (3.12) by the simpler equation

$$i\hbar \frac{\partial \beta_{qn}}{\partial t} = \hbar \Omega_q \beta_{qn} + \frac{1}{N^{1/2}} \sum_q F(q) |\varphi_n|^2. \quad (3.14)$$

We shall look for solutions of this equation in the form of modulated plane waves [see (2.10)]

$$\beta_{qn}(t) = \beta_{qn}(0) \exp(i|q|Vt), \quad (3.15)$$

where V is a constant velocity. Substituting (3.15) into (3.14) we find

$$\beta_{qn}(t) = -F(q) |\varphi_n|^2 / \hbar |q| N^{1/2} (V_a + V). \quad (3.16)$$

In the same way we get from the equation which is the complex conjugate of (3.14)

$$\beta_{-q,n}(t) = -F(q) |\varphi_n|^2 / N^{1/2} \hbar |q| (V_a - V). \quad (3.17)$$

Substituting these values into (3.11) we get a non-linear equation for the function φ_n

$$i\hbar \frac{\partial \varphi_n}{\partial t} - \left(\mathcal{E}_0 + \frac{\hbar^2}{ma^2} \right) \varphi_n + \frac{\hbar^2 \exp(-\bar{W}_n)}{2ma^2} (\varphi_{n-1} + \varphi_{n+1}) + G |\varphi_n|^2 \varphi_n = 0, \quad (3.18)$$

where

$$G = \sigma^2 / MV_a^2 (1-s^2), \quad s = V/V_a, \quad (3.19)$$

$$\bar{W}_n = |\varphi_n|^2 Bf(\Theta). \quad (3.20)$$

Here

$$B = q_0 a^2 \sigma^2 / 4MV_a^2 \hbar (1-s^2) \quad (3.20a)$$

is a dimensionless parameter, $q_0 = \pi/a$,

$$f(\Theta) = \frac{1}{Nq_0} \sum_q (1+2\nu_q) |q| \approx \frac{1}{q_0^2} \int_0^{q_0} q (1+2\nu_q) dq = \frac{1}{2} + \frac{2\Theta^2}{\hbar^2 \Omega_0^2} \int_0^{q_0} \frac{xdx}{e^x - 1} \quad (3.20b)$$

is a function which depends on the temperature Θ . In the limiting cases it has the form

$$f(\Theta) \approx \begin{cases} 1/2 + 2\Theta/\hbar\Omega_0, & \text{when } \hbar\Omega_0/\Theta \ll 1, \quad \Omega_0 = V_a q_0 \\ 1/2 + \pi^2 \Theta^2 / 6\hbar^2 \Omega_0^2, & \text{when } \hbar\Omega_0/\Theta \gg 1 \end{cases}$$

Equation (3.18) has a solution, normalized by the condition (2.11), which is non-vanishing in some range of n values. In the region of the lattice covered by the excitation the distances between neighboring molecules decrease proportional to $|\varphi_n|^2$. Indeed,

$$\rho_n(t) = \langle \nu | U_n^+ (\xi_n - \xi_{n-1}) U_n | \nu \rangle = \sum_q \left(\frac{\hbar}{2M\Omega_q N} \right)^{1/2} (1 - e^{-iqa}) (\beta_{qn} + \beta_{-q,n}^*).$$

Substituting the values (3.16) and (3.17) into this expres-

sion we obtain

$$\rho_n(t) = - \frac{\sigma |\varphi_n|^2}{MV_a^2 (1-s^2)} \frac{1}{N} \sum_q \frac{q \sin qa}{q^2} \approx - \frac{a\sigma |\varphi_n|^2}{MV_a^2 (1-s^2)}. \quad (3.21)$$

4. CONTINUUM APPROXIMATION

The explicit form of the solutions of the equations given in Sec. 3 can be obtained in the continuum approximation which is valid when $s \ll 1$. In that case the function $\varphi_n(t)$ can be replaced by the function $\varphi(z, t)$ of the continuous variable z/a which is normalized by the condition

$$\frac{1}{a} \int |\varphi(z, t)|^2 dz = 1. \quad (4.1)$$

In accordance with (3.18) this function will satisfy the equation

$$i\hbar \frac{\partial \varphi}{\partial t} - \left[\mathcal{E}_0 + \frac{\hbar^2 (1 - e^{-\bar{W}})}{ma^2} \right] \varphi + \frac{\hbar^2 e^{-\bar{W}}}{2m} \frac{\partial^2 \varphi}{\partial z^2} + G |\varphi|^2 \varphi = 0. \quad (4.2)$$

The equation obtained is as yet too complicated since the function \bar{W} depends, according to (3.20), on $|\varphi(z, t)|^4$. We shall therefore look for its approximate solution.

For some restriction on the velocity of displacement of the excitation ($s \ll 1$) and at not too high a temperature the following inequality holds

$$Bf(\Theta) \ll 1, \quad (4.3)$$

in which the values of B and $f(\Theta)$ are determined by Eqs. (3.20a) and (3.20b). In that case we can put $W(z, t) \approx 0$ in Eq. (4.2) in the zeroth approximation. It then transforms to the well studied non-linear Schrödinger equation

$$\left(i\hbar \frac{\partial}{\partial t} - \mathcal{E}_0 + \frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2} + G |\varphi_0(z, t)|^2 \right) \varphi_0(z, t) = 0. \quad (4.4)$$

Normalized by the condition (4.1) the solution of Eq. (4.4) has the form

$$\varphi_0(z, t) = \frac{(a\alpha_0)^{1/2} \exp\{i[k(z-z_0) + (\hbar/2m^*) (\alpha_0^2 - k^2)t - \mathcal{E}_0 t]\}}{2^{1/2} \text{ch}[\alpha_0(z-z_0 - Vt)]}, \quad (4.5)$$

in which $k = mV/\hbar$

$$\alpha_0 = \frac{maG}{2\hbar^2} = \frac{ma\sigma^2}{2MV_a^2 \hbar^2 (1-s^2)}, \quad s \ll 1. \quad (4.6)$$

To obtain solutions of Eqs. (4.2) in the next approximation we carry out in it simplifications of the factors which stand, respectively, in front of φ and $\partial^2 \varphi / \partial z^2$:

$$(1 - e^{-\bar{W}}) \varphi \approx 1/2 a \alpha_0 |\varphi(z, t)|^2 Bf(\Theta) \varphi(z, t), \quad (4.7)$$

$$e^{-\bar{W}} \frac{\partial^2 \varphi}{\partial z^2} \approx \exp\left[-\frac{a^2 \alpha_0^2}{4} Bf(\Theta)\right] \frac{\partial^2 \varphi(z, t)}{\partial z^2}.$$

The quantity $\frac{1}{2} a \alpha_0$ occurring in these expressions is the maximum value of $|\varphi_0(z, t)|^2$. After the simplifications (4.7) Eq. (4.2) again becomes the non-linear Schrödinger equation

$$\left[i\hbar \frac{\partial}{\partial t} - \mathcal{E}_0 + \frac{\hbar^2}{2m(\Theta)} \frac{\partial^2}{\partial z^2} + G(\Theta) |\varphi(z, t)|^2 \right] \varphi(z, t) = 0, \quad (4.8)$$

in which the coefficients $m(\Theta)$ and $G(\Theta)$ depend on the temperature. With increasing temperature the exciton mass increases, since

$$m(\Theta) = m \exp[1/2 a^2 \alpha_0^2 Bf(\Theta)], \quad (4.9)$$

while the non-linearity coefficient

$$G(\Theta) = G[1 - 1/2 Bf(\Theta)] \quad (4.10)$$

decreases.

The increase in the exciton mass is caused by the effective decrease in the resonance interaction between the molecules, a decrease produced by the violation of the phase coherence of the intra-molecular excitations. The decrease in the non-linearity parameter when the temperature rises reflects the effective decrease in the coupling of the exciton with the lattice deformations. At a sufficiently high temperature the parameter $G(\Theta)$ may become negative. In that case Eq. (4.8) will not have localized (soliton) solutions. This conclusion has, unfortunately, only a qualitative meaning, since our formulas are valid only when inequality (4.3) is satisfied.

When $s < 1$ an increase in the velocity V of the displacement of the excitation leads, according to (3.20a), to an increase in the parameter B and acts hence, in the same direction as an increase in the lattice temperature which causes an increase in the exciton mass. The change in the non-linearity parameter (4.10) is more complicated. As $V \rightarrow V_a$ the value of G increases, according to (3.19), while the factor $[1 - 1/2 Bf(\Theta)]$ decreases. At sufficiently high temperatures a change in sign of that factor is even possible and leads to a loss of localization of the excitation. This fact, apparently, removes the difficulty discovered in Refs. 1 to 5: the fact that the soliton energy tends to infinity and its size to zero as the soliton velocity approaches the longitudinal sound velocity. The n -dependence of the unitary operator of the displacements was not taken into account in those papers, it was chosen in the form

$$U = \prod_n U_n.$$

The range of values $V \approx V_a$, of course, needs a special study.

Solving Eq. (4.8) we find that the probability for the distribution of the excitations along the lattice is determined by the function

$$|\varphi(z, t)|^2 = \frac{a\alpha(\Theta)}{2 \operatorname{ch}^2 \{ \alpha(\Theta) [z - z_0 - Vt] \}}, \quad (4.11)$$

where

$$\alpha(\Theta) = (a/2\hbar^2) m(\Theta) G(\Theta). \quad (4.12)$$

In accordance with (3.21) the decrease in the equilibrium distances between neighboring molecules is determined by the function

$$\rho(z, t) = - \frac{a^2 \sigma(\Theta) \alpha(\Theta)}{2M V_a^2 \{ \alpha(\Theta) [z - z_0 - Vt] \}}. \quad (4.13)$$

The energy of a soliton moving with a velocity $V \ll V_a$ is proportional to the square of the velocity:

$$E_{\text{sol}}(V) = E_{\text{sol}}(0) + 1/2 m_{\text{sol}} V^2, \quad (4.14)$$

with a soliton mass

$$m_{\text{sol}} = m(\Theta) \left[1 + \frac{a^2}{6\hbar^2 V_a^2} G^2(\Theta) \right] \quad (4.15)$$

and a rest energy

$$E_{\text{sol}}(0) = \mathcal{E}_0 - m(\Theta) a^2 G^2(\Theta) / 12\hbar^2. \quad (4.16)$$

The size of the soliton is, in accordance with (4.11), determined by the quantity

$$l \approx \pi / \alpha(\Theta) = 2\pi\hbar^2 / a m(\Theta) G(\Theta). \quad (4.17)$$

We substitute in that expression the values (4.9) and (4.10). When the condition for the continuum approximation ($a\alpha_0 \ll 1$) and inequality (4.3) is satisfied, we then get, using (4.6),

$$l \approx 2\pi\hbar^2 / maG[1 - 1/2 Bf(\Theta)]. \quad (4.18)$$

With increasing temperature the size of the soliton thus increases and its properties increasingly approach those of an exciton. Whether the transition from a soliton to an exciton proceeds continuously or with a jump can be sorted out only when we develop a new theory which is valid in the region $V \approx V_a$.

¹The operator (2.2) also describes the motion of an extra electron in the conduction band of a one-dimensional dielectric. In that case m is the effective mass of the electron, \mathcal{E}_0 the energy of the bottom of the conduction band, and A_n^+ and A_n^- the operators for the presence or absence of an electron in the neighborhood of the molecule n . All the results of the present paper refer therefore also to the case of the migration of an electron through a one-dimensional molecular chain from a donor to an acceptor molecule. This effect plays, apparently, an important role in biological phenomena.

²Restricting ourselves to the linear approximation in the displacements we do not take into account possible changes in the frequencies Ω_n of the vibrational oscillations of the lattice when there are intra-molecular excitations. We can neglect these changes since we consider collective excitations which correspond to merely a single intra-molecular excitation in a very large lattice.

³In what follows we shall show that

$$|\varphi_n|^2 \ll ma^2 \sigma^2 / 2M V_a^2 \hbar^2.$$

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