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SOLITON-LIKE SOLUTIONS OF EQUATIONS DESCRIBING EXCITONS IN ONE-DIMENSIONAL MOLECULAR CRYSTALS

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SOLITON-LIKE SOLUTIONS OF EQUATIONS DESCRIBING EXCITONS IN ONE-DIMENSIONAL MOLECULAR CRYSTALS

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Солитоноподобные решения уравнений, описывающих возбуждения в одномерных молекулярных кристаллах

Найдены частные решения солитоноподобного типа для уравнений, описывающих экситон-фононные взаимодействия.

Работа выполнена в Лаборатории теоретической физики и в Лаборатории вычислительной техники и автоматизации ОИЯИ.

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Soliton-Like Solutions of Equations Describing Excitons in One-Dimensional Molecular Crystals

The family of soliton-like solutions to equations describing excitons in one-dimensional molecular crystals are obtained and discussed. It is shown that terms due to resonance interaction between excitons and molecules give rise to a change root and branch of a solution spectrum of the Schrödinger equation with cubic nonlinearity even if such an interaction is small.

The investigation has been performed at the Laboratory of Theoretical Physics and Laboratory of Computing Techniques and Automation, JINR.

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The set of equations describing excitons in one-dimensional molecular crystals has been obtained in the preceding papers of this series [1,2] with the help of the transformation suggested in [3]. The effects of the resonance interaction between excitons and molecules as well as the interaction of excitons and phonons have been taken into account. The exciton spectrum of this system has been derived and examined.

In dimensionless variables and long-wave limit (see [2]) such system assumes the form

$$F(\varphi,\alpha) \equiv i\varphi_t - \varphi + \alpha\varphi^*_x + \varphi_{xx} + |\varphi|^2\varphi = 0$$
$$F^*(\varphi,\alpha) \equiv -i\varphi^*_t - \varphi^* + \alpha\varphi_x + \varphi^*_{xx} + |\varphi|^2\varphi^* = 0, \qquad (1)$$

where φ is the Schrödinger amplitude and dimensionless parameter α is small ($\alpha \ll 1$) . The system (1) is a non-Lagrangian one and possesses the whole series of particular properties which we intend to discuss here. In the following part of this work the results of a numerical investigation of the dynamics of soliton type solutions of system (1) including the formation, the interaction and the stability of solitons are supposed to be published. The physical sense of the model, notations and validity limits of system (1) has been discussed earlier so we refear reader to the cited papers [1,2] and [4] as well.

The first integral of (1) can be obtained with convensional method, upon multiplying $F(\varphi,\alpha)$ by φ^* and subtracting from it $F^*(\varphi,\alpha)$ times φ . As a result we arrive at the law of the quantum number conservation in a divergent form.

$$\frac{\partial}{\partial t}|\varphi|^2 = i\frac{\partial}{\partial x}\left\{\frac{\alpha}{2}(\varphi^{*2}-\varphi^2)+(\varphi^*\varphi_x-\varphi\varphi_x^*)\right\}. \qquad (2)$$

This relation may be thought of as a "change" conservation law in nonrelativistic limit with

$$\rho = |\varphi|^2, \qquad (3a)$$

$$j = i\left\{\frac{\alpha}{2}(\varphi^2-\varphi^{*2}) + (\varphi_x^*\varphi-\varphi^*\varphi_x)\right\} \qquad (3b)$$

being respectively the "charge" (or probability) and "current" densities. One can see from the latter relation that, in our case unlike the well-known one of Lagrangian systems, "current" density consists of two parts

$$j = j^{(a)} + j^{(2)}, \qquad (4a)$$

where

$$j^{(a)} = i\frac{\alpha}{2}(\varphi^2-\varphi^{*2}) \qquad (4b)$$

and

$$j^{(2)} = i(\varphi\varphi_x^*-\varphi^*\varphi_x) \qquad (4c)$$

coincides with conventional Lagrangian "current" density. As we shall see $j^{(a)}$ may be thought of as a "dissipative" part of the overall current.

Upon integrating (2) over x we get the constant of motion for soliton type solutions (i.e., solutions with $\varphi(\pm\infty) = 0$)

$$\frac{d}{dt}Q = 0, \quad Q = \int\rho(x)\,dx \qquad (5)$$

that is usually interpreted as a law of the quantum number conservation.

Making likewise one can obtain

$$\frac{\partial}{\partial t}\left(|\varphi_x|^2-\frac{1}{2}|\varphi|^4\right) = i\frac{\partial}{\partial x}\left\{\frac{\alpha}{2}(\varphi_x^{*2}-\varphi_x^2)+i(\varphi_x^*\varphi_{xx}-\varphi_x\varphi_{xx}^*)+ \right. \qquad (6a)$$
$$\left. + \rho j^{(2)}\right\} + \rho\frac{\partial}{\partial x}j^{(a)},$$

that makes a functional

$$H^{(0)} = \int\left(|\varphi_x|^2-\frac{1}{2}|\varphi|^4\right)dx$$

the energy integral in $\alpha\to 0$ limit, to alter with time. Thus, $H^{(0)}$ associated with only the exciton energy may no longer be thought of as total energy of the system. Recall that $\alpha\varphi_x^*$ and $\alpha\varphi_x$ terms describe the reversible resonance interaction between excitons and molecules which can lead to broadening of the spectrum line.

Proceeding in the same fashion we have

$$i\frac{\partial}{\partial t}(\varphi^*\varphi_x-\varphi_x^*\varphi) = 2\alpha(\varphi_x^2+\varphi_x^{*2}) + \frac{\partial}{\partial x}\left\{-\alpha(\varphi^*\varphi_x^*+\varphi\varphi_x)+ \right. \qquad (6b)$$
$$\left. + 2\left(|\varphi_x|^2-\frac{1}{2}|\varphi|^4\right) - (\varphi^*\varphi_{xx}+\varphi_{xx}^*\varphi)\right\}.$$

Finally, integrating (6) over x yields

$$\frac{dH^{(0)}}{dt} = \int|\varphi|^2\frac{\partial}{\partial x}j^{(a)}dx, \quad \frac{dP^{(0)}}{dt} = 2\alpha\int(\varphi_x^{*2}+\varphi_x^2)\,dx, \qquad (7)$$

where $P^{(0)} = -i\int(\varphi^*\varphi_x-\varphi_x^*\varphi)$ is the momentum of a packet in $\alpha\to 0$ limit. That is why we supply values H and P with (0) superscript.

After transition to the conventional "polar" representation of complex function

$$\varphi = \psi\exp i\theta,$$

we have

$$\frac{dH^{(0)}}{dt} = -\frac{\alpha}{2}\int\theta_x\psi^4\cos 2\theta\,dx, \qquad (8)$$

$$\frac{dP^{(0)}}{dt} = 4\alpha\int\left\{(\psi_x^2-\psi^2\theta_x^2)\cos 2\theta - 2\psi\psi_x\theta_x\sin 2\theta\right\}dx.$$

Let us consider qualitatively possible soliton solution of the system (1). In $\alpha \ll 1$ limit one can derive a series in a small parameter starting from a well-known soliton solution for the Schrödinger equation with the cubic nonlinearity (S3). However, in this way one may hardly obtain a qualitatively new result.

Consider first the stability of some solutions to eq. (1). In the large amplitude region $\left(|\varphi|^2 \simeq 1\right)$ the solution

$$\varphi(x,t) = A \exp\{-i(\omega_c t - \vartheta_o)\} \tag{9}$$

(with $A = 1 - \omega_c$ arbitrary ϑ_c and $\omega_c \ll 1$) turns out to be unstable with respect to small perturbations which frequency $\Omega \gg \omega_c$ and wave number $\varkappa$ are related by the dispersion equation*)

$$\Omega = \pm\sqrt{\frac{a}{2}}\left\{\sqrt{1+\sqrt{1+b^2/a^2}} - i\sqrt{\sqrt{1+b^2/a^2} - 1}\right\}, \tag{10}$$

where

$$a = \varkappa^2(\varkappa^2 + \alpha^2 - 2A^2), \quad b = 2\alpha A^2 \varkappa \cos\vartheta_c . \tag{11}$$

This instability is analogous to that of a monochromatic plane wave in the framework of S3 equation, except the asymptotic behaviour of the growth rate: (10) yields $\mathrm{Im}\,\Omega \propto 1/\varkappa$ when $\varkappa \to \infty$.

In the small amplitude domain ($A \ll 1$, $\omega_c \simeq 1$) the instability of the wave

$$\varphi = A\left\{\left(1 - i\frac{\alpha k}{\omega_o}\right)\cos(kx - \omega_c t) + i\frac{1+k_o^2}{\omega_c}\sin(kx - \omega_c t)\right\} \tag{12}$$

$$\omega_c^2 = (1+k^2)^2 + \alpha^2 k^2 - 2A^2 .$$

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*) Eq. (10) may be easily obtained via standard technique.

(or of the wave packet) is also described by formula (10), where now

$$a = \varkappa^2\left(\varkappa^2 + \tfrac{1}{2}\alpha^2\varkappa^2 - 2A^2\right), \quad b = \alpha\varkappa^3 A^4/4 . \tag{13}$$

But in this case to get (10) we have to employ quite a general and successive Bogolubov method, known in the theory of nonlinear equations /5/, that enables one, in principle, to calculate terms of higher order in A^2 ($\propto A^6$ and so on, though the calculations become more complicated and dull). A more visual and "straight" formalism of averaging over fast time ($\tau \simeq \frac{1}{\omega_c} \ll \frac{1}{\Omega}$) is not able to give dissipative terms $\sim O(A^4)$ so we have $b \equiv 0$.

The growth rate of the instability of plane waves with various amplitudes may be seen from (10) to have a peak near $\varkappa_c \simeq A$ like in the case of S3 equation. But the spectrum due to (10) is enriched with short-wave harmonics.

The fact that the character of the instability of solutions to (1) both for large and small amplitudes is qualitatively identical seems to be noteworthy to us. The instability (10) results in the formation of self-localized wave packets of a soliton type. Such solutions may be examined in more detail in a particular case when the group, i.e., soliton velocity, is equivalent to the phase velocity of constituent waves, $V_{gr} = \omega/k$. Having used the polar form for φ and introducing $\xi = x - vt$, $\eta = kx - \omega t$ one comes to

$$\begin{aligned} -v\psi_\xi - \alpha\psi_\xi \sin 2\vartheta - \alpha\vartheta_\eta \psi\cos 2\vartheta + 2\psi_\xi\vartheta_\eta + \psi\vartheta_{\eta\eta} = 0 \\ v\vartheta_\eta\psi + \psi_{\xi\xi} - \psi + \psi^3 - \vartheta_\eta^2\psi + \alpha\psi_\xi\cos 2\vartheta - \alpha\vartheta_\eta\psi\sin 2\vartheta = 0 \end{aligned} \tag{14}$$

Letting $\eta = k\xi$ we can integrate once the first equation of (14)

$$\psi^2\left(\vartheta_\xi - \tfrac{1}{2}(v + \alpha\sin 2\vartheta)\right) = \text{const} \quad . \tag{15}$$

Soliton solutions imply $\psi(\pm\infty) \to 0$ therefore $\text{const} = 0$ and (15) may be further integrated to give

$$\xi + C = \begin{cases} 2(v^2-\alpha^2)^{1/2}\,\text{arctg}\,\dfrac{v\,\text{tg}\,\vartheta + \alpha}{\sqrt{v^2-\alpha^2}}, & v^2 > \alpha^2 \\ -\frac{1}{v}\text{tg}\,(\vartheta - \frac{\pi}{4}), & v^2 = \alpha^2 \\ (\alpha^2 - v^2)^{-1/2}\,\ln\dfrac{v\,\text{tg}\,\vartheta + \alpha - \sqrt{\alpha^2 - v^2}}{v\,\text{tg}\,\vartheta + \alpha + \sqrt{\alpha^2-v^2}}, & v^2 < \alpha^2 \end{cases} \tag{16}$$

Taking in (16) v/α or α/v as a small parameter some approximate solutions $\psi_s(\xi)$ of the second eqution of (14) might be obtained. Here as an example we describe the most curious situation arisen at $v = 0$, when the phase

$$\vartheta = \text{arctg}\left\{\exp\alpha(x - x_0)\right\} + \vartheta_0 \; , \quad \vartheta_0 = \pm\frac{\pi}{2} \pm \pi n \tag{17}$$

is subject to sine-Gordon equation*) $\vartheta_{xx} = (\alpha^2/4)\sin 4\vartheta$. It is a kink-soliton describing the rotation of the phase by the angle $\pi/2$ when x varies from $x = -\infty$ to $x = +\infty$. Note that the phase rotation occurs in the region of order $1/\alpha$.

The second equation of (14) then assumes the form

$$\psi_{xx} - \psi + \psi^3 - \tfrac{3}{4}\alpha^2\psi\sin 2\vartheta + \alpha\psi_x\cos 2\vartheta = 0 \tag{18}$$

Its asymptotic behaviour at $|x| \gg 1/\alpha$ depends essentially on the "initial" phase ϑ_0 at $x \to -\infty$. In the case $\vartheta_0 \geq 0$ $\left(\vartheta_0 = \pi(n + \tfrac{1}{2}),\ n = 0,1,2,\ldots\right)$ we have equation

$$\psi_{xx} - \psi + \psi^3 - \text{sgn}(x)\,\alpha\psi_x = 0 \qquad |x| \gg 1/\alpha \tag{19}$$

possessing soliton-like solutions if $\alpha < \sqrt{2}$. The "initial" phase $\vartheta_0 = -\pi(n + \tfrac{1}{2}),\ n = 0, 1, \ldots$ leads to the equation

$$\psi_{xx} - \psi + \psi^3 + \text{sgn}(x)\,\alpha\psi_x = 0 \tag{20}$$

that has as a solution either a narrow soliton of S3 equation or a set of solitons with nodes of the field function $\psi(x)$ /6/ (at any rate for the solutions of the $x \to -x$ symmetry).

That the higher conservation laws are absent for system (1) at $\alpha \neq 0$ **) and that it has a rich spectrum of soliton-like solutions will naturally rise to a qualitatively new dynamics of initial packets. The formation as well as the inelastic interaction of solitons may be expected in the framework of system (1).

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**) Unlike the complete integrable S3 equation not permitting inelastic interaction of solitons /7/.

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