NANOSCALE EXCITATIONS OF SOLIDS IN THE FORM OF AXIALLY SYMMETRIC SOLITONS

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Introduction

Soliton excitations in solids is a development of the concept of traditional electronic excitations (injected electrons, excitons), or excitations of a different physical nature (magnon, polarons, etc.). The main feature that distinguishes soliton excitations from analogous traditional excitations is the appearance of an amplitude distributed in space. In this case, the spatial distribution of the amplitude of the soliton excitation has dimensions that do not exceed several nanometers. The studies carried out are of practical interest, since they make it possible to use soliton excitations to control the processes of directed point transfer of energy or charge

The excited states of materials with a crystal structure taking into account the nonlinear response of the crystal lattice to excitation

A general system of equations for soliton excitations is formulated, and its exact 3-D solution is constructed in the form of an amplitude modulated plane wave. For the modulating factor, a nonlinear equation of the type of the nonlinear Schrödinger equation (NLS equation) is formulated. Only movement in the *z*-direction is considered. Then the components of the vector of dimensionless wave momentum: $\boldsymbol{p} \equiv b\mathbf{k}$, where *b* is the crystal lattice constant, satisfy the condition: $p_x = p_y = 0,\ \ p_z \neq 0$; the components of the dimensionless velocity vector satisfy the condition: $\beta_x = \beta_y = 0,\ \ \beta_z = sin(p_z)$; the components of the dimensionless mass tensor satisfy the condition: $\mu_x = \mu_y = 1$, $\mu_z \equiv 1/cos(p_z) \equiv 1/\sqrt{1-\beta_z^2}$. The equation for the amplitude in this case takes the form:

$$\frac{1}{2}\frac{\partial^2\varphi_f}{\partial\xi_x^2}+\frac{1}{2}\frac{\partial^2\varphi_f}{\partial\xi_y^2}+\frac{1}{2\mu_z}\frac{\partial^2\varphi_f}{\partial\xi_z^2}+g_f\varphi_f^3+\varepsilon_f\varphi_f=0 \qquad (1)$$

Here *f* is the quantum state to which the excitation occurred, and g_f is the nonlinearity parameter, which depends on the crystal parameters. The ξ_α variables are the components of the vector $\boldsymbol{\xi} = \mathbf{r} - \mathbf{r}_0(\tau)$. The variable $\mathbf{r}$ is the quantum spatial variable of excitation in the crystal frame of reference, and $\mathbf{r}_0(\tau) = \boldsymbol{\beta}\tau$ is the point of conditional localization of excitation. It is a variable of the classical type and it describes the motion of the point $\mathbf{r}_0(\tau)$ in the crystal frame of reference. Equations (1) are formulated in eigen reference frame relative to the point $\mathbf{r}_0$.
Equation (1) is exactly satisfied by the function:

$$\varphi_f(\xi) = H_f(\xi_\perp)\Phi_f(\xi_z), \qquad (2)$$

where $\xi_\perp = \sqrt{\xi_x^2+\xi_y^2}$. In this solution: $H_f(\xi_\perp) = \theta\_\big(1-\lambda_f^\perp\xi_\perp\big)$, where $\theta\_(x)$ is the Heaviside step function, which has the following properties: $\theta\_(x) = 1$, for $x \geq 0$; and $\theta\_(x) = 0$, for $x < 0$. The $\lambda_f^\perp$ parameter is the reciprocal of the radius of the area inside which the function $H_f(\xi_\perp)$ is nonzero, and outside this area it is equal to zero. This choice of the factor $H_f(\xi_\perp)$ is associated with two important properties, namely: $H_f^q(\xi_\perp) = H_f(\xi_\perp)$, where *q* is any integer degree, and $\partial H_f/\partial\xi_\perp = 0$. These properties make it possible to consider the representation $\varphi_f(\xi) = H_f(\xi_\perp)\Phi_f(\xi_z)$ as an exact solution of equation (1), which has a finite norm. Substitution of (2) into (1) leads to the expression:

$$\theta_-\left(1-\lambda_f^\perp\xi_\perp\right)\left\{\frac{1}{2\mu_z}\frac{d^2\Phi_f}{d\xi_z^2}+g_f\Phi_f^3+\varepsilon_f\Phi_f\right\}=0$$

This equation is satisfied outside the region $\xi_\perp = 1/\lambda_f^\perp$ (i.e., when $\lambda_f^\perp\xi_\perp > 1$) due to the properties of the $\theta\_$ – function. Inside this region (for $\lambda_f^\perp\xi_\perp \leq 1$), it is satisfied by the differential equation:

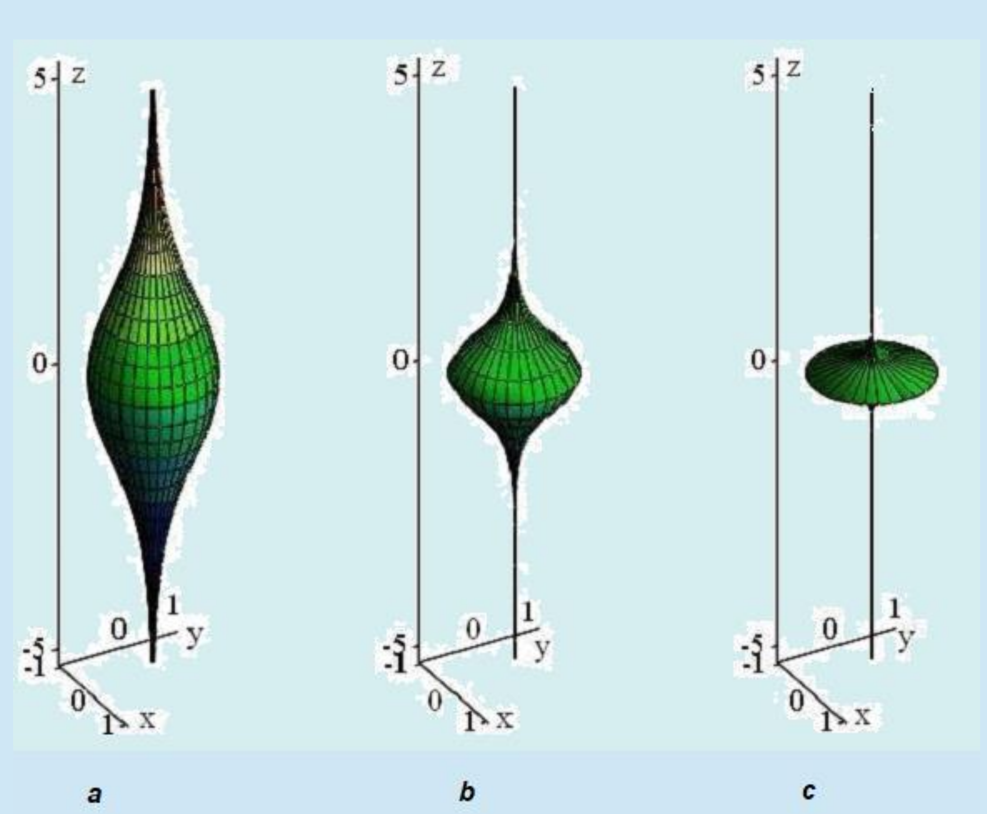
$$\frac{1}{2\mu_z}\frac{d^2\Phi_f}{d\xi_z^2}+g_f\Phi_f^3+\varepsilon_f\Phi_f=0$$

and creates solutions in the form: $\Phi_f(\xi_z) = B_f/\mathrm{ch}\big(\lambda_f\ \xi_z\big)$. The complete solution (2), taking into account the normalization condition: $\iiint_{(\infty)}\varphi_f^2(\xi)d\xi_x d\xi_y d\xi_z = 1$, is reduced to the following

$$\varphi_f^2(\xi)=\mu_z\left(g_f\cdot\left(\lambda_f^\perp\right)^4\Big/4\pi\right)\theta_-\left(1-\lambda_f^\perp\xi_\perp\right)\mathrm{ch}^{-2}\left(\left(g_f\cdot\left(\lambda_f^\perp\right)^2\Big/2\sqrt{\pi}\right)\mu_z\,\xi_z\right)$$

It is the square of the solution that has a physical meaning and is called a soliton.
Two circumstances attract attention on themselves. First, the product $\mu_z\xi_z$ in the argument of the function $\mathrm{ch}^{-2}(\ldots)$, when taking into account the explicit form of the factors ($\mu_z = 1/\sqrt{1-\beta_z^2}$, $\xi_z \equiv z - \beta_z\tau$), takes on the following explicit form: $\mu_z\xi_z \equiv (z-\beta_z\tau)/\sqrt{1-\beta_z^2}$, and has a Lorentz-invariant form in the dynamic direction. Secondly, the entire factor $\varphi_f^2(\xi)$, on the one hand, is proportional to the component of the dynamic mass μ_z, and on the other hand, the function $\varphi_f^2(\xi)$ is proportional to the change in the lattice constant: $\Delta\mathbf{b}_f(\xi) \sim -\varphi_f^2(\xi)$. This leads to the appearance of curvature in the space of the crystal lattice in the vicinity of the point of localization of excitation: $z_0(\tau) = \beta_z\tau$. Formally, it looks as if the quasiparticle mass creates a curvature of the space of crystal.
If we introduce the notation: $\sigma_f \equiv \left(\lambda_f^\perp\right)^4 g_f^2/8\pi$, then due to the values of the σ_f parameter and the velocity $\beta_z = \sin(p_z)$, the shape of the soliton can continuously vary from an almost ellipsoid of rotation elongated along the dynamic direction (along the *z* axis) (Fig.1a) to an almost flattened ellipsoid of rotation (Fig. 1.c) Of course, there are also such parameter values for which the excitation has an almost spherical shape (Fig. 1.b). $\sqrt{2\sigma_f/(1-\beta_z^2)}$. That is, the spatial forms of the soliton are presented for the function: $\Psi(r,z) = \theta\_(1-r)/\mathrm{ch}^2(\chi z)$, where for the convenience of numerical implementation redesignated: $\lambda_f^\perp\xi_\perp \equiv r = \sqrt{x^2+y^2}$.
Figure 1 shows the spatial forms of the soliton for the quantity $\Psi \equiv \varphi_f^2(\xi)\sqrt{4\pi}/\left(\left(\lambda_f^\perp\right)^2\chi\right)$, where $\chi \equiv$, $\xi_z = z$. In this representation, the shape of the soliton is determined exclusively by the parameter χ. The higher the velocity β_z of a soliton at a fixed value of σ_f, the more flattened it's form.

Figure 1.
Spatial forms of solitons for values: $\chi = 0.5$ (a), $\chi = 1.3$ (b) and $\chi = 5$ (c). The soliton propagates in the positive direction of the z axis.



Conclusions

The excited states of materials with a crystal structure are considered taking into account the nonlinear response of the crystal lattice to excitation. The possibility of constructing an analytically soliton solution with axial symmetry and a finite norm is analyzed. The corresponding solution was received.
It is known that an NLS equation with cubic nonlinearity has analytic solutions on the class of hyperbolic functions only for the spatially one-dimensional case. It turned out that there is a physically consistent case when in a three-dimensional NLS equation it is possible to perform an exact separation of variables in terms of generalized functions. New analytical solutions of the NLS equation with cubic nonlinearity are obtained. The solutions have the form of axially symmetric 3D solitons.
It is shown that the soliton has a nanoscale axially symmetric spindle-like spatial shape. It can vary from strongly elongated along the dynamic direction (along the *z*-axis) to strongly oblate, depending on the parameter values. Varying these parameters makes it possible to control the spatial form of soliton excitation.