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дубна

E17-84-752

D.I.Pushkarov

QUANTUM BEHAVIOUR OF SOLITONS IN LATTICE STRUCTURES

Submitted to
"Solid State Communications"

1984

1. INTRODUCTION

Quantum behaviour of solitons in solids has been apparently considered first in 1972 [1] in the case of crowdion propagation in crystals at low temperatures. Obviously, the crowdion configuration represents a unique example of one-dimensional structure in 3-dimensional solids. It arises when the deformation caused by an extra atom occurs only in one of the crystallographic directions. Thus, the extra atom is in more or less close-packed row in which even the remote atoms are displaced from their equilibrium positions (Fig.1). The model used in [1] is similar to the Frenkel'-Kontorova dislocation model [2]. It has been shown that the crowdion turns into a quasi-particle (the crowdion wave) that is no longer characterized by its mass centre and velocity but by its quasi-wave vector, k, and dispersion law $\epsilon(k)$. It has been also shown that the crowdion can move with a supersonic velocity and irradiate Cherenkov phonons.

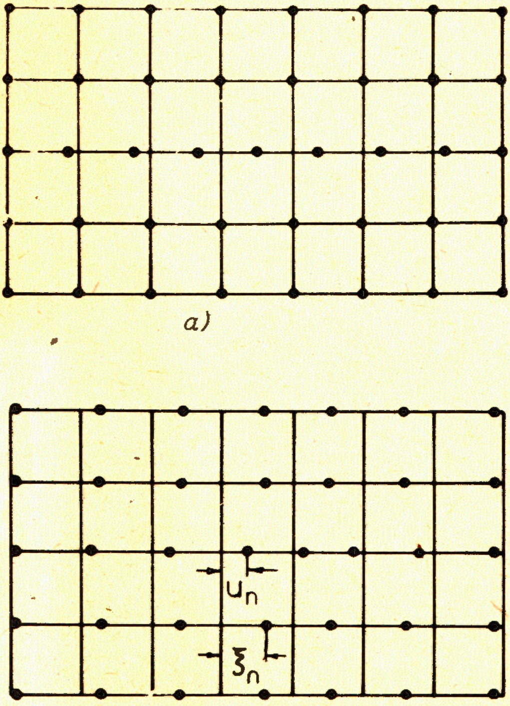

Fig.1. Crowdion configuration: a) in an undeformed crystal and b) in a crystal deformed by an elastic wave.

From a mathematical point of view the problem has been reduced to the sine-Gordon model. However, the consideration made in [1] is quite more general and the physical results can be also applied to some other models (e.g., SSH [3], ϕ^4-model [4], etc.) used for describing solitons in polyacetylene, $NbSe_3$ and other quasi-one-dimensional substances. It is of interest therefore to point out the main consequences of the effects predicted in [1] and consider their applicability to other model structures. It will be shown, e.g., that the quantum effects make impossible the pinning of the soliton to the lattice not only in the case of crowdions but also in polyacetylene in contrast to the classical results /4/.

2. MODEL. CONTINUUM APPROXIMATION

Crowdion behaviour in crystals /1/ and the soliton behaviour in quasi-one-dimensional structures like polyacetylene described usually by SSH and ϕ^4-models have many common features which can be treated in a common way by means of a Lagrangian of the form

$$\tilde{L} = \frac{m}{2}\sum_n \dot{u}_n^2 - \sum_n \left\{\frac{mc^2}{2}(u_{n+1}-u_n)^2 + W(u_n)\right\} \qquad (1)$$

describing a chain of particles of mass m interacting with their neighbours via elastic forces and placed in a potential $W(u)$. u_n is the displacement of n-th particle, and c corresponds to the sound velocity in the isolated chain. The lattice constant $a = 1$. In the continuum approximation (n continuous) the equations of motion are reduced to the following differential equation

$$\frac{\partial^2 u_n}{\partial t^2} - c^2\frac{\partial^2 u_n}{\partial n^2} = -\frac{1}{m}\frac{\partial W}{\partial u_n}. \qquad (2)$$

If the potential is assumed to be of the form

$$W(u) = \frac{1}{2}A(1-\cos 2\pi u), \qquad (3)$$

then (2) coincides with the sine-Gordon equation. The one-soliton solution of interest has the form

$$u(n-vt) = \frac{2}{\pi}\,\mathrm{arctg}\left(\exp\frac{x-n+vt}{L}\right), \qquad (4)$$

where x is the crowdion centre, and the crowdion length is

$$L = L_0\sqrt{1-w^2}, \quad L_0 = \frac{1}{\pi}\sqrt{mc^2/2A}, \quad w = v/c. \qquad (5)$$

For the validity of the continuum approximation the inequality $L \gg 1$ must be satisfied. The crowdion energy in the same approach is

$$E = U_0/\sqrt{1-w^2} \qquad (6)$$

which can be obtained from the static energy $U_0 = 2mc^2/\pi^2 L_0$ by the Lorents transformation. At small velocities ($v \ll c$) the soliton behaves like a particle of mass

$$\mu = U_0/c^2 = 2m/(\pi^2 L_0) \qquad (7)$$

which obviously is much smaller than the atomic mass, m.

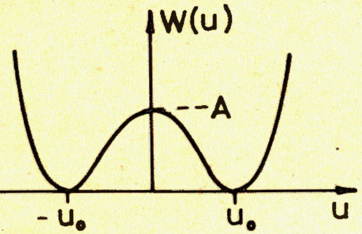

Fig.2. A double-well potential form used in ϕ^4 and SSH models.

Now consider the case of double-well potential $W(u)$ (Fig.2). Obviously, $W(\pm u_0) = W'(\pm u_0) = 0$, where $\pm u_0$ are the coordinates of the equivalent potential minima, and (') denotes the derivative with respect to u. As we are interested in solutions of the form $u((n-vt)/\ell)$ eq.(2) becomes

$$\frac{mc^2}{\ell^2}(1-w^2)\frac{d^2u}{dz^2} = \frac{dW}{du}, \qquad (8)$$

where $z \equiv (n-vt)/\ell$.

The energy first integral of (8) is

$$\frac{mc^2}{2}\left(\frac{du}{dz}\right)^2 = \frac{\ell^2}{1-w^2}W(u). \qquad (9)$$

As the left-hand side and $W(u)$ are positive, the condition $v < c$ appears. On the other hand, eq.(9) must be satisfied for arbitrary $v < c$. Hence, $\ell = \ell_0\sqrt{1-w^2}$.

Taking into account (9), the strain energy, $W_{e\ell}$, can be written in the form

$$W_{e\ell} = \frac{mc^2}{2}\int_{-\infty}^{\infty}\left(\frac{\partial u}{\partial n}\right)^2 dn = \frac{mc^2}{2\ell}\int\frac{du}{dz}du = \frac{1}{2}U_0/\sqrt{1-w^2}, \qquad (10)$$

where

$$U_0 = \sqrt{2mc^2}\int_{-u_0}^{u_0}\sqrt{W(u)}\,du. \qquad (11)$$

In the same way the kinetic energy is found to be

$$\frac{m}{2}\int_{-\infty}^{\infty}\dot{u}^2 dn = w^2 W_{e\ell} \qquad (12)$$

and the energy connected with the potential $W(u)$ is

$$\int W(u(n))\,dn = \ell\int W(u)\frac{dz}{du}du = \frac{1}{2}U_0\sqrt{1-w^2}. \qquad (13)$$

Finally the total energy is

$$E = U_0/\sqrt{1-w^2}\,. \qquad (14)$$

Note that the contributions of terms (10,12,13) to the effective mass μ are equal in magnitude but differ in sign.

Hence, the soliton energy and effective mass can be obtained by means only of the potential W(u) without knowing the solution of (8). So, for the ϕ^4-model one has

$$W(u) = \frac{1}{4}\gamma u_0^2 [(\frac{u}{u_0})^2 - 1]^2 \qquad (15)$$

and making use of (11) obtains

$$U_0 = \frac{4mc^2}{3\ell_0} u_0^2 \qquad (16)$$

and

$$\mu = \frac{4}{3}\frac{m}{\ell_0} u_0^2\,. \qquad (17)$$

where

$$\ell_0 = (2mc^2/\gamma)^{1/2}. \qquad (18)$$

In the same notations the soliton solution of (8) has the form

$$u(n-vt) = u_0 \tanh(\frac{x+n-vt}{\ell})\,. \qquad (19)$$

In this case U_0 and μ contain an additional small factor $(u_0/a)^2$ in comparison with (6) and (7). The same parameter appears also in SSH model [3], and owing to its small value ($\sim 10^{-3}$) the effective mass of the soliton in polyacetylene turns out to be of the order of several electronic masses.

However note that u_0 and ℓ_0^{-1} may not be extremely small, because this leads to very small potential minima not able to pin atoms. In other words u_0 has to be larger than the zero oscillation amplitude. Unfortunately this is not the case realized in SSH model where the barrier height $A = W(0) - W(u_0) \approx$ ≈ 150 K (called in [3] the condensation energy) is much smaller as compared to the first quantum level $\hbar\omega/2 \approx 10^3$K. In the notations of SSH [3] one has

$$\frac{2A}{\hbar\omega} = u_0^2(\frac{\lambda MK}{\hbar^2})^{1/2} \ll 1\,; \quad \lambda = \frac{2a^2}{\pi K t_0} = 0.20; \quad u_0 = 0.04\,\text{Å}.$$

As a result, the atomic coordinates become bad characteristics, the existence of a real dimerization is questionable, and a more accurate quantum analysis has to be carried out.

3. LATTICE PERIODICITY EFFECT. PINNING PROBLEM

If the soliton length is much larger than the lattice constant, solutions (4) and (19) describe well the atomic positions. However, the soliton energy calculated in the continuum approximation is degenerated with respect to the coordinate of centre x. The lattice discreteness can be taken into account in a good approximation substituting the solutions into the sum

$$E = \sum_n E_n\,, \quad E_n = \frac{m}{2}\dot{u}_n^2 + \frac{mc^2}{2}(u_{n+1} - u_n)^2 + W(u_n)\,. \qquad (20)$$

Making use of a standard method yields

$$E = \int dk \sum_n \delta(n-k) E_k = \int dk E_k + \int dk E_k \cos 2\pi k + \dots\,. \qquad (21)$$

The first integral in the right-hand side is the energy (14). It can be shown that each subsequent integral is smaller by a factor $\sim e^{-\pi^2 \ell}$. Hence, one may limit oneself to the second term. The calculation (for v = 0) yields (see Appendix).

$$\mathcal{E}_1 = \frac{1}{2} U_1 \cos 2\pi x, \quad U_1 = a e^{-\pi^2 \ell_0}. \qquad (22)$$

where the value of the coefficient a depends on the model used. For the sine-Gordon system

$$a_{SG} \approx 4\pi^2/9 \qquad (23)$$

and for the ϕ^4-model

$$a_4 = 8\pi^2(\frac{\pi^2}{3} - 1)\ell_0^2 u_0^2 \qquad (24)$$

(This value differs from that of [4], see Appendix).

Hence, the soliton moves in a periodic potential with the periodicity of the lattice. The amplitude of this potential, U_1, has been considered in [4] as a pinning energy. From the comparison of this energy with the soliton-soliton interaction energy the critical soliton concentration necessary for the depinning and free soliton propagation has been evaluated. The barrier height has been evaluated also in [3] and the conclusion has been made that pinning can take place at low temperatures ($T < 20 \div 40$ K). An attempt of a more precise calculation of the pinning energy has been made in /5/. However, as it was shown in 1972 /1/ the pinning of the soliton in such a potential cannot take place even at $T = 0$ due to quantum effects. As a criterion of the quantum behaviour one may use the quantity

$$\delta = \frac{U_1}{\pi^2 \hbar^2/\mu a^2}$$

(in a quantum case $\delta \leq 1$). Owing to the small effective mass and exponentially small barrier height δ turns out to be smaller than 1 in all physically reasonable cases. In fact, the condition $\delta \lesssim 1$ can be rewritten as

$$\pi^2 \ell e^{\pi^2 \ell} \gtrsim \alpha \left(\frac{mc^2}{\theta_D}\right)^2 \left(\frac{u_0}{a}\right)^2$$

(θ_D being the Debye temperature) which is satisfied even at $\ell = 1$.

4. SOLITON AS A QUASI-PARTICLE

Hence, the soliton is a quantum object. It is delocalized and must be considered as a quasi-particle (soliton wave) that is no longer characterized by the coordinate and velocity of its centre but by its quasi-wave vector, k, and dispersion law, $\epsilon(k)$. Note that as a consequence of the delocalization there is no sense to calculate the "pinning energy" in more detail (taking into account the dependence of the soliton shape on the position of its centre within a unit cell). In fact, tunneling occurs between equivalent states. On the other hand, the contribution to the soliton effective mass is negligible (see below).

To find the soliton wave dispersion law, one has to obtain the eigenvalue spectrum of the Schrödinger equation

$$\Psi'' + \frac{2\mu}{\hbar^2}\left(\mathcal{E} - \frac{1}{2} U_1 \cos 2\pi x\right)\Psi = 0$$

that allows solutions of the form of Bloch waves $\Psi = N^{-1/2} e^{ikx} \phi_k(x)$, where $\phi_k(x+1) = \phi_k(x)$. This spectrum is quite complicated in the general case. However, in the case of interest ($\delta \ll 1$) the dependence of the energy on the quasi-wave vector k can be determined from the following equation

$$\cos k = \cos k_0 + \frac{\pi^2 \delta^2}{4(1 - k_0^2/\pi^2)} \frac{\sin k_0}{k_0}, \quad k_0^2 = 2\mu\mathcal{E}/\hbar^2 .$$

This leads for small $k_0 \ll 1$ to the dispersion law

$$\epsilon(k) = U_0 + \frac{1}{4} U_1 \delta + \hbar^2 k^2 / 2\mu^* ,$$

where the effective mass $\mu^* = \mu\left(1 - \frac{1}{2}\delta^2\right)$.

5. SUPERSONIC SOLITON BEHAVIOUR. PHONON EMISSION

All the consideration above is obviously restricted by the condition of small velocity v as compared to velocity c called here the sound velocity in the isolated chain. However, the actual sound velocity, s, in complex lattices (the only lattices where crowdions occur) can be drastically different from velocity c. In fact, the sound propagation is connected with displacements of heavy lattice cells containing several atoms. On the other hand the effective strain constant can also be widely different. Therefore the crowdion can move with a supersonic velocity. In such a case the propagation of an elastic wave in the crystal amounts to a change in the amplitude A and in the period of the potential $W(u)$ which now become functions of the deformation tensor Δ:

$$W(u_n, \Delta) = A(\Delta)\left\{1 - \cos\left(2\pi \frac{u_n - \xi_n}{1 + \Delta_1(n)}\right)\right\},$$

where ξ_n is the component of the deformation vector ξ along the crowdion chain (chosen as x-axis). Assuming axial symmetry the diagonal elements of Δ are $\Delta_1(n) = \xi_{n+1} - \xi_n$, $\Delta_2(n)$, $\Delta_3(n)$.

The analysis made in /1/ shows that the problem can be fully considered (analytically) in the most interesting case when the phonon quasi-wave vector components in the crowdion direction are small ($q_x L \ll 1$). The other components have to satisfy $q_\perp a \ll 1$. In this case the soliton length takes the form

$$\mathcal{L} = \frac{1 + \Delta_1}{2\pi} \sqrt{2mc^2/A(\Delta)} = L(1 + \lambda_i \Delta_i),$$

where λ_i are determined through the coefficients in the expansion of A in powers of Δ_i: $A(\Delta) = A[1 - 2(\lambda_1 - 1)\Delta_1 - 2\lambda_2(\Delta_2 + \Delta_3)]$. The bottom of the crowdion energy band is also shifted and, as a result, the crowdion wave can be described by a local dispersion law

$$\epsilon(k, \Delta) = U_0 + \epsilon_i \Delta_i + \hbar^2 k^2 / 2\mu^* ,$$

where $\epsilon_1 = U_0(1 - \lambda_1)$, $\epsilon_2 = \epsilon_3 = \lambda_2/(1 - \lambda_1)$.

To consider the phonon emission, the deformation potential method can be used /1/. If the wave propagates along the chain, the emission probability, W^+, is found to be

$$W^+ \approx \frac{\epsilon_1^2}{2\hbar M s^2 N}\left(\frac{q_x}{2p}\right)^2 \left(\exp\frac{\hbar s q_x}{T} - 1\right)^{-1},$$

where $M = \Sigma\, m_i$ is the total mass of a lattice cell, $p = \mu s/\hbar$, and N is the cell number. Since in this case phonons with wave vectors $q_x \sim k$ are emitted (or absorbed) $\hbar s q_x/T \sim \hbar s k/T \sim (\mu s^2/T)^{1/2}$.

Thus, for $T \gg \mu s^2$ $\quad W^+ \approx \frac{\epsilon_1^2}{8Ms^2N}\frac{q_x}{\mu s}\frac{T}{\mu s^2}$.

If oscillations with all possible directions of $\vec{q}$ are excited in the crystal, then $q \sim T/\hbar s$ whereas $q_x \sim k \sim (2\mu T/\hbar)^{1/2}$. Consequently, $q_x/q \sim (\mu s^2/T)^{1/2} \sim s/v \ll 1$ which is typical of the Cherenkov emission cone. In this case, however, the phonon energy can be of the order of the crowdion excitation itself, and therefore the process, in general, could be inelastic.

It has been recently reported /6/ about the possibility of supersonic propagation of solitons in SSH model. The numerical calculations made there show that a soliton of the form $u_0 \tanh\left(\frac{x - vt}{\ell}\right)$ can move with a velocity v larger than the sound velocity in the "metallic" state. But the physical nature of the new restricting velocity seems not to be clear enough. On the other hand, if the soliton configuration is formed by means of a small deformation transfer from a cell to cell the sound velocity (correctly defined) seems to play a very important role. This problem will be considered elsewhere.

Acknowledgements are due to Professor E.A.Kaner and S.Drechsler for discussions.

APPENDIX

To obtain U_1 one has to calculate (at $v = 0$) the following integrals

$$I_1 = \int_{-\infty}^{\infty} W(u(n)) \cos 2\pi n\, dn, \quad I_2 = \frac{mc^2}{2}\int_{-\infty}^{\infty} [u(n+1) - u(n)]^2 \cos 2\pi n\, dn.$$

Note that the strain energy in I_2 has to be written in a finite difference form. If the difference is substituted by a derivative, the latter must be taken at the point $n + 1/2$ and one obtains

$$\frac{mc^2}{2}\int \left(\frac{\partial u}{\partial n}\right)^2_{n+1/2} \cos 2\pi n\, dn = -\frac{mc^2}{2}\int \left(\frac{\partial u}{\partial n}\right)^2_n \cos 2\pi n\, dn = -\int W(u) \cos 2\pi n\, dn,$$

where the second equality follows from (9). As a result, in the continuum approximation $\frac{1}{2} U_1 = I_1 + I_2 = 0$ (in contrast to the value $2I_1$ obtained in /4/).

For the ϕ^4 model I_1 and I_2 are exactly integrable in elementary functions. Using (15) and (18) yields /7/

$$I_1 = \frac{mc^2}{2\ell^2} u_0^2 \int_{-\infty}^{\infty} \frac{\cos 2\pi n}{\mathrm{ch}^4 n/\ell}\, dn = \frac{2\pi^4}{3}\frac{mc^2 \ell u_0^2}{\mathrm{sh}\, \pi^2 \ell}\left(1 + \frac{1}{\pi^2\ell^2}\right), \quad \ell \equiv \ell_0$$

Substituting (19) into I_2 one obtains after some transformations

$$I_2 = \frac{mc^2}{2} u_0^2 \mathrm{sh}\frac{1}{\ell}\int_{-\infty}^{\infty} \frac{\cos 2\pi n\, dn}{\left(\mathrm{ch}^2 \frac{n+1/2}{\ell} + \beta_0^2\right)^2} = \frac{mc^2}{2} u_0^2 \mathrm{sh}\frac{1}{\ell} \cdot \ell \left(\frac{\partial I_3}{\partial \beta^2}\right)_{\beta=\beta_0}, \quad \text{(A1)}$$

where $\beta_0 \equiv \mathrm{sh}\frac{1}{2\ell}$, and /7/

$$I_3 = \int_{-\infty}^{\infty} \frac{\cos 2\pi \ell x}{\mathrm{ch}^2 x + \beta^2}\, dx = 2\pi \frac{\sin(\pi\ell\, \mathrm{arch}(2\beta^2+1))}{\sqrt{(2\beta^2+1)^2}\ \mathrm{sh}\,\pi^2\ell}.$$

Substituting the derivative into (A1) and taking into account that $2\beta_0^2 + 1 = \mathrm{ch}\frac{1}{\ell}$ one obtains

$$I_2 = -2\pi^2 mc^2 \frac{u^2 \ell}{\mathrm{sh}\,\pi^2\ell}.$$

Finally

$$U_1 = 2(I_1 + I_2) \approx 8\pi^2\left(\frac{\pi^2}{3} - 1 + \frac{1}{3\ell^2}\right)\ell^2 u_0^2 mc^2 e^{-\pi^2\ell}$$

which coincides (after neglecting $1/3\ell^2 \ll 1$) with (21) and (22).

For the sine-Gordon equation the potential $W(u)$ and the soliton solution are given by (3) and (4), respectively. Hence /7/

$$I_1 = 2A\int \frac{\cos 2\pi n}{\mathrm{ch}^2 n/L}\, dn = \frac{mc^2}{L\, \mathrm{sh}\,\pi^2 L}, \quad I_2 = \frac{2mc^2}{\pi^2} L \int \mathrm{arctg}^2\left(\frac{\beta_0}{\mathrm{ch}(x + \frac{1}{2})}\right)\cos 2\pi x\, dx.$$

The expansion $\mathrm{arctg}^2(t) = \sum_{k=1}^{\infty} C_k t^{2k}$, $C_k = \frac{(-1)^{k+1}}{k}\sum_{n=1}^{k}\frac{1}{2n-1}$ and termwise integration /7/ yield

$$I_2 = -2L\,\mathrm{sh}\frac{1}{2L} I_1 - \frac{mc^2}{\pi^2 \mathrm{sh}\,\pi^2 L}\sum_{k=2}^{\infty}\frac{C_k}{(2k-1)!}\left(2\pi L\cdot\mathrm{sh}\frac{1}{2L}\right)^{2k}\left[1+\frac{1}{(\pi L)^2}\right]\ldots\times$$

$$\times\left[1+\left(\frac{k-1}{\pi L}\right)^2\right].$$

Finally (at $2L \gg 1$),

$$U_1 \approx \frac{4\pi^2}{9} mc^2 e^{-\pi^2 L}.$$

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Пушкарев Д.И. E17-84-752

Квантовое поведение солитонов в решеточных структурах

Рассмотрено квантовое поведение нелинейных возбуждений /солитонов/ и их взаимодействие с учетом периодичности решетки. Квантовые эффекты приводят к делокализации солитона, и он превращается в квазичастицу, которая характеризуется своим волновым вектором и законом дисперсии. Рассмотрено сверхзвуковое движение солитона и излучение черенковских фононов. Полученные результаты могут найти применение при рассмотрении распространения солитонов в твердых телах и кинков в полиацетилене. Показано, в частности, что пиннинг на решетке /напр., в полиацетилене/ невозможен, в отличие от результатов других авторов.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Препринт Объединенного института ядерных исследований. Дубна 1984

Pushkarov D.I. E17-84-752

Quantum Behaviour of Solitons in Lattice Structures

Quantum behaviour of nonlinear excitations (solitons) and their interaction with phonons is treated taking into account the lattice periodicity. Due to quantum effects the soliton is delocalized and turns into a quasi-particle characterized by its quasi-wave vector and dispersion law. The supersonic solitons in crystals are considered, and Cherenkov phonon emission is discussed. The results obtained can be applied to crowdion propagation in solids as well as to kinks in polyacetylene and in other quasi-one-dimensional structures. It is shown, in particular, that no pinning to the lattice (e.g., in polyacetylene) can take place in contrast to results of some other authors.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

Preprint of the Joint Institute for Nuclear Research. Dubna 1984