Helium diffusion as sine-Gordon kink in disordered quartz structure

E. Kalashnikov1). I.Tolstikhin3), N. Belova1).

1)Moscow Region University, Radio str.,10a, Moscow,105005, Russia
2)Geological Institute KSR, RAS, Fersman str., 14, Apatity, Murmansk Region 1842, Russia

e-mail: ekevkalashnikov1@gmail.com

Abstract. Discrete model ( local chains approach) reveals the influence of heterogeneity of structure on the movement of a helium atom in the form of a soliton Frenkel-Kontorova. The transition to the field form of this equation - to the Klein-Fock-Gordon equation or, simply, to the sine-Gordon equation, allows us to calculate the diffusion coefficient of such a soliton, taking into account the collective nature of the movement of the atom and the accompanying reversible displacements of the atoms of the environment through the medium in the form of a soliton and taking into account the details of the structure of nanostructures.

1. Discret model

The traditional approach to diffusion is based on the theory of random walks – jumps of an atom from one position to another [1]. This does not take into account the equation of motion of the atom, which, moreover, is accompanied by the movement of the atoms of the environment. It is shown [2,3,4] that the transition of an atom from one position to another, firstly, is described by the equation of motion of the atom itself, and secondly, is accompanied by the movement of atoms of the environment. This leads to a new form of movement in the form of a kink (Frankel-Kontorova soliton) - a collective composed of the atom itself and the accompanying reversible displacements of the atoms of the environment. The behavior of such a soliton allows us to describe it the Lagrangian $\mathcal{L}$

$$\mathcal{L} = \sum_{n} \left[ \frac{m}{2} \left( \frac{d\vec{r}_n}{dt} \right)^2 - \frac{1}{2} \alpha \gamma (1 \pm \sum_k \sigma_k) (\vec{r}_n - \vec{r}_{n+1})^2 - A(1 - \cos(2\pi \Gamma_n/a_n)) \right]$$

(1)

which describes the movement of a helium atom in the form of a Frenkel-Kontorova soliton (F-K). Here $\vec{r}_n$ is the displacement vector at the $n$-th node, $m$ is the mass of the helium atom, $\alpha \gamma$ is the interaction constant of the helium atom with the nearest environment, $a_n$ is the minimum distance in the direction of the $\vec{n}$, vector indicating the position. $\sigma_k$ is the reduced "area" of the corresponding shape of the nanostructure. Subsequent progress in considering the movement of the atom as a soliton and finding the diffusion coefficient of such a collective is associated with the transition to the field description of this collective. In this case, instead of the Frenkel-Kontorova equation arises sine-Gordon equation

$$m \left( \frac{\partial^2 \Gamma(x)}{\partial t^2} \right) = \gamma \left( \frac{\partial^2 \Gamma(x)}{\partial x^2} \right) - \left( \frac{2\pi}{a} \right) A \sin \left( \frac{2\pi \Gamma(x)}{a} \right)$$

(2)
\[ \gamma = \alpha_p (1 - \sum_k \sigma_k) \]  

The advantage of using this equation is that it is (in contrast to the Frenkel-Kontorova equation) invariant with respect to the Lorentz transformations [5, 6] (in which the role of the limiting velocity of propagation of disturbances in the medium plays the speed of sound). The advantage of using this equation is that it is (in contrast to the Frenkel-Kontorova equation) invariant with respect to the Lorentz transformations [5, 6, 9] (in which the role of the limiting velocity of propagation of disturbances in the medium plays the speed of sound). To make the transition to the field description of the collective in the form of a soliton, it is necessary to consider the peculiarities of the movement (movement) of the atom in the crystal.

2. The trajectory of a foreign atom in a crystal

The result of the movement of a foreign atom in a solid is a complex, continuous, broken line in three-dimensional space, consisting of straight segments. This line – trajectory – consists of separate rectilinear "parts" of different length and oriented relative to each other randomly. So that the movement in one direction can be, exactly, continued in the opposite direction. And in this sense, both (or any) directions are equivalent. This means that the atom starts from each new position regardless of how it got into it. (approximation of the Markov process). In this case, the movement of the atom along this trajectory remains one-dimensional. Some "pieces" of such a trajectory can be extended (at least by an order of magnitude greater than the interatomic distance) and rectilinear. But this length of trajectories is not the result of the free movement of an atom in a solid body, which would indicate the absence of interaction with the environment, but quite the contrary - the result of a specific interaction with the environment, which promotes the movement of a foreign atom in a solid over long distances in a straight path. Parts of such a broken trajectory correspond to the movement of the atom in a regular structure (without defects). Other parts of the trajectory correspond to the movement of the atom in the structure with defects. The minimal parts of such trajectory correspond to the transition of a foreign atom between the nearest neighboring positions [4]. The transition of a foreign atom between the nearest neighbors, in this case, is described by the Frenkel-Kontorova equation. And the transition itself (the solution of this equation) between the nearest positions is described by kink the Frankel-Kontorova soliton-type, determined up to an arbitrary momentum transmitted to the atoms of the nearest environment and does not violate the kink [2]. Thus, through the crystal (ordered or disordered) moves not a foreign atom, and the collective, which is a foreign atom itself, accompanied by reversible displacements of the atoms of the environment. That is, a soliton formed by reversible displacements of the lattice atoms moves in the field of reversible displacements of the lattice atoms. Within the discrete model, the soliton moves as if it were in a tube. The "diameter" of such a virtual tube is equal to the minimum "diameter" of a foreign atom, which varies depending on its polarizability [2]. This, in particular, follows from the law of conservation of the projection of the angular momentum of a foreign atom on the "axis" of the virtual tube at its transition from one position to the next. In this case, the complex three-dimensional motion of a foreign atom through a crystal (ordered or disordered) can be represented as the displacement of the soliton along the axis of a very broken tube that is never interrupted. Such movement can now be considered as one-dimensional, the only coordinate of which is the x-coordinate on the continuous axis of the broken tube.

3. Field form of the equations of motion of an atom

So the Lagrangian (1) now is transformed into a Lagrangian describing the displacement density \( \Gamma(x) \) along x

\[ \mathcal{L}(x) = \left( \frac{m}{2a} \right) \left( \left( \frac{\partial \Gamma(x)}{\partial t} \right)^2 - c^2 \left( \frac{\partial \Gamma(x)}{\partial x} \right)^2 - A \left( 1 - \cos \left( \frac{2\pi \Gamma(x)}{a} \right) \right) \right) \]  

(4)

here \( c \) is speed of sound, \( c = \left( \gamma \cdot 2a/m \right)^{1/2} \) (4a)
An analogue of this Lagrangian is the Lagrangian for the real scalar field [10], which admits a solution in the form of a soliton for the one-dimensional case $x^y = \{t, x\}$:

$$L(x, t) = \left(\frac{1}{2}\right)\partial_\mu \Phi \partial^\mu \Phi - V(\Phi)$$

$$V(\Phi) = (1 - \cos \Phi)$$  \hspace{1cm} (5)

energy-momentum tensor for which

$$T^{\mu\nu} = \partial_\mu \Phi \partial^\nu \Phi - g^{\mu\nu}L$$  \hspace{1cm} (6)

So for our case, at $(\Phi \rightarrow \Gamma)$, the component $(0, 0)$ of the energy-momentum tensor is a Hamiltonian [10]:

$$T^{0,0} = H = \left(\frac{m}{2}\right) \left[\left(\partial^\Gamma / \partial t\right)^2 + c^2 \left(\partial^\Gamma / \partial x\right)^2\right] + V(\Gamma)$$  \hspace{1cm} (7)

Then the total energy

$$E = \int_{-\infty}^{+\infty} \left\{ \left(\frac{m}{2}\right) \left[\left(\partial^\Gamma / \partial t\right)^2 + c^2 \left(\partial^\Gamma / \partial x\right)^2\right] + V(\Gamma) \right\} dx/\alpha = E_0/\sqrt{1 - (v/c)^2}$$  \hspace{1cm} (8)

$$E_0 = \left(\frac{4\alpha}{\pi}\right)^{1/2} \left(\frac{\gamma A}{2}\right)^{1/2}$$  \hspace{1cm} (9)

here $A$–$G$ is the shear modulus [2].

As follows from the expression (9), the rest energy, $E_0$ is completely determined by the structure of the nanostructure and the nature of interaction with the environment (3). This value makes it possible to determine the displacement of the soliton $\Delta_q$ interacting with the field of vibrations of the crystal atoms from the considerations of invariance of the sine – Gordon equation with respect to the Lorentz transformations (in which the speed of light plays the role of sound velocity $(4a)$ in the medium) [5, 6, 7]:

$$\Delta_q = \left(\frac{E_{ph}}{E_0}\right) \Lambda_{ph}(q)$$  \hspace{1cm} (10)

where $E_{ph}$ and $\Lambda_{ph}(q)$ are the energy of the phonon wave packet and its shift in interaction with the soliton. In turn, this allows us to find the diffusion coefficient for the collective "Helium atom+ reversible displacements of the medium lattice" in the form of a soliton [5, 6, 7]

$$D = \lim_{t \rightarrow 0} \left(\frac{1}{2\pi}\right) \sum_2 (\Delta_q)^2 \left(\langle n_2^2 \rangle - \langle n_q \rangle \langle n_q \rangle \right)$$  \hspace{1cm} (11)

here

$$\langle n_2^2 \rangle - \langle n_q \rangle \langle n_q \rangle \sim \langle n_q \rangle (\langle n_q \rangle + 1)$$

At temperatures above Debye one [3] works high-temperature approximation [5, 6]

$$\langle n_q \rangle \sim kT / E_{ph}$$  \hspace{1cm} (12)

4. Calculation of the diffusion coefficient

The final form for $D$ from (11) taking into account (12) has the form [6]:

$$D = \left(\frac{3}{2\pi}\right) \cdot \left(\frac{kT}{E_0}\right)^2$$

The diffusion coefficient significantly depends of what the quantum state of the helium atom is, as this affects the polarizability of the atom and the features of the interaction with the environment.

So if the helium atom is in the ground state $(1^1S_0)$, its polarizability $\beta_2 = 0.0203$ nm$^3$ (i.e., the interaction with the environment almost does not change the helium atom and it can be considered as a ball), the rest energy (activation) $E_0(\beta_2) = 6.18$ ev [2]. The activation energy (9) is exactly the same as calculated in [2]. A diffusion coefficient

$$D(\beta_2)(T = 300K) \sim 10^{-19} cm^2/s$$

Acknowledgments

I. Tolstikhin thanks Grant 18-05-70004 for support of his work with this contribution.
References
[1] Mehrer H. Diffusion in Solids. (Springer, Berlin)
[2] Kalashnikov E.V., Tolstikhin I.N, Lehmann B.E, Pevzner B.Z. 2003 Journ. Phys. Chem. Solids. 64 2293.
[3] Kalashnikov E.V., Tolstikhin I.N, Pevzner B.Z. 2010 Journ. Phys. Solid State 52 1372
[4] Kalashnikov E.V., Tolstikhin I.N., Krylova N.A. 2017 Defect and Diffusion Forum 380 98
[5] Theodorakopoulos N. 1970 Z.Physik B33 385
[6] Theodorakopoulos N., Klein R. 1980 Phys. Stat. Sol. A61 107
[7] Hasenfratz W., Klein R. 1977 Physica 89A 191
[8] Wang D., Wu H., Schwartz D.K. 2017 Phys.Rev.Lett., 119 268001
[9] Boiko G.G., Berezjnoi G.V. 2003 Physics and Chemistry Glasses 29 65
[10] Berestetskii V.B., Lifshitz E.M., Pitaevskii L.P. Relativistic Quantum Theory. Part I (Pergamon Press)