SOLITON LATTICES IN CARBON NANOTUBES

M.B. Belonenko[(1)], E.V. Demushkina[(1)], Lebedev N.G.*
Volgograd State University, University Avenue, 100, Volgograg, 400062, Russia
[(1)] Volgograd State Architectural-Building University, Academic Street, 1, Volgograd, 400074, Russia
* *E-mail: nikolay.lebedev@volsu.ru*

Introduction

The recently researches have shown that carbon nanotubes have unique properties: by very high durability, conductivity (semi-conductor or metal) and number of other properties causing unlimited opportunities of their applications, for example in microelectronics [1]. Among all specialties of carbon nanotubes the non-linear properties (acoustical or electromagnetic descent) are special interesting last years. In particular, one should to notice that the non-linear properties of nanotubes connecting with inharmonious potential of the interaction between neighboring carbon atoms have been researched using a reduction to Korteweg-de Vries and other non-linear equations in works [2 - 4].

In present paper the attention focuses primarily on non-linear properties of nanotube [5] because of the strong electron interaction described by Hubbard Hamiltonian. Our choosing of Hubbard model of the electron states deals with that the model can describe electrical and magnetic properties and high temperature superconductivity effects also.

Results and discussion

In given it is supposed to concentrate attention on nonlinear properties of NT caused by strong electron interaction described by Hubbard's Hamiltonian.

We shall consider single walled carbon nanotube (SWNT) with low limit of radius (fig. 1). This implies that the transition to continual approach is imposable in SWNT perimeter. On the figure the Z axis is directed along nanotube axis and I axis – along SWNT perimeter. Graphite sheet consists of carbon hexagons oriented so that some C-C bonds are parallel to SWNT axis. On the other words we study so-called "zig-zag" or (n,0) SWNT, where n – a number of hexagons on the tube perimeter. In order to apply Fourier analysis it is assumed the (n, 0) tube is infinite in Z axis direction.

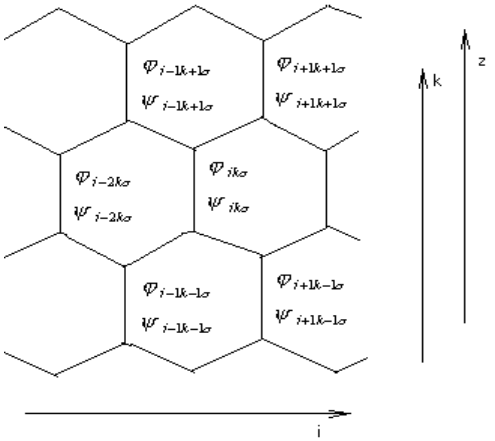

Fig. 1. Geometry of the system. Z axis is directed along nanotube axis.

According to above mentioned reason the Hubbard model [6] has been used to study the electron states of carbon nanotube. The model includes the terms of the energy of the electron jump from one to next carbon atom and the energy of Coulomb's repulsion of two electrons localized on same carbon atom. Hubbard Hamiltonian for the described system [6] is following:

$$H = -\sum_{j\Delta\sigma} t(a^{+}_{j+\Delta\sigma} a_{j\sigma} + a^{+}_{j\sigma} a_{j+\Delta\sigma}) + \\ + \mu \sum_{j\Delta} a^{+}_{j\sigma} a_{j\sigma} + U \sum_{j} a^{+}_{j\sigma} a_{j\sigma} a^{+}_{j+\sigma} a_{j-\sigma} \quad , (1)$$

where $a^{+}_{j\sigma}, a_{j\sigma}$ – an electron appearance and annihilation operators on j point (j = {i, k}) with σ spin, t – transfer integral, U – Coulomb electron energy; μ – chemical potential.

Further the Heisenberg's equations of the operator movements have been solved within the framework of following approximations. The lattice of NT has been consisted from two carbon sublattices. Wave functions of both sublattice electrons are considered as φ and ψ with character distance of changing along NT axis being much more than the interatomic distance. The phase portraits of Heisenberg's equations solutions have been constructed and the soliton behavior of electron wave functions (soliton lattices) has been shown.

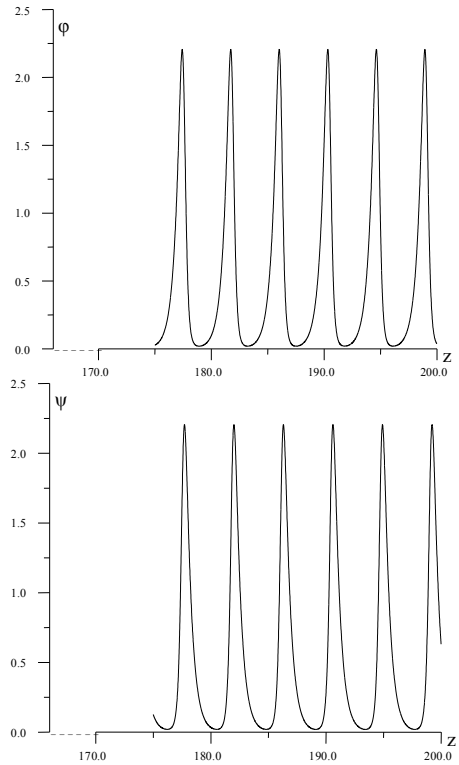

Fig. 2. The dependences of φ(z-vt), ψ(z-vt) function modules on the argument.

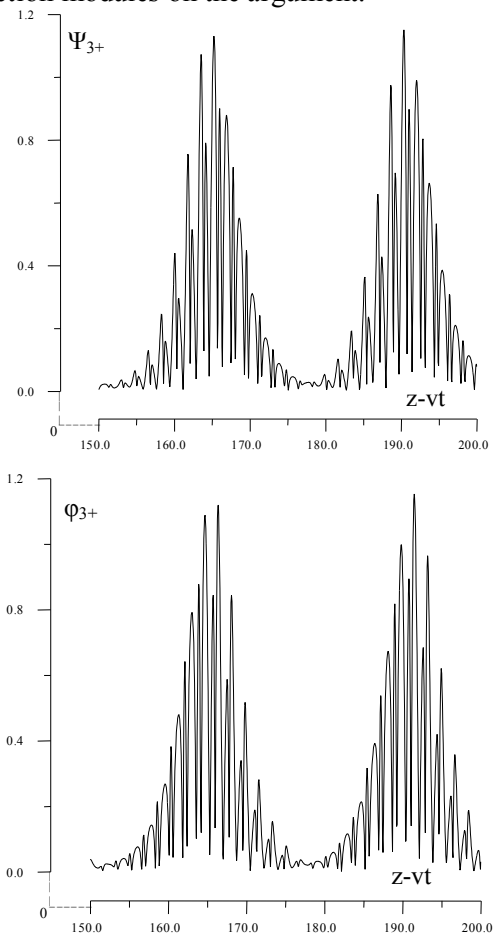

Fig. 3. The dependences of φ_{3+}(z-vt), ψ_{3+}(z-vt) function modules on the argument.

Conclusions

In conclusion we would like to resume the main results of soliton grids appearance in carbon nanotubes.

First, the similar lattices easily enough can be found out by diffraction methods. The research by similar methods will allow to define the parameters of lattices and to connect them with the appropriate sizes in microscopic Hamiltonian.

Secondly, the given lattices form the regular structure, which is actually domain. Here domains are the areas with various electron densities. The presence of domain structure will contribute in NT susceptibility and allows to hope for a detection of memory effects in an electronic subsystem of NT.

In third, the existence of regular periodic structure results at movement along such structure an additional electron in quantization of its energy (Flocke's theorem). The similar quantization results in presence of additional energy levels in carbon NT spectrum. Also similar quantization can result to suppression of electron-phonon interaction and to increasing of carbon NT conductivity.

Acknowledgements

The work has been partly supported by Russian Foundation for Basic Researches (project 04-03-96501).

References

1. P.J.F. Harris, Carbon nanotubes and relative structures. New materials of twenty-first century, Cambridge University Press, 1999, 336 p.
2. T.Yu. Astakhova, O.D. Gurin, M. Menon, G.A. Vinogradov, Phys. Rev. B 64 (2001) 035418.
3. T.Yu. Astakhova, G.A. Vinogradov, O.D. Gurin, M. Menon, Khimicheskaya Fizika. 23, (2004).
4. T.Yu. Astakhova, V.A. Dmitrieva, G.A. Vinogradov, Fullerenes, nanotubes and carbon nanostructures, 12(1,2) (2004) 133.
5. M.B. Belonenko, E.V. Demushkina, N.G. Lebedev, Abstracts of symposium and summer school "Nano and Giga challenges in microelectronics: research and development opportunities", Cracow, Poland, 2004, September 13-17, p. 152.
6. Solitons, Edited by R.K. Bullough, P.J. Caudrey, Mir, Moscow, 1983, 408 p.