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Original article

Mathematical model of weakly coupled spherical resonator chains under the influence of external magnetic field

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ABSTRACT The Schrödinger operators with constant magnetic field in a bent chain and Y-type chain of coupled balls are considered. Coupling exists due to point-like openings at the touching points of neighbor spheres. The mathematical background of the model is the theory of self-adjoint extensions of symmetric operators. The spectral equations for the model operators in each case were derived and analyzed.

KEYWORDS spectrum; operator extensions theory; balls chain; magnetic field

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1. Introduction

Last decades various nanostructures attract attention of researches. Single-walled nanotubes (SWNTs) were first seen in 1993 as cylinders rolled from a single graphene sheet. In 1998, the first peapod was observed by B. Smith, M. Monthioux and D. Luzzi [1]. Carbon peapod is a hybrid nanomaterial consisting of spheroidal fullerenes encapsulated within a carbon nanotube. It is named due to their resemblance to the seedpod of the pea plant. There are a number of works dealing with mathematical modelling of mechanical, optical and electronic properties of nano-peapods [2–5]. Since the properties of carbon peapods differ from those of nanotubes and fullerenes, the carbon peapod can be recognized as a new type of a self-assembled graphitic structure [6]. Possible applications of nano-peapods include nanoscale lasers, single electron transistors, spin-qubit arrays for quantum computing, nanopipettes, and data storage devices thanks to the memory effects and superconductivity of nano-peapods [7–10]. Spectral problems for a chain of coupled resonator attract a special interest due to its usefulness for micro and nanoelectronics, radio physics, acoustics [3, 11, 12].

In the present paper, we suggest a solvable model of a chain of weakly coupled spheres. A presence of a magnetic field is assumed. The mathematical background of the model is given by the theory of self-adjoint extensions of symmetric operators. This approach appeared initially as a mathematical justification of zero-range potential method in atomic physics [13]. Later, it became a well-developed method of construction of solvable models for systems with singular interactions [14–16]. We consider two systems shown in Fig. 1, bent chain and Y-type chain of coupled spheres. Coupling exists due to point-like openings at the touching points of neighbor spheres. The spectral equations for the model operators in each case was derived and analyzed.

2. Model construction

At all junction points of the resonators, the presence of the so-called condition δ- connection, and it is assumed that its intensity $\alpha \in \mathbb{R}$ is the same for all junction points of the resonators. At the boundary of the resonators, which is not involved in their connection, it is placed Neumann boundary condition. It is also believed that all balls making up the chain have same radius. We consider the magnetic field to be uniform and directed along an axis perpendicular to the plane containing all the junction points of the circuit resonators.

To study the stationary states of a non-relativistic spinless particle placed in the described chain structure, it is necessary to consider the stationary Schrödinger equation:

$$H^B \psi(\mathbf{x}) = E\psi(\mathbf{x}), \qquad (1)$$

where H^B is the Hamiltonian of the system under the influence of an external magnetic field $\mathbf{B}$, $\psi(\mathbf{x})$ is the wave function of the three-dimensional spatial coordinate $\mathbf{x}$, and E is the energy of the system. The main goal of the work is to describe the spectrum of the Hamiltonian of the system $\sigma(H^B)$ depending on its physical and geometric parameters.

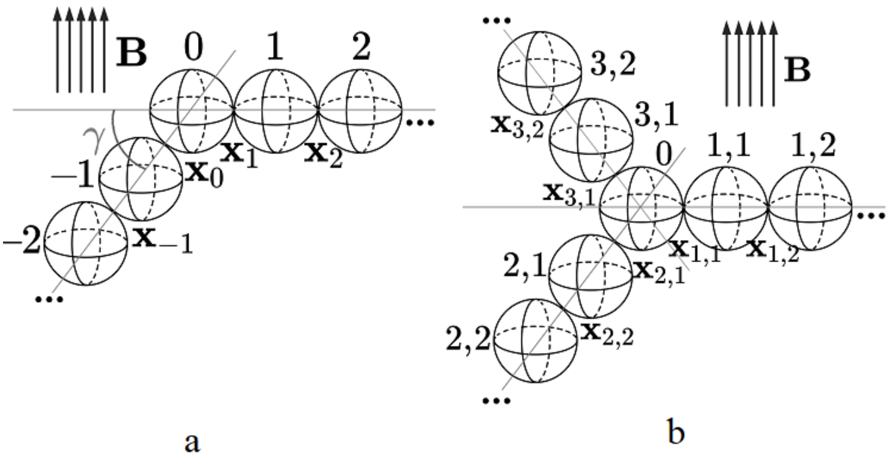

FIG. 1. Geometrical configuration of the system: a - bent chain, b- Y-type chain.

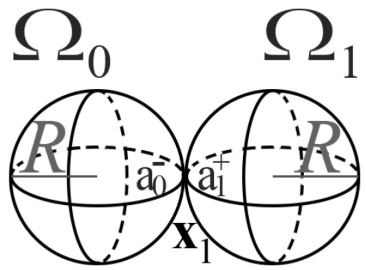

FIG. 2. Two coupled balls.

A mathematical model of interacting resonators is constructed within the framework of the theory of self-adjoint extensions of symmetric operators [17]. The scheme for constructing a model of interacting resonators under the influence of an external magnetic field is similar to that in [3].

The operator H_j^B defined for the j-th resonator in the chain ($j \in \mathbb{Z}$) takes the form:

$$H_j^B = \frac{1}{2m}\left(-i\hbar\nabla - \frac{e(\mathbf{B}\times\mathbf{r})}{2}\right)^2, \tag{2}$$

where i is the imaginary unit, $\hbar$ is the reduced Planck constant, e is the particle charge, $\mathbf{B} = B\mathbf{k}$ is the magnetic field induction vector, $\mathbf{r}$ is the radius vector: $\mathbf{r} = \{x, y, z\}$, and m is the particle mass. We choose the symmetric gauge for the magnetic field.

To understand the scheme for constructing a model of a chain of interacting resonators at exposure to an external magnetic field, consider the simplest chain - two coupled resonators Ω_0 and Ω_1, having one common point x_1 (Fig. 2).

Starting with the orthogonal sum of the self-adjoint Hamiltonians for each ball, we restrict it to the set of functions vanishing at the common point of two balls and come to the symmetric operator. Its self-adjoint extension gives us a model of coupled resonators. To construct it, one can restrict the domain of the adjoint operator [13]. The corresponding limitation is that the following boundary form annihilates for elements from the domain of the adjoint operator:

$$\left((H^B)^* u, v\right) - \left(u, (H^B)^* v\right) = \int\limits_{\Omega_0\cup\Omega_1} \left((H^B)^* u\overline{v} - u\overline{(H^B)^* v}\right) d(\Omega_0\cup\Omega_1), \tag{3}$$

where the bar denotes complex conjugation, and $d(\Omega_0 \cup \Omega_1)$ is the volume element $\Omega_0 \cup \Omega_1$. The function $u \in \mathrm{dom}\left((H^B)^*\right)$ can be represented in the following form [3]:

$$u = \begin{pmatrix} u_0^0 + a_{0(u)}^- G_0^B(\mathbf{x}, \mathbf{x}_1, \lambda_0) + b_{0(u)}^- \\ u_1^0 + a_{1(u)}^+ G_1^B(\mathbf{x}, \mathbf{x}_1, \lambda_0) + b_{1(u)}^+ \end{pmatrix}, \tag{4}$$

where $G_j^B(\mathbf{x}, \mathbf{x}_1, \lambda_0)$ are Green's functions for the problem $(j = 0, 1)$, are the deficiency elements of the symmetric operator $\overset{\circ}{H}{}^B$.

By direct calculation, one obtains the boundary form and, correspondingly, the condition of its annihilation:

$$((H^B)^*u,v)-(u,(H^B)^*)=\overline{a^-_{0(v)}}b^-_{0(u)}-a^-_{0(u)}\overline{b^-_{0(v)}}+\overline{a^+_{1(v)}}b^+_{1(u)}-a^+_{1(u)}\overline{b^+_{1(v)}}=0. \quad (5)$$

Expression (5) is similar to that for the boundary form in the absence of external fields [17].

3. Results

Based on all of the above, the following theorem is valid:

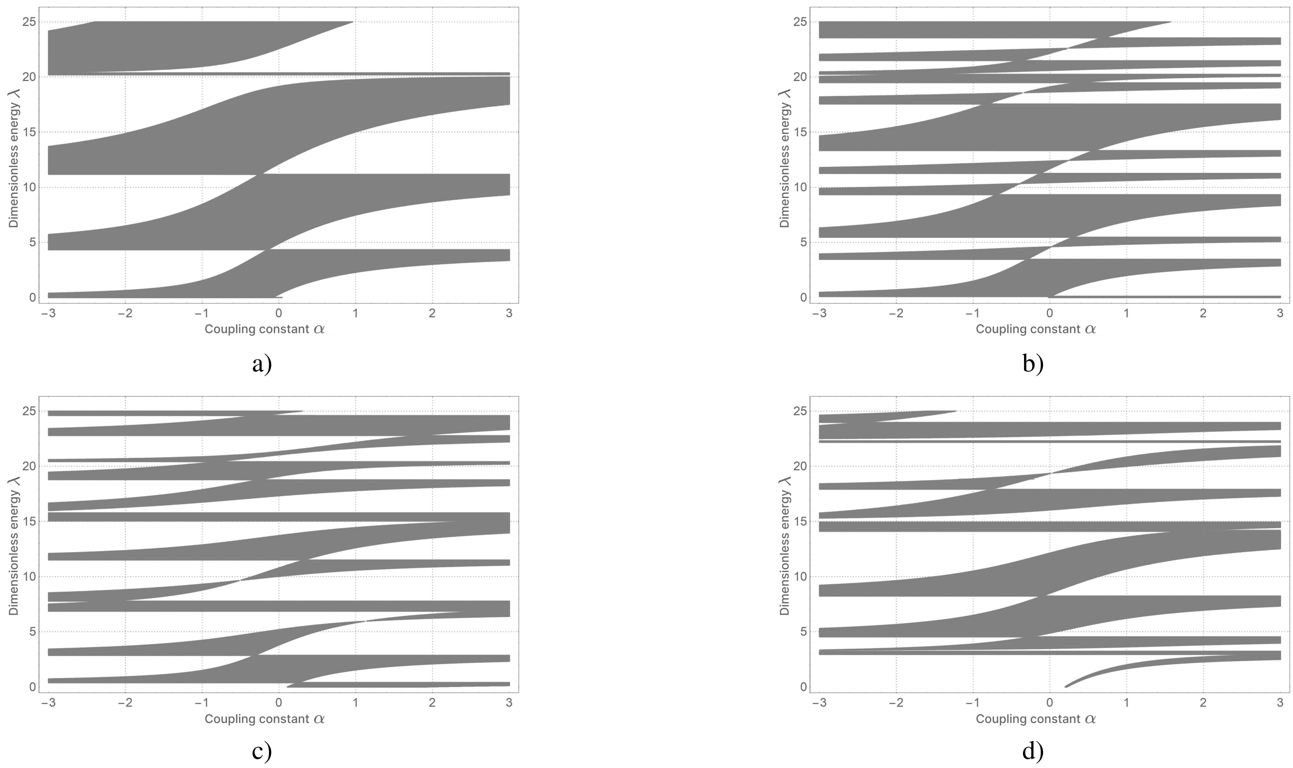

FIG. 3. Structure of the continuous spectrum of a chain with a break (or branching) depending on the connection parameter α at a fixed magnetic field: a) $B = 0$, b) $B = 0.5$, c) $B = 1$, d) $B = 3$

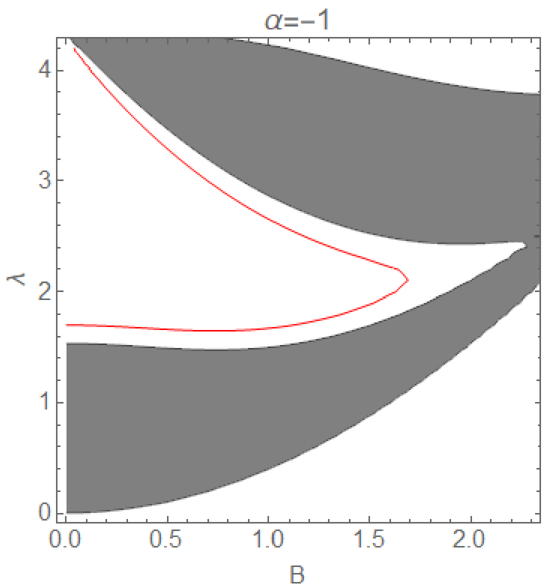

FIG. 4. Structure of the spectrum of the basic Y-branch of the chain depending on B at $\alpha = -1$ (gray areas — continuous spectrum zones; solid line — energy values belonging to the discrete spectrum)

Theorem 1. Let the chain break angle γ be such that $\gamma \in [0, \frac{2\pi}{3})$. Then the essential spectrum of the model Hamiltonian of a chain with a kink and with the condition of δ-connection at the junction points of the resonators, subject to the influence of the magnetic field $\mathbf{B}$, consists of eigenvalues of infinite multiplicity — the eigenvalues of the Neumann Laplacian in the ball, corresponding to the eigenfunctions equal to 0 at both junction points of the resonators ($\mathbf{x}_{j-1}$ and $\mathbf{x}_j$), and continuous spectrum. The continuous spectrum of the model Hamiltonian has a band structure completely described by inequality (6)

$$|\mu_B^{\pm}| = 1 \quad \Leftrightarrow \quad \left|\frac{X_B}{2G^B}\right| \leqslant 1. \tag{6}$$

At $\gamma = 0$, the discrete spectrum of the model Hamiltonian is empty.

Let now the chain break angle γ be such that $\gamma \in (0, \frac{2\pi}{3})$. The discrete spectrum of the model Hamiltonian consists of all λ that resolve equation (11) and satisfy conditions (7)-(8):

$$|\mu_B^{+}| < 1 \quad \Leftrightarrow \quad \frac{X_B}{2G^B} < -1, \tag{7}$$

$$|\mu_B^{-}| < 1 \quad \Leftrightarrow \quad \frac{X_B}{2G^B} > 1, \tag{8}$$

where $X_B = \lim\limits_{\mathbf{x}\to\mathbf{x}_j} \left(G^B(\mathbf{x}, \mathbf{x}_1, \lambda) - G^B(\mathbf{x}, \mathbf{x}_1, \lambda_0)\right)$. We also present here the eigenvalues μ_B of this transfer matrix and the corresponding eigenvectors ν_B (for $j \neq 1$):

$$\mu_B = \frac{X_B}{2G^B} \pm \sqrt{\left(\frac{X_B}{2G^B}\right)^2 - 1}, \tag{9}$$

$$\nu_B = \varrho \begin{pmatrix} 1 \\ -\mu_B \end{pmatrix}, \tag{10}$$

where $G^B = G^B(\mathbf{x}_{j-1}, \mathbf{x}_j, \lambda) = G^B(\mathbf{x}_j, \mathbf{x}_{j-1}, \lambda)$ ($j \neq 1$), ϱ is some constant ($\varrho \neq 0$).

$$\frac{|Z_\gamma^B|^2 - (G^B)^2}{G^B Z_\gamma^B} = 0. \tag{11}$$

For Y-type chain of balls, the structure of the spectrum is described by the following theorem [7]:

Theorem 2. The essential spectrum of the model Hamiltonian of a Y-branched chain with the condition of δ-connection at the junction points of the resonators, subject to the influence of the magnetic field $\mathbf{B}$, consists of eigenvalues of infinite multiplicity - the eigenvalues of the Neumann Laplacian in the ball, corresponding to the eigenfunctions equal to 0 at both junction points of the resonators ($\mathbf{x}_{j-1}$ and $\mathbf{x}_j$), and continuous spectrum. The continuous spectrum of the model Hamiltonian has a band structure completely described by inequality (6). The discrete spectrum of the model Hamiltonian consists of all λ that resolve equation (12) and satisfy conditions (7) – (8)

$$\frac{1}{(G^B)^3}\Big((X_B - \mu_B G^B)^3 - (X_B - \mu_B G^B)\left(|G_{[2],3}|^2 + |G_{[1],2}|^2 + |G_{[1],3}|^2\right) + \\ + G_{[1],2}G_{1,[3]}G_{[2],3} + \overline{G_{[1],2}G_{1,[3]}G_{[2],3}}\Big) = 0. \tag{12}$$

The picture of the dependence of the continuous spectrum on the magnitude of the magnetic field in the case of a Y-branched chain has the same form as in the case of a chain with a break It is shown in Fig. 4 (the gap between the first and second zones of the continuous spectrum contains energy values belonging to the discrete spectrum).

4. Conclusion

Explicitly solvable model was constructed for electron in a system of bent chain and Y-type chain of weakly coupled balls in a magnetic field. The model is based on the theory of self-adjoint extensions of symmetric operators in the Hilbert space. The spectral problems are of special interest for systems of such type (see, e.g., [18–22]). Spectral equations were derived. The continuous and the point spectra of the model operator were described.

References

[1] Smith, Brian W., Monthioux, Marc, Luzzi, David E. Carbon nanotube encapsulated fullerenes: A unique class of hybrid materials. Chemical Physics Letters. 1999, **315**(1-2), P. 31–36.

[2] Lee J.Y., Lee Ch., Osawa E., et.al. Snapshots of the Fragmentation for C70@Single-Walled Carbon Nanotube: Tight-Binding Molecular Dynamics Simulations. *International Journal of Molecular Science*, 2021, **22**(8), p. 3929.

[3] Melikhova A.S., Popov I.Y. Spectral problem for solvable model of bent nanopeapod. Applicable Analysis. 2017, **96**(2), P. 215–224.

[4] Li Y., Kaneko T. and Hatakeyama R. Photoresponse of fullerene and azafullerene peapod field effect transistors, 2009 9th IEEE Conference on Nanotechnology (IEEE-NANO), Genoa, Italy, 2009, P. 86–89.

[5] Matsuno T., Terasaki S., Kogashi K. et al. A hybrid molecular peapod of sp2- and sp3-nanocarbons enabling ultrafast terahertz rotations. Nat Commun 12, 5062 (2021).

[6] Iijima, Sumio. Carbon nanotubes: Past, present, and future. Physica B: Condensed Matter, 2002, **323**(1-4), P. 1–5.

[7] Utko P., Nygerd J., Monthioux M., Noe L. Sub-Kelvin transport spectroscopy of fullerene peapod quantum dots. *Applied Physics Letters*, 2006, **89**(23), P. 233118.

[8] Pichler T., Kuzmany H., Kataura H., Achiba Y. Metallic Polymers of C60 Inside Single-Walled Carbon Nanotubes. *Physical Review Letters*, 2001, **87**(26), P. 267401.

[9] Enyashin A.N., Ivanovskii A.L. Nanotubular composites: modeling of capillary filling of nanotubes of disulfide of molybdenum by molecules of TiCl4. *Nanosystems: Phys. Chem. Math.*, 2010. **1**(1) P. 63–71.

[10] Tao X., Zhang Zh., et.al. Peapod-Like Structured B/N Co-Doped Carbon Nanotube Array Encapsulating MxPy (M = Fe, Co, and Ni) Nanoparticles for High-Rate Potassium Storage. *ACS Appl Mater Interfaces*, 2024, **16**(1), P. 772–783.

[11] Pazynin V. Multiplet properties in the spectrum of oscillations of coupled waveguide resonators chain. *Radiofizika i Elektronika*, 2017, **22**(1), P. 3–14.

[12] Gao Z., Gao F., Shastri K. et al. Frequency-selective propagation of localized spoof surface plasmons in a graded plasmonic resonator chain. *Sci. Rep.*, 2016, **6**, P. 25576.

[13] Berezin F.A., Faddeev L.D. Remark on the Schrödinger equation with singular potential. *Dokl. Akad. Nauk SSSR.*, 1961, **137**(5), P. 1011–1014.

[14] Pavlov B.S. *Extensions theory and explicitly solvable models*. *Russian Math. Surveys*, 1987, **42**(6), P. 127–168.

[15] Popov I.Y. The resonator with narrow slit and the model based on the operator extensions theory. *J. Math. Phys.*, 1992, **33**(11), P. 3794–3801.

[16] Albeverio S., Kuracov P. *Singular Perturbations of Differential Operators: Solvable Schrödinger-type Operators (London Mathematical Society Lecture Note Series, Series Number 271)*, Cambridge, Cambridge University Press, 2000, 444 p.

[17] Popov I.Yu. The extension theory and localization of resonances for the domain of trap type, *Matematicheskii sbornik*, 1990, **181**(10), P. 1366–1390. English: *Mathematics of the USSR-Sbornik*, 1992, **71**(1), P. 209–234.

[18] Duclos P., Exner P., Turek O. On the spectrum of a bent chain graph. *J. Phys. A: Math. Theor.*, 2008, **41**, P. 415206.

[19] Popov I.Yu., Smirnov P.I. Spectral problem for branching chain quantum graph. *Phys. Lett. A*, 2013, **377**(6), P. 439–442.

[20] Popov I.Y., Skorynina A.N., Blinova I.V. On the existence of point spectrum for branching strips quantum graph. *J. Math. Phys.*, 2014, **55**, P. 033504/1-20.

[21] Blinova I.V., Popov A.I., Bosova A.A. Spectral gaps for star-like quantum graph and for two coupled rings. *Nanosystems: Phys. Chem. Math.*, 2022, **13**(3), P. 245–249.

[22] Borisov D.I., Pankrashkin K.V. Gap opening and split band edges in waveguides coupled by a periodic system of small windows. *Math. Notes*, 2013, **93**(5-6), P. 660–675.

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