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Electron energy spectrum for a bent chain of nanospheres

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Abstract. An infinite bent chain of nanospheres connected by wires is considered. We assume that there are δ-like potentials at the contact points. A solvable mathematical model based on the theory of self-adjoint extensions of symmetric operators is constructed. The spectral equation for the model operator is derived in an explicit form. It is shown that the Hamiltonian has non-empty point spectrum. The positions of the eigenvalues for different values of the system parameters (the length of the connecting wires, the intensities of δ-interactions and the bent angle) are found.

1 Introduction

The spectral properties of Hamiltonians for nanosystems play an important role in the prediction of transport properties (see, e.g., [1–4]). It is impossible to create a new nanodevice without the spectral analysis of the corresponding Hamiltonian, however, direct computations of the Hamiltonians are rather difficult. Usually, physicists use simplifying models, such as the widely used and very attractive quantum graph models. In the framework of such models, the problem is reduced to a quasi-one-dimensional problem. In spite of its simplicity, the model retains the features of the corresponding realistic system. In many cases, the model of a nanodevice consists of a few leads attached to some compact finite graph, which can be considered as a local perturbation of the corresponding infinite graph (including the leads). The spectral problem for a locally perturbed infinite quantum graph was considered in [5], where the authors presented the specific spectral behavior of the operator. Chain type structures are intensively investigated last time. The chain elements may be quantum rings, quantum dots, quantum graphs, etc. For these systems, the quantum graph model is transformed to the so-called decorated quantum graph model. If the chain is periodic, then the spectrum has the band structure. As for the discrete spectrum, one observes the most interesting situation when there is a local perturbation of such graph. In this case the point spectrum can appear, which is an interesting physical phenomenon. This is why it is important to be able to identify the condition for its realisation. Duclos et al. [6] considered the quantum graph of bent chain of rings. In this work they posed the question: "What is a condition for the discrete spectrum to appear?" It is interesting that the considered bent chain has a point spectrum only in the case when there are δ-like perturbations at the contact points of the neighbor rings. To construct the eigenfunctions, they used the transfer matrix approach. This method was applicable given that the model system was quasi-one-dimensional. More complicated cases of branching chains of rings and branching strips graphs are considered in [7,8].

Due to the physical significance of the problem of bound states caused by a local perturbation, it is interesting to investigate other types of bent chain systems. In this work we study the bent chain of spheres connected by wires (see Fig. 1). It can be used as a model of one newly created nanostructure, the so-called nano peapod. It is a nanotube filled by a chain of fullerene molecules. There is a number of experimental works describing the properties of such systems and the processes for their creation [9–14], and it would therefore be useful to construct an effective mathematical model for the system. This is the goal of the present paper.

Let us begin with a description of the mathematical background of the model. To avoid unnecessary difficulties, we will use dimensionless values. From a physical point of view, this means that we choose the system of units in which $e = \hbar = c = 2m = 1$, where e, m are the charge and the mass of the particle, correspondingly, c is the speed of light, $\hbar$ is Planck's constant. The state space for the model is $\bigoplus_{n=-\infty}^{+\infty}(L^2(S_j) \oplus L^2(0,\ell))$. Here S_j is the jth sphere of the chain. Let $H_n^S = -\Delta_{LB}$ denote the Laplace-Beltrami operator on the sphere S_n, $H_n^w = -\dfrac{d^2}{dx^2}$ denotes the Hamiltonian for the wire with number n. The operator of the system has the following form:

$$H = \bigoplus_{n=-\infty}^{+\infty} \left(H_n^S \oplus H_n^w\right).$$

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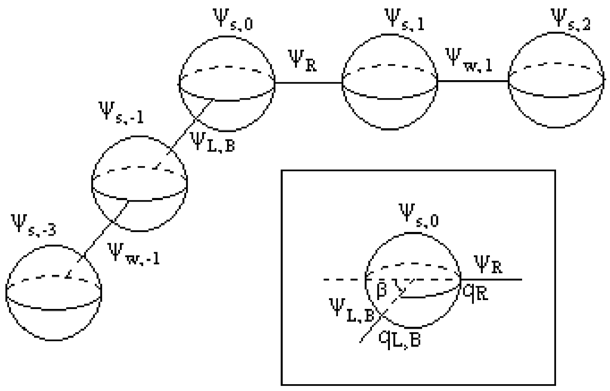

Fig. 1. Geometry of the system. The inset shows the central cell.

The domain of this operator is $\bigoplus_{n=-\infty}^{+\infty}(W_2^2(S_n) \oplus W_2^2(0,\ell))$. Here W_2^2 is the Sobolev space. In addition, we assume that there are the δ-potentials at the contacts points.

To give rigorous mathematical description of our system we use the operator extension theory. In particular, the δ-potential at segment $[0,\ell]$ is introduced in the following way. Let $\xi \in [0,\ell]$. Consider the restriction of the operator $-\dfrac{d^2}{dx^2}$ in the set of smooth functions, which are equal to zero at the point ξ simultaneously with their derivative. The obtained operator is a symmetric operator. Its self-adjoint extensions give us a one-parameter family of operators H^α, where the parameter α characterises the power of the δ-perturbation in the chosen point ξ. Actually, the existence of a δ-like potential at the point ξ means that functions from the domain of H^α satisfy the following conditions at the point ξ:

$$\begin{cases} \psi(\xi+0) = \psi(\xi-0), \\ \psi'(\xi+0) - \psi'(\xi-0) = \alpha\psi(\xi). \end{cases} \tag{1}$$

In addition we give a brief description of the "gluing" process for a sphere and a wire. Denote by ψ_s and ψ_w the wave functions at the sphere and the wire, respectively. We restrict the operator $H^S \oplus H^w$ onto the set of elements, for which ψ_S, ψ_w, ψ_w' vanish at the connection points. Then, we construct self-adjoint extensions of this symmetric operator. The extensions are parameterised by a few numbers related to the contact characteristics. In fact, to realise this procedure, it is necessary to consider functions with logarithmic singularities at the connecting points to the sphere and establish the correlation between the coefficients. Namely, we consider functions of the following form:

$$\psi_S(x) = -u(\psi_S)\frac{1}{2\pi}\ln\rho(x,q) + v(\psi_S) + R(x),$$

where $\rho(x,q)$ means the geodesic distance between point x and the contact point q on the sphere, $R(x)$ is the remainder term, which tends to zero if $x \to q$, parameters u, v $(u, v \in \mathbb{C})$ are coefficients which play the role of boundary values for ψ_S at the point q.

It is obvious, that the boundary conditions for the wave function at the contact points are linear relations between $\psi_w(q), \psi_w'(q)$ and $u(\psi), v(\psi)$. Following [15,16], we choose these relations in the form

$$\begin{cases} v(\psi_S) = Nu(\psi_S) - M\psi_w'(q), \\ \psi_w(q) = M^*u(\psi_S) - P\psi_w'(q). \end{cases}$$

The coefficients M, N, P are related to the physical properties of the connection at points q_j. We will assume that $M = 1$, and $N = P = 0$. This is analogous to the well-known Kirchhoff conditions [17,18].

2 Transfer matrix

To find the point spectrum for the system we use the transfer matrix (monodromy matrix) approach (see, e.g., [6,7,19,20]). It is necessary to construct the matrix for each cell of the chain. The cell consists of a sequence of elements. The transfer matrix for the whole cell is the product of the transfer matrices for all elements. Let us construct the transfer matrix for one cell of our chain step-by-step.

First, we have δ-potentials at the ends of our segments. The transfer matrix corresponding to a 1D δ-potential is known (see Eq. (1)):

$$\begin{pmatrix} \psi_{n-1}(\ell+0) \\ \psi_{n-1}'(\ell+0) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ \alpha & 1 \end{pmatrix} \begin{pmatrix} \psi_{n-1}(\ell-0) \\ \psi_{n-1}'(\ell-0) \end{pmatrix}.$$

Our goal is to find the eigenvector for the Hamiltonian. Note, that the eigenfunction corresponding to the eigenvalue $E = k^2$ should have the following form.
For the segment:

$$\psi_{w,n}(x) = D_{n,1}\sin kx + D_{n,2}\cos kx.$$

For the sphere:

$$\psi_{S,n}(\varphi,\theta) = C_n^L G\left(\varphi,\theta;\pi,\frac{\pi}{2};E\right) + C_n^R G\left(\varphi,\theta;0,\frac{\pi}{2};E\right),$$

where φ, θ are the spherical coordinates, and G is the Green function for the sphere [21]

$$G(x,y;E) = \frac{1}{4\cos\left(\pi\sqrt{\frac{1}{4}+E}\right)} \times \mathcal{P}_{-\frac{1}{2}+\sqrt{\frac{1}{4}+E}}(-\cos\rho(x,y)),$$

where $\mathcal{P}_\nu(x)$ is the Legendre function, and $\rho(x,y)$ is the geodesic distance on the sphere.

As in [15], we have for the left contact point

$$\begin{aligned} u^L &= \psi_{n-1}(\ell-0) = C^L, \\ v^L &= \alpha\psi_{n-1}(\ell-0) + \psi_{n-1}'(\ell-0) \\ &= Q_{LL}C^L + Q_{LR}C^R, \end{aligned}$$

that is:

$$C^L = \psi_{n-1}(\ell - 0),$$
$$C^R = \frac{1}{Q_{LR}}(\alpha\psi_{n-1}(\ell-0) + \psi'_{n-1}(\ell-0) - Q_{LL}\psi_{n-1}(\ell-0)).$$

Here we use the inputs of the Krein Q-matrix

$$Q = \begin{pmatrix} Q_{LL} & Q_{LR} \\ Q_{RL} & Q_{RR} \end{pmatrix}, \tag{2}$$

where

$$Q_{LL}(E) = \lim_{x\to q_L}\left(G(x,q_L;E) + \frac{1}{2\pi}\ln\rho(x,q_L)\right),$$
$$Q_{RR}(E) = \lim_{x\to q_R}\left(G(x,q_R;E) + \frac{1}{2\pi}\ln\rho(x,q_R)\right),$$
$$Q_{RL}(E) = Q_{LR}(E) = G(q_L,q_R;E), \tag{3}$$

and q_L, q_R are the corresponding contact points.

For our model we have $\rho(q_l,q_R) = 1$ in accordance with the contacts locations. Therefore $\mathcal{P}_\nu(1) \equiv 1$. We obtain the following expression for the non-diagonal elements of Q-matrix:

$$Q_{LR} = Q_{RL} = \frac{1}{4\cos(\pi t(E))}\mathcal{P}_{t(E)-1/2}(-\cos(\rho(q_l,q_R))) = \frac{1}{4\cos(\pi t(E))}, \tag{4}$$

where $t(E) = \sqrt{E+1/4}$.

For the diagonals elements we have [15,22]:

$$Q_{LL} = Q_{RR} = -\frac{1}{2\pi}\left[\psi(1/2+t(E)) - \frac{\pi}{2}\tan(\pi t(E)) - \ln 2 + C_E\right], \tag{5}$$

where $\psi(x)$ is the logarithmic derivative of the Gamma-function, and C_E is the Euler's constant.

Similarly, we obtain the analogous result for the right contact point

$$\psi_n(-0) = u^R = C^R = \frac{1}{Q_{LR}}(\alpha\psi_{n-1}(\ell-0) + \psi'_{n-1}(\ell-0) - Q_{LL}\psi_{n-1}(\ell-0)),$$
$$\psi'_n(-0) = -v^R = -Q_{RR}C^R - Q_{RL}C^L = -\frac{Q_{RR}}{Q_{LR}}(\alpha\psi_{n-1}(\ell-0) + \psi'_{n-1}(\ell-0) - Q_{LL}\psi_{n-1}(\ell-0)) - Q_{RL}\psi_{n-1}(\ell-0).$$

Transition through the δ-potential gives us the following expressions for the value of the wave function and its derivative:

$$\psi_n(+0) = \frac{1}{Q_{LR}}(\alpha\psi_{n-1}(\ell-0) + \psi'_{n-1}(\ell-0) - Q_{LL}\psi_{n-1}(\ell-0)),$$
$$\psi'_n(+0) = \frac{\alpha}{Q_{LR}}(\alpha\psi_{n-1}(\ell-0) + \psi'_{n-1}(\ell-0) - Q_{LL}\psi_{n-1}(\ell-0)) - \frac{Q_{RR}}{Q_{LR}}(\alpha\psi_{n-1}(\ell-0) + \psi'_{n-1}(\ell-0) - Q_{LL}\psi_{n-1}(\ell-0)) - Q_{RL}\psi_{n-1}(\ell-0).$$

We express the values at the end point of the segment using the values at the beginning of the segment by solving the corresponding Cauchy problem for the equation $\psi''_n + k^2\psi = 0$ on the segment $[0,\ell]$. The result is as follows:

$$\psi_n(\ell-0) = \frac{\psi'_n(+0)}{k}\sin kl + \psi_n(+0)\cos kl,$$
$$\psi'_n(\ell-0) = \psi'_n(+0)\cos kl - k\psi_n(+0)\sin kl.$$

Therefore, we obtain the following relation

$$\begin{pmatrix} \psi_n(\ell-0) \\ \psi'_n(\ell-0) \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix}\begin{pmatrix} \psi_{n-1}(\ell-0) \\ \psi'_{n-1}(\ell-0) \end{pmatrix}, \tag{6}$$

where M_{ij}, $i,j = 1,2$, the inputs of the transfer matrix M, are as follows:

$$M_{11} = \frac{\alpha - Q_{LL}}{Q_{LR}}\cos k\ell + \frac{\sin k\ell}{k}\left(\frac{(\alpha-Q_{RR})(\alpha-Q_{LL})}{Q_{LR}} - Q_{RL}\right),$$
$$M_{12} = \frac{\cos k\ell}{Q_{LR}} + \frac{\alpha - Q_{RR}}{Q_{LR}}\frac{\sin k\ell}{k},$$
$$M_{21} = \left(\frac{(\alpha-Q_{RR})(\alpha-Q_{LL})}{Q_{LR}} - Q_{RL}\right)\times\cos k\ell - \frac{k\sin k\ell}{Q_{LR}}(\alpha - Q_{LL}),$$
$$M_{22} = \frac{\alpha - Q_{RR}}{Q_{LR}}\cos k\ell - \frac{k\sin k\ell}{Q_{LR}}. \tag{7}$$

3 Model of bent chain of spheres

Our system consists of three elements: a central cell (see the inset in Fig. 1) and two semi-infinite chains. The transfer matrix for the semi-infinite chain is the matrix M which was found in the previous section.

Note, that the point spectrum of the model operator includes the points $E = k^2$, corresponding to the eigenvalues $\lambda = \lambda(k)$ of the transfer matrix M, such that

$|\lambda| < 1$, and the continuous spectrum consists of the points $E = k^2$, for which the eigenvalues λ satisfy the condition: $|\lambda| = 1$ (see, e.g., [23,24]). As has been shown elsewhere (see, e.g., [25,26]), a local perturbation of a system does not change the continuous spectrum. Hence, in our case it is sufficient to consider the semi-infinite chains to determine the continuous spectrum.

The spectral equation for the transfer matrix (see (6) and (7)) has the form:

$$\lambda^2 - 2y\lambda + 1 = 0,\ y = \frac{1}{2}\left(M_{11} + M_{22}\right). \tag{8}$$

It is clear that if $|y| \le 1$ then $|\lambda_{1,2}(k)| = 1$ and the corresponding energy values $k^2 = E$ give us the band.

Furthermore, we introduce the notation

$$X = \frac{1}{2\pi}\left[\psi(1/2 + t(E)) - \ln 2 + C_E\right].$$

Then, one has

$$\begin{aligned} M_{11} + M_{22} = {} & 2(\alpha + X) \\ & \times \left(4\cos(kl)\cos(\pi t)) - \frac{1}{k}\sin(kl)\sin(\pi t)\right) \\ & - 4k\sin(kl)\cos(\pi t) \\ & + \frac{4}{k}\sin(kl)\cos(\pi t)\left((\alpha + X)^2) - \frac{1}{16}\right) \\ & - 2\cos(kl)\sin(\pi t). \end{aligned}$$

Thus, we obtain the condition for the continuous spectrum

$$\begin{aligned} \Big|(\alpha + X)\left(4\cos(kl)\cos(\pi t) - \frac{1}{k}\sin(kl)\sin(\pi t)\right) \\ -2k\sin(kl)\cos(\pi t) \\ +\frac{2}{k}\sin(kl)\cos(\pi t)\left((\alpha + X)^2 - \frac{1}{16}\right) \\ -\cos(kl)\sin(\pi t)\Big| \le 1. \end{aligned} \tag{9}$$

In comparison with the continuous spectrum, the derivation of the point spectrum is more complicated. The procedure is as follows. We obtain the eigenvalue $\lambda, |\lambda| < 1$, of the matrix M and the corresponding eigenvector. Then, we consider the Cauchy problem for the central cell with the initial conditions given at the left-hand limit by the eigenvector. The solution of the Cauchy problem gives us the Cauchy data at the right-hand limit. These Cauchy data, in their turn, should belong to the invariant subspace corresponding to the eigenvalue $\lambda, |\lambda| < 1$. Thus, there are two conditions for $E = k^2$ to be an eigenvalue of the Hamiltonian: $|\lambda(k)| < 1$ and proper correlation between the Cauchy data at the left and the right-hand limit of the central cell.

Let us take the first step. If in the spectral equation one has (8) $|y| > 1$ then $|\lambda_1(k)| < 1,\ |\lambda_2(k)| > 1$. The eigenvalue corresponding to λ_1,

$$\lambda_1 = \begin{cases} y - \sqrt{y^2 - 1}, & y > 1, \\ y + \sqrt{y^2 - 1}, & y < -1, \end{cases}$$

gives us the Hamiltonian eigenvalue satisfying the first condition for the point spectrum. The eigenvector corresponding to $\lambda_1(k)$ presents the proper Cauchy data:

$$\begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = \begin{pmatrix} M_{12} \\ \lambda_1 - M_{11} \end{pmatrix}. \tag{10}$$

To obtain the second condition for the point spectrum we need to solve the Cauchy problem for the central cell. The procedure is similar to that used for the transfer matrix construction. The central cell matrix M^0 transforming the Cauchy data is obtained as a product of the seven matrices for each step. The steps, consequently, are: ℓ-shift – δ-potential – input to sphere – transmission from q_B to q_R through the sphere – output from the sphere – δ-potential – ℓ-shift. The matrices for each step have been described above (the central cell differs from other cells only in the positions of the connecting points).

As a result, the corresponding matrix is as follows:

$$M^0 = \begin{pmatrix} M^0_{11} & M^0_{12} \\ M^0_{21} & M^0_{22} \end{pmatrix},$$

where

$$\begin{aligned} M^0_{11} = {} & \frac{\alpha - Q_{BB}}{Q_{BR}}\cos^2 k\ell - \frac{\alpha - Q_{RR}}{Q_{BR}}\sin^2 k\ell \\ & + \left(\frac{(\alpha - Q_{RR})(\alpha - Q_{BB}) - k^2}{Q_{BR}} - Q_{RB}\right) \\ & \times \frac{1}{k}\sin k\ell\cos k\ell, \\ M^0_{12} = {} & -\frac{1}{Q_{BR}}\cos^2 k\ell \\ & - \left(\frac{(\alpha - Q_{RR})(\alpha - Q_{BB}) - k^2}{Q_{BR}} - Q_{RB}\right)\frac{\sin^2 kl}{k^2} \\ & - \frac{2\alpha - Q_{BB} - Q_{RR}}{Q_{BR}}\frac{1}{k}\sin k\ell\cos k\ell, \\ M^0_{21} = {} & \left(\frac{(\alpha - Q_{RR})(\alpha - Q_{BB})}{Q_{RB}}\right)\cos^2 k\ell + \frac{k^2}{Q_{BR}}\sin^2 k\ell \\ & - \frac{2\alpha - Q_{BB} - Q_{RR}}{Q_{BR}}k\sin k\ell\cos k\ell, \\ M^0_{22} = {} & -\frac{\alpha - Q_{RR}}{Q_{BR}}\cos^2 k\ell + \frac{\alpha - Q_{BB}}{Q_{BR}}\sin^2 k\ell \\ & - \left(\frac{(\alpha - Q_{RR})(\alpha - Q_{BB}) - k^2}{Q_{BR}} - Q_{RB}\right) \\ & \times \frac{1}{k}\sin k\ell\cos k\ell. \end{aligned}$$

Here $Q_{RR}, Q_{BR}, Q_{RB}, Q_{BB}$ are given by formulae (2)–(5).

Taking into account the fact that the initial data at the entrance of the central cell are formed by the corresponding eigenvector (10) of the transfer matrix, and that the output data should belong to the corresponding (the same as at the entrance) eigenspace of the transfer-matrix, one obtains the second condition for the point spectrum:

$$M^0_{21}a_1^2 - M^0_{12}a_2^2 + \left(M^0_{22} - M^0_{11}\right)a_1a_2 = 0. \tag{11}$$

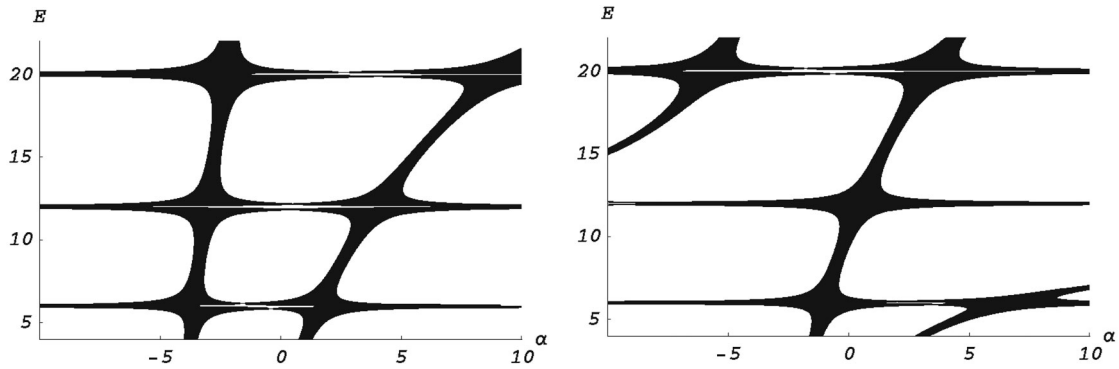

Fig. 2. The dependence of the continuous spectrum on the intensity α of the δ-interactions for the parameters (dimensionless units): $\ell = 0.5$ (left), $\ell = 1$ (right).

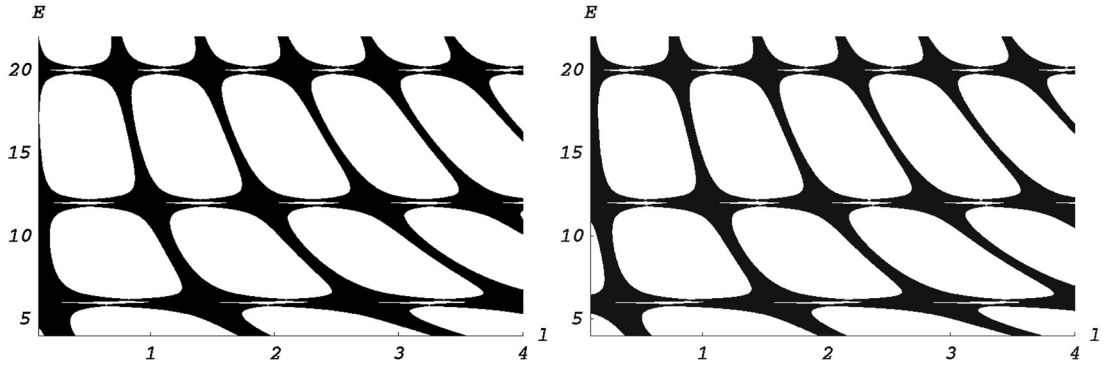

Fig. 3. The dependence of the continuous spectrum on the connecting wires length for the parameters (dimensionless units): $\alpha = 0.5$ (left), $\alpha = 1$ (right).

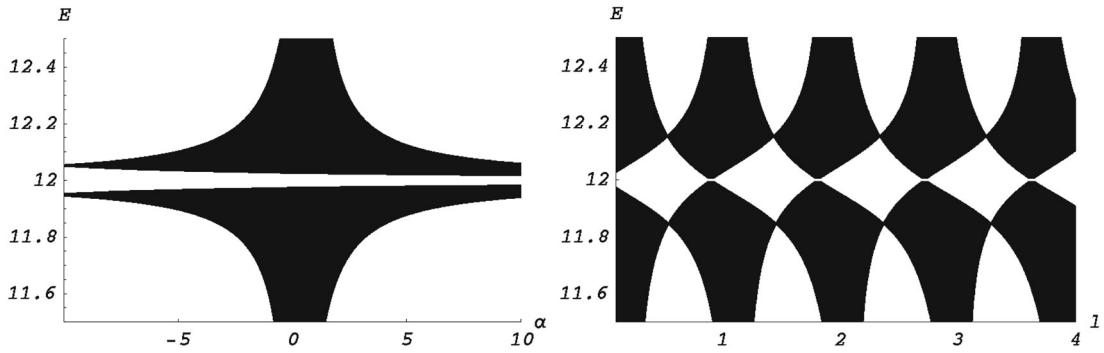

Fig. 4. Gap of the continuous spectrum in a neighborhood of the Green function pole $E = 12$ for the sphere. Left: $\ell = 1$, right: $\alpha = 1$ (dimensionless units).

As a result, for the bent sphere chain, we come to the following conclusion:

Theorem. 1. If $|M_{11} + M_{22}| > 2$, then solution k of equation (11) corresponds to an eigenvalue $E = k^2$ of the model Hamiltonian.
2. If $|M_{11} + M_{22}| \leq 2$, then $E = k^2$ belongs to the continuous spectrum of the model Hamiltonian.

4 Results and discussion

The spectrum of the model Hamiltonian was calculated for different values of the system parameters. Namely, we varied the length of the connecting wires, the intensity of the δ-interactions and the bent angle.

As for the continuous spectrum, it is determined by equation (9). The bands positions depend on the length of the connecting wires and the intensity of the δ-interactions (Figs. 2 and 3). They do not depend on the bent angle (it is natural from the point of view of the general theory: local perturbation does not effect on the continuous spectrum).

We note that there are gaps in the continuous spectrum in the neighbourhoods of the Green function poles for the sphere ($E = n(n+1), n \in \mathbb{N}$) (Fig. 4).

The dependence of the eigenvalues on the bent angle for different values of α and ℓ is shown in Figures 5 and 6.

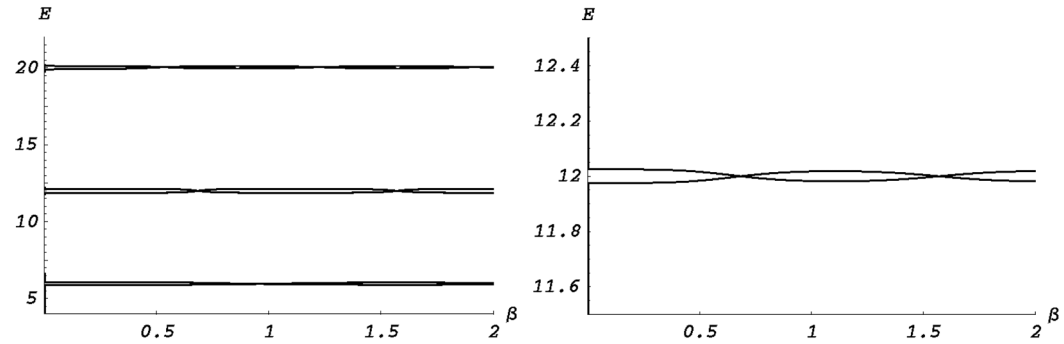

Fig. 5. The dependence of the eigenvalue on the bent angle for the parameters (dimensionless units): $\alpha = 1, \ell = 0.5$ (left), $\alpha = 1, \ell = 1$ (right). The bands are shown as bold segments at the energy axis.

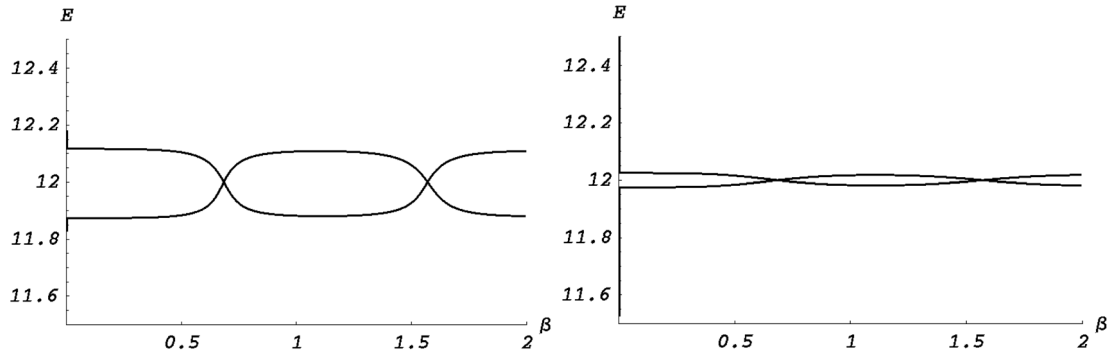

Fig. 6. The dependence of the eigenvalue on the bent angle for the parameters (dimensionless units): $\alpha = 1, \ell = 1.5$ (left), $\alpha = 1.5, \ell = 1$ (right). The bands are shown as bold segments at the energy axis.

The eigenvalues belong to gaps of the continuous spectrum. The bands are shown at the energy axis as bold segments. One can see that the variation of ℓ has a greater influence on the point spectrum of the bent chain than the variation of α. If the bent angle tends to zero, then the eigenvalue tends to the edge of the continuous spectrum. The discrete spectrum is empty for the straight periodic chain, i.e. for zero bent angle. This is natural because in this case the system becomes purely periodic.

Thus, in the present paper we have constructed a solvable model based on the theory of self-adjoint extensions of symmetric operators for an infinite bent chain of coupled nanospheres. The spectrum of the corresponding model Hamiltonian is described.

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