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On the rate of convergence for a class of Markovian queues with group services

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There are many queuing systems that accept single arrivals, accumulate them and service only as a group. Examples of such systems exist in various areas of human life, from traffic of transport to processing requests on a computer network. Therefore, our study is actual. In this paper some class of finite Markovian queueing models with single arrivals and group services are studied. We considered the forward Kolmogorov system for corresponding class of Markov chains. The method of obtaining bounds of convergence on the rate via the notion of the logarithmic norm of a linear operator function is not applicable here. This approach gives sharp bounds for the situation of essentially non-negative matrix of the corresponding system, but in our case it does not hold. Here we use the method of 'differential inequalities' to obtaining bounds on the rate of convergence to the limiting characteristics for the class of finite Markovian queueing models. We obtain bounds on the rate of convergence and compute the limiting characteristics for a specific non-stationary model too. Note the results can be successfully applied for modeling complex biological systems with possible single births and deaths of a group of particles.

Key words and phrases: queuing system, Markovian queues, forward Kolmogorov system, rate of convergence, limiting characteristics

1. Introduction

Consider a Markovian queueing model on the finite state space $\{0, 1, \dots, N\}$ with single arrivals and group services, see the first motivation in [1] and more recent studies in [2], [3].

Let $X(t)$ be the corresponding queue-length process for any $t \geqslant 0$. Denote by $p_{ij}(s,t) = P\{X(t) = j \,|X(s) = i\}$, $i, j \geqslant 0$, $0 \leqslant s \leqslant t$ the transition probabilities of $X(t)$ and by $p_i(t) = P\{X(t) = i\}$ — the probability that the Markov chain $X(t)$ is in state i at time t. Let $\mathbf{p}(t) = (p_0(t), p_1(t), \dots, p_N(t))^T$ be the vector of state probabilities at the moment t.

The probabilistic dynamics of the process $X(t)$ is described by the forward Kolmogorov system

$$\frac{d\mathbf{x}}{dt} = A(t)\mathbf{x}, \tag{1}$$

where $A(t) = Q^T(t)$ is the transposed intensity matrix. All column sums of this matrix are zeros for any $t \geqslant 0$, and $A(t)$ is essentially nonnegative (i.e. all its off-diagonal elements are nonnegative for any $t \geqslant 0$), and all 'intensity functions' $a_{ij}(t)$ are analytical in t.

We suppose that $a_{ij}(t) = 0$ for $i > j-1$, all rates service do not depend on the size of a queue, i.e. $a_{i,i+k}(t) = b_k(t)$ for $k \geqslant 1$, arrival rates $a_{i,i-1}(t) = \lambda_i(t)$. The process $X(t)$ belongs to class (III), see [3]. The matrix $A(t)$ for $X(t)$ has the following structure:

$$A\,(t) = \begin{pmatrix} a_{00}(t) & b_1(t) & b_2(t) & b_3(t) & \cdots & b_{N-1}(t) & b_N(t) \\ \lambda_1(t) & a_{11}(t) & b_1(t) & b_2(t) & \cdots & b_{N-2}(t) & b_{N-1}(t) \\ 0 & \lambda_2(t) & a_{22}(t) & b_1(t) & \cdots & b_{N-3}(t) & b_{N-2}(t) \\ 0 & 0 & \lambda_3(t) & a_{33}(t) & \ddots & b_{N-4}(t) & b_{N-3}(t) \\ \vdots & \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \ddots & a_{N-1N-1}(t) & b_1(t) \\ 0 & 0 & 0 & 0 & \cdots & \lambda_{N-1}(t) & a_{NN}(t) \end{pmatrix}. \tag{2}$$

2. Stationary Markovian queueing model

In this paper we consider a subclass of the class (III) satisfying additional suppositions $b_i(t) = 0$, $1 \leqslant i \leqslant N-1$, $b_N(t) = b(t)$ and $\lambda_i(t) = \lambda(t)$ for any i, $t \geqslant 0$.

The difficulty of studying this model is due to the fact that it is not possible to apply the most convenient method of the logarithmic norm for it, see [3].

Now we get the following expression for the transposed intensity matrix:

$$A\,(t) = \begin{pmatrix} a_{00}(t) & 0 & 0 & \cdots & 0 & b(t) \\ \lambda(t) & a_{11}(t) & 0 & \cdots & 0 & 0 \\ 0 & \lambda(t) & a_{22}(t) & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & a_{N-1N-1}(t) & 0 \\ 0 & 0 & 0 & \cdots & \lambda(t) & a_{NN}(t) \end{pmatrix}. \tag{3}$$

We perform the following system transformations. Since $p_0\,(t) = 1 - \sum\limits_{i \geqslant 1} p_i\,(t)$, one can rewrite the system (1) as

$$\frac{d\mathbf{z}}{dt} = B\,(t)\,\mathbf{z} + \mathbf{f}\,(t)\,, \tag{4}$$

where $\mathbf{f}(t) = (\lambda(t), 0, \dots, 0)^T$, $\mathbf{z} = (p_1(t), p_2(t), \dots, p_N(t))^T$,

$$B(t) = \begin{pmatrix} a_{11}-\lambda & -\lambda & -\lambda & -\lambda & \cdots & -\lambda & -\lambda \\ \lambda & a_{22} & 0 & 0 & \cdots & 0 & 0 \\ 0 & \lambda & a_{33} & 0 & \cdots & 0 & 0 \\ 0 & 0 & \lambda & a_{44} & \ddots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \ddots & a_{N-1N-1} & 0 \\ 0 & 0 & 0 & 0 & \cdots & \lambda & a_{NN} \end{pmatrix}. \tag{5}$$

All bounds on the rate of convergence to the limiting regime for $X(t)$ correspond to the same bounds of the solutions of system

$$\frac{d\mathbf{y}}{dt} = B(t)\mathbf{y}(t). \tag{6}$$

Denote by T upper triangular matrix

$$T = \begin{pmatrix} 1 & 1 & 1 & \cdots & 1 \\ 0 & 1 & 1 & \cdots & 1 \\ 0 & 0 & 1 & \cdots & 1 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \end{pmatrix}. \tag{7}$$

Let $\mathbf{u}(t) = T\mathbf{y}(t)$, then

$$\frac{d\mathbf{u}}{dt} = B^*(t)\mathbf{u}(t), \tag{8}$$

where

$$B^*(t) = TB(t)T^{-1} = \begin{pmatrix} -\lambda & 0 & 0 & \cdots & 0 & -b \\ \lambda & -\lambda & 0 & \cdots & 0 & -b \\ 0 & \lambda & -\lambda & \cdots & 0 & -b \\ 0 & 0 & \lambda & \ddots & 0 & -b \\ \vdots & \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \lambda & -(\lambda+b) \end{pmatrix}. \tag{9}$$

Let us remark that the matrix $B^*(t)$ is not essentially non-negative. This means that the method of the logarithmic norm is inconvenient to apply (it gives poor results). That's why we use the method of 'differential inequalities', which was described in [4]–[6].

Let $\mathsf{D} = \operatorname{diag}(d_1, d_2, \dots d_N)$ be a diagonal matrix and d_i, $i = 1, \dots, N$ be nonzero numbers. By $\mathbf{w}(t)$ denote a product $\mathsf{D}\mathbf{u}(t)$, then one can rewrite (8) as following system

$$\frac{d\mathbf{w}}{dt} = B^{**}(t)\mathbf{w}(t), \tag{10}$$

where

$$B^{**}(t) = \mathsf{D}B^{*}(t)\mathsf{D}^{-1} = \begin{pmatrix} -\lambda & 0 & 0 & 0 & \cdots & 0 & -b\cdot\frac{d_1}{d_N} \\ \lambda\cdot\frac{d_2}{d_1} & -\lambda & 0 & 0 & \cdots & 0 & -b\cdot\frac{d_2}{d_N} \\ 0 & \lambda\cdot\frac{d_3}{d_2} & -\lambda & 0 & \cdots & 0 & -b\cdot\frac{d_3}{d_N} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & -\lambda & -b\cdot\frac{d_{N-1}}{d_N} \\ 0 & 0 & 0 & 0 & \cdots & \lambda\cdot\frac{d_N}{d_{N-1}} & -\lambda - b \end{pmatrix}.$$

By $\mathbf{u}(t)$ denote an arbitrary solution of system (8), then we can consider an interval (t_1, t_2) with fixed signs of the coordinates $u_i(t)$ and choose the elements of the diagonal matrix such that signs of the entries d_i are equal with signs of corresponding coordinates $u_i(t)$ of the solution of system (8).

Since any $d_k u_k(t) \geqslant 0$ on the corresponding time interval, the sum $\sum\limits_{k=1}^{N} d_k u_k(t) = \|\mathbf{w}\|$ can be considered as the corresponding norm.

Denote $B^{**}(t) = \left(b_{ij}^{**}(t)\right)_{i,j=1}^{N}$. Now, if the function $\alpha_D(t)$ is such that $\sum\limits_{i=1}^{N} b_{ij}^{**}(t) \leqslant -\alpha_D(t)$, $j = 1, \ldots, N$, then the following bound holds:

$$\frac{d\,\|\mathbf{w}\|}{dt} = \frac{d\left(\sum\limits_{i=1}^{N} w_k\right)}{dt} = \sum_{j=1}^{N}\sum_{i=1}^{N} b_{ij}^{**}(t) w_j \leqslant -\alpha_D(t)\,\|\mathbf{w}\|\,.$$

We set $\alpha^* = \min\{\alpha_D(t)\}$, where the minimum is taken over all intervals with different combinations of coordinate signs of the solution. Hence for any such combination we have the inequality

$$\|\mathbf{w}(t)\| \leqslant e^{-\int_s^t \alpha^*(\tau)d\tau}\|\mathbf{w}(s)\|.$$

If we compared all the norms, then one can obtain the final bound

$$\|\mathbf{y}(t)\| \leqslant Ce^{-\int_0^t \alpha^*(\tau)d\tau}\|\mathbf{y}(0)\|, \tag{11}$$

where C is a corresponding constant.

In our case (in general, all intensities depend on the time t)

$$\sum_{i=1}^{N-1} w_i' = -\lambda\cdot\left(1-\frac{d_2}{d_1}\right)\cdot w_1 - \lambda\cdot\left(1-\frac{d_3}{d_2}\right)\cdot w_2 - \lambda\cdot\left(1-\frac{d_4}{d_3}\right)\cdot w_3 - \cdots -$$

$$- \left(\lambda + b \cdot \left(1 + \frac{d_1}{d_N} + \frac{d_2}{d_N} + \cdots + \frac{d_{N-1}}{d_N} \right) \right) \cdot w_{N-1}$$

1) Let all $u_1, \ldots, u_N$ be positive. Since $\left(1 - \frac{d_{i+1}}{d_i}\right)$ must be positive, we have $d_i > d_{i+1}$. Suppose $d_1 := h$, $d_2 := h^2$, ..., $d_N := h^N$, then

$$\begin{aligned}
\sum_{i=1}^{N-1} w_i' &= -\lambda \cdot \left(1 - \frac{d_2}{d_1}\right) \cdot w_1 - \lambda \cdot \left(1 - \frac{d_3}{d_2}\right) \cdot w_2 - \lambda \cdot \left(1 - \frac{d_4}{d_3}\right) \cdot w_3 - \cdots - \\
&\quad - \left(\lambda + b \cdot \left(1 + \frac{d_1}{d_N} + \frac{d_2}{d_N} + \cdots + \frac{d_{N-1}}{d_N} \right) \right) \cdot w_{N-1} = \\
&= -\lambda \cdot (1-h) \cdot w_1 - \lambda \cdot (1-h) \cdot w_2 - \lambda \cdot (1-h) \cdot w_3 - \cdots - \\
&\quad - \left(\lambda + b \cdot \left(1 + \frac{1}{h} + \frac{1}{h^2} + \cdots + \frac{1}{h^{N-1}} \right) \right) \cdot w_{N-1},
\end{aligned}$$

and we have $\alpha_D = \lambda \cdot (1-h)$.

2) Let all u_1, ..., u_k be positive, and all u_{k+1}, ..., u_N negative. Similarly $|d_i| > |d_{i+1}|$. Suppose $d_1 := h^{N-k+1}$, $d_2 := h^{N-k+2}$, ..., $d_k := h^N$, $d_{k+1} := -h$, $d_{k+2} := -h^2$, ..., $d_N := -h^{N-k}$, then

$$\begin{aligned}
\sum_{i=1}^{N-1} w_i' &= -\lambda \cdot \left(1 - \frac{d_2}{d_1}\right) \cdot w_1 - \lambda \cdot \left(1 - \frac{d_3}{d_2}\right) \cdot w_2 - \lambda \cdot \left(1 - \frac{d_4}{d_3}\right) \cdot w_3 - \cdots - \\
&\quad - \left(\lambda + b \cdot \left(1 + \frac{d_1}{d_N} + \frac{d_2}{d_N} + \cdots + \frac{d_{N-1}}{d_N} \right) \right) \cdot w_{N-1} = \\
&= -\lambda \cdot (1-h) \cdot w_1 - \lambda \cdot (1-h) \cdot w_2 - \lambda \cdot (1-h) \cdot w_3 - \cdots - \\
&\quad - \lambda \cdot (1-h) \cdot w_{k-1} - \lambda \cdot \left(1 + \frac{1}{h^{N-1}}\right) \cdot w_k - \cdots - \\
&- \left(\lambda + b \cdot \left(1 - h - h^2 - \ldots - h^k + \frac{1}{h^{N-k-1}} + \frac{1}{h^{N-k-2}} + \cdots + \frac{1}{h} \right) \right) \cdot w_N,
\end{aligned}$$

In this case $\alpha_D = \lambda \cdot (1-h)$ too.

3) Let all u_1, ..., u_k be positive, and all u_{k+1}, ..., u_s negative and all u_{s+1}, ..., u_N be positive too. As before $|d_i| > |d_{i+1}|$. Suppose $d_1 := h^{N-k+1}$, $d_2 := h^{N-k+2}$, ..., $d_k := h^N$, $d_{k+1} := -h^{N-s+1}$, $d_{k+2} := -h^{N-s+2}$, ..., $d_s := -h^{N-k}$, $d_{s+1} := h$, $d_{s+2} := h^2$, ..., $d_N := -h^{N-s}$.

$$\begin{aligned}
\sum_{i=1}^{N-1} w_i' &= -\lambda \cdot \left(1 - \frac{d_2}{d_1}\right) \cdot w_1 - \lambda \cdot \left(1 - \frac{d_3}{d_2}\right) \cdot w_2 - \lambda \cdot \left(1 - \frac{d_4}{d_3}\right) \cdot w_3 - \cdots - \\
&\quad - \left(\lambda + b \cdot \left(1 + \frac{d_1}{d_N} + \frac{d_2}{d_N} + \cdots + \frac{d_{N-1}}{d_N} \right) \right) \cdot w_{N-1} =
\end{aligned}$$

$$= -\lambda \cdot (1-h) \cdot w_1 - \lambda \cdot (1-h) \cdot w_2 - \lambda \cdot (1-h) \cdot w_3 - \cdots -$$

$$-\lambda \cdot (1-h) \cdot w_{k-1} - \lambda \cdot \left(1 + \frac{1}{h^{s-1}}\right) \cdot w_k - \lambda \cdot (1-h) \cdot w_{k+1} - \cdots - \lambda \cdot (1-h) \cdot w_{s-1} -$$

$$- \lambda \cdot \left(1 + \frac{1}{h^{N-k}}\right) \cdot w_s - \lambda \cdot (1-h) \cdot w_{s+1} - \cdots -$$

$$-\left(\lambda + b\left(1 + h^{s-k+1} + \cdots + h^s - h - h^2 - \cdots - h^{s-k} + \frac{1}{h^{N-k-1}} + \cdots + \frac{1}{h}\right)\right) \cdot w_N,$$

as before $\alpha_D = \lambda \cdot (1-h)$.

In the general case, we do the same. Then we have $C = h^{1-N}$ and the following bound

$$\|y(t)\| \leqslant 2Nh^{1-N} \cdot e^{-\lambda \cdot (1-h)t} \|y(0)\|. \tag{12}$$

In general non-stationary situation

$$\|y(t)\| \leqslant 2Nh^{1-N} \cdot e^{-(1-h)\int_0^t \lambda(\tau)d\tau} \|y(0)\|. \tag{13}$$

3. Non-stationary Markovian queueing model

Here we consider a specific queueing model with 1-periodic intensities: $\lambda(t) = 2 + \sin(2\pi t)$ and $b(t) = (2 + \cos(2\pi t))$, then

$$A(t) = \begin{pmatrix} a_{00} & 0 & 0 & 0 & \cdots & 0 & 2 + \cos(2\pi t) \\ 2 + \sin(2\pi t) & a_{11} & 0 & 0 & \cdots & 0 & 0 \\ 0 & 2 + \sin(2\pi t) & a_{22} & 0 & \cdots & 0 & 0 \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ 0 & 0 & 0 & 0 & \cdots & a_{N-1N-1} & 0 \\ 0 & 0 & 0 & 0 & \cdots & 2 + \sin(2\pi t) & a_{NN} \end{pmatrix}$$

and $B^{**}(t) = \left(b_{ij}^{**}(t)\right)_{i,j=1}^{N}$, where $b_{ii}^{**}(t) = -2 - \sin(2\pi t)$, if $1 \leqslant i \leqslant N-1$; $b_{NN}^{**}(t) = -4 - \sin(2\pi t) - \cos(2\pi t)$, $b_{iN}^{**}(t) = -(2 + \cos(2\pi t)) \cdot \frac{d_i}{d_N}$, if $1 \leqslant i \leqslant N-1$; $b_{i(i-1)}^{**}(t) = (2 + \sin(2\pi t)) \cdot \frac{d_i}{d_{i-1}}$, if $2 \leqslant i \leqslant N$, all other elements are zero.

Then we have the following bound on the rate of convergence

$$\|y(t)\| \leqslant 2N \cdot h^{1-N} \cdot e^{-\int_0^t (1-h)\lambda(\tau)d\tau} \|y(0)\|, \tag{14}$$

namely

$$\|y(t)\| \leqslant 2N \cdot h^{1-N} \cdot e^{-(1-h)\int_0^t (2+\sin(2\pi\tau))d\tau} \|y(0)\|, \tag{15}$$

hence

$$\|\mathbf{y}(t)\| \leqslant 2N \cdot h^{1-N} \cdot e^{-(1-h)t} \|\mathbf{y}(0)\|. \tag{16}$$

The right-hand side of estimate (16) decreases rather slowly with increasing t. However, this does not mean that the estimate is inaccurate because the real

rate of convergence is rather slow. For example, let $N = 50$ and $h = \frac{1}{2}$. In Figures 1–3 we can see the state probability of an empty queue $p_0(t)$ as low convergence rate function of time t.

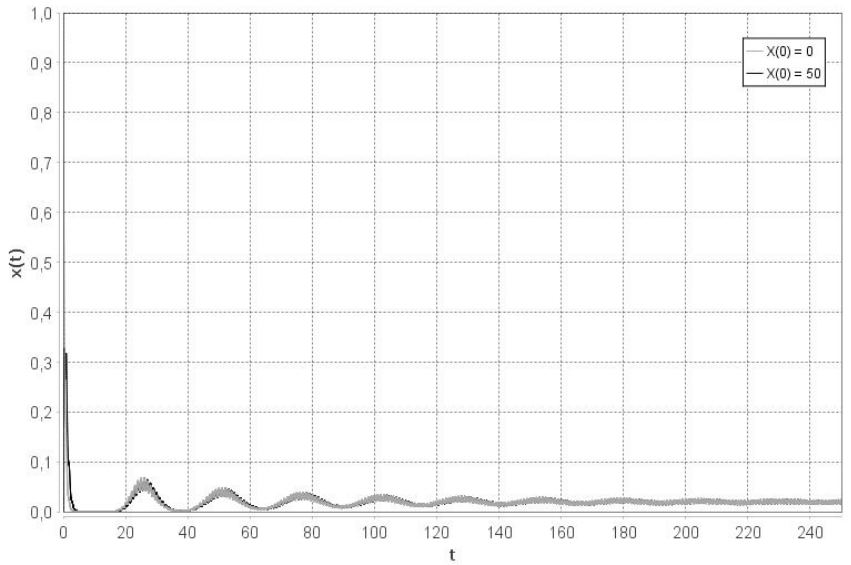

Figure 1. Probability of the empty queue $p_0(t)$ for $t \in [0, 250]$ with initial conditions $X(0) = 50$ (black) and $X(0) = 0$ (gray)

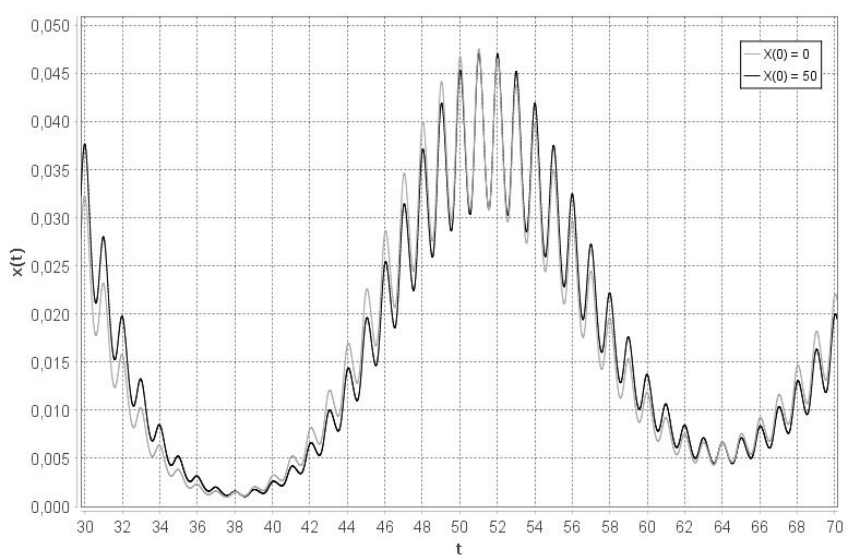

Figure 2. Probability of the empty queue $p_0(t)$ for $t \in [30, 70]$ with initial conditions $X(0) = 50$ (black) and $X(0) = 0$ (gray)

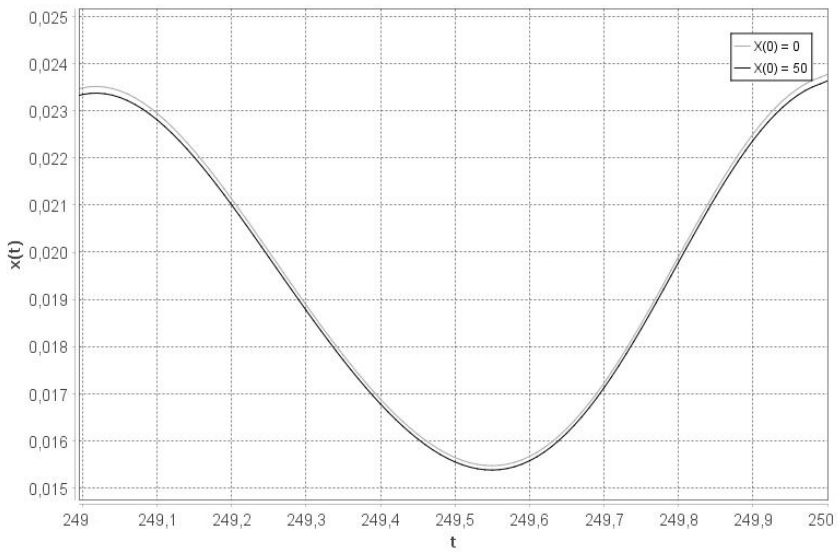

Figure 3. Probability of the empty queue $p_0(t)$ for $t \in [249, 250]$ with initial conditions $X(0) = 50$ (black) and $X(0) = 0$ (gray)

4. Conclusions

Some new class of finite Markovian queueing models with single arrivals and group services was considered. Bounds on the rate of convergence for these models and computations of the limiting characteristics for a specific non-stationary model were obtained.

The obtained results belong to the theory of queueing systems and can be applied, for example, in medical and biological stochastic systems, which satisfy the adopted assumptions.

For describing possibility of applications of Markovian queues we can refer to [7]–[17], which contains a broad overview and a classification of time-dependent queueing systems.

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References

[1] R. Nelson, D. Towsley, and A. N. Tantawi, "Performance analysis of parallel processing systems," *IEEE Transactions on Software Engineering*, vol. 14, no. 4, pp. 532–540, 1988. DOI: 10.1109/32.4676.

[2] J. Li and L. Zhang, "$M^X/M/c$ Queue with catastrophes and state-dependent control at idle time," *Frontiers of Mathematics in China*, vol. 12, no. 6, pp. 1427–1439, 2017. DOI: 10.1007/s11464-017-0674-8.

[3] A. Zeifman, R. Razumchik, Y. Satin, K. Kiseleva, A. Korotysheva, and V. Korolev, "Bounds on the rate of convergence for one class of inhomogeneous Markovian queueing models with possible batch arrivals and services," *International Journal of Applied Mathematics and Computer Science*, vol. 28, pp. 141–154, 2018. DOI: 10.2478/amcs-2018-0011.

[4] A. Zeifman, A. Sipin, V. Korolev, G. Shilova, K. Kiseleva, A. Korotysheva, and Y. Satin, "On Sharp Bounds on the Rate of Convergence for Finite Continuous-time Markovian Queueing Models," in *Computer Aided Systems Theory — EUROCAST 2017. EUROCAST 2017. Lecture Notes in Computer Science*, R. Moreno-Díaz, F. Pichler, and A. Quesada-Arencibia, Eds., vol. 10672, 2018, pp. 20–28. DOI: 10.1007/978-3-319-74727-9_3.

[5] A. Zeifman, Y. Satin, A. Kryukova, R. Razumchik, K. Kiseleva, and G. Shilova, "On the Three Methods for Bounding the Rate of Convergence for some Continuous-time Markov Chains," *International Journal of Applied Mathematics and Computer Science*, vol. 30, pp. 251–266, 2020. DOI: 10.34768/amcs-2020-0020.

[6] Y. Satin, A. Zeifman, and A. Kryukova, "On the Rate of Convergence and Limiting Characteristics for a Nonstationary Queueing Model," *Mathematics*, vol. 7, no. 678, pp. 1–11, 2019. DOI: 10.3390/math7080678.

[7] B. Almasi, J. Roszik, and J. Sztrik, "Homogeneous finite-source retrial queues with server subject to breakdowns and repairs," *Mathematical and Computer Modelling*, vol. 42, no. 5, pp. 673–682, 2005. DOI: 10.1016/j.mcm.2004.02.046.

[8] A. Brugno, C. D'Apice, A. Dudin, and R. Manzo, "Analysis of an $MAP/PH/1$ queue with flexible group service," *International Journal of Applied Mathematics and Computer Science*, vol. 27, no. 1, pp. 119–131, 2017. DOI: 10.1515/amcs-2017-0009.

[9] A. Di Crescenzo, V. Giorno, B. K. Kumar, and A. Nobile, "A Time-Non-Homogeneous Double-Ended Queue with Failures and Repairs and Its Continuous Approximation," *Mathematics*, vol. 6, no. 5, p. 81, 2018. DOI: 10.3390/math6050081.

[10] A. N. V. Giorno and S. Spina, "On some time non-homogeneous queueing systems with catastrophes," *Applied Mathematics and Computation*, vol. 245, pp. 220–234, 2014. DOI: 10.1016/j.amc.2014.07.076.

[11] B. Granovsky and A. Zeifman, "Nonstationary Queues: Estimation of the Rate of Convergence," *Queueing Systems*, vol. 46, pp. 363–388, 2004. DOI: 10.1023/B:QUES.0000027991.19758.b4.

[12] H. LI, Q. Zhao, and Z. Yang, "Reliability Modeling of Fault Tolerant Control Systems," *International Journal of Applied Mathematics and Computer Science*, vol. 17, no. 4, pp. 491–504, 2007. DOI: 10.2478/v10006-007-0041-0.

[13] A. Moiseev and A. Nazarov, "Queueing network $MAP - (GI/\infty)K$ with high-rate arrivals," *European Journal of Operational Research*, vol. 254, no. 1, pp. 161–168, 2016. DOI: 10.1016/j.ejor.2016.04.011.

[14] J. Schwarz, G. Selinka, and R. Stolletz, "Performance analysis of time-dependent queueing systems: Survey and classification," *Omega*, vol. 63, pp. 170–189, 2016. DOI: 10.1016/j.omega.2015.10.013.

[15] N. Vvedenskaya, A. Logachov, Y. Suhov, and A. Yambartsev, "A Local Large Deviation Principle for Inhomogeneous Birth-Death Processes," *Problems of Information Transmission*, vol. 54, no. 3, pp. 263–280, 2018. DOI: 10.1134/S0032946018030067.

[16] A. Zeifman, S. Leorato, E. Orsingher, Y. Satin, and G. Shilova, "Some universal limits for nonhomogeneous birth and death processes," *Queueing Systems*, vol. 52, no. 2, pp. 139–151, 2006. DOI: 10.1007/s11134-006-4353-9.

[17] A. Zeifman, V. Korolev, Y. Satin, A. Korotysheva, and V. Bening, "Perturbation Bounds and Truncations for a Class of Markovian Queues," *Queueing Systems*, vol. 76, no. 2, pp. 205–221, 2014. DOI: 10.1007/s11134-013-9388-0.

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О скорости сходимости одного класса марковских цепей с групповым обслуживанием требований

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Существует множество систем массового обслуживания, которые принимают единичные требования, накапливают их и обслуживают только как группу. Примеры таких систем можно найти в различных областях человеческой жизни — от трафика транспортных перевозок до обработки запросов в компьютерных сетях. Этим обуславливается актуальность нашего исследования. В этой статье изучается некоторый класс конечных марковских моделей массового обслуживания с одиночным прибытием и групповым обслуживанием. Рассмотрена прямая система Колмогорова для соответствующего класса цепей Маркова. Метод определения границ сходимости, основанный на понятии логарифмической нормы, здесь не применим. Такой подход даёт точные оценки для моделей, для которых матрица соответствующей системы существенно неотрицательна, но в нашем случае это не так. Здесь мы использовали новый метод «дифференциальных неравенств» для получение оценки скорости сходимости для этого класса конечных марковских моделей. Кроме того, мы получили оценки скорости сходимости и вычислили предельные характеристики и для соответствующей нестационарной модели. Заметим, что результаты могут быть успешно применены для моделирования сложных биологических систем, в которых возможны рождения новых особей только по одной и гибель групп.

Ключевые слова: система массового обслуживания, марковский процесс, прямая система Колмогорова, скорость сходимости, предельные характеристики

Research article

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Application of a computer algebra systems to the calculation of the $\pi\pi$-scattering amplitude

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The aim of this work is to develop a set of programs for calculation the scattering amplitudes of the elementary particles, as well as automating the calculation of amplitudes using the appropriate computer algebra systems (Mathematica, Form, Cadabra). The paper considers the process of pion-pion scattering in the framework of the effective Nambu–Iona–Lasinio model with two quark flavours. The *Package-X* for Mathematica is used to calculate the scattering amplitude (starting with the calculation of Feynman diagrams and ending with the calculation of Feynman integrals in the one-loop approximation). The loop integrals are calculated in general kinematics in *Package-X* using the Feynman parametrization technique. A simple check of the program is made: for the case with zero temperature, the scattering lengths $a_0 = 0.147$ and $a_2 = -0.0475$ are calculated and the total cross section is constructed. The results are compared with other models as well as with experimental data.

Key words and phrases: Feynman integrals, one-loop approximation, total sross section, scattering length, a computer algebra, *Package*-X

1. Introduction

The heavy ion collision experiment is an instrument for the study of the matter properties under critical conditions. The modern experiment is a multi-stage process, which includes the event selection, the event reconstruction (the reconstruction of the primary particles) and the simulation of the collision process. The simulation is made on the base of the chosen model and the final result has to reproduce the real data. The fulfil of such analysis or simulation among other things requires a good understanding and a strict description of the final state particle interaction.

The information about the particles properties and their interactions can be extracted from the probabilities of the processes occurring during their

collision. The interaction probability is associated with the cross section of the given reaction and the phase volume, which is uniquely determined by the laws of conservation of energy-momentum, i.e., by the kinematics of the reaction. From the theoretical point of view, the cross section is defined by the scattering amplitude, which is described in the framework of the model under consideration. The model can include description of the quantum mechanical properties of the particles, describe the type of the interaction, take into account the matter properties or the quark structure of the colliding particles, etc. That is why to obtain the scattering amplitude is not the trivial task both from theoretical and computing point of view.

This paper is dedicated to the calculation of $\pi\pi$-scattering amplitude. As the lightest hadron with Goldstone nature, the pion occupies a special position in hadronic physics. The elastic $\pi\pi$-scattering is a fundamental process for quantum chromodynamics (QCD) at low energies as it provides an ideal testing for the mechanism of spontaneous chiral symmetry breaking. During the heavy ion collision, pions can be quickly created in the early phase, for example, by the Schwinger mechanism and their number is quasi-conserved over the time scale of the heavy ion collision until freeze- out. Then, in the hadron phase, two and more pions are the final state of many hadronic interactions. Accordingly, $\pi\pi-$ scattering attracts considerable interest even though the cross section is not directly measurable.

In this work the $\pi\pi$-scattering is considered in the frame of two-flavour Nambu–Jona-Lasinio model (NJL) [1]. The most important advantage of the NJL model is that it introduces a mechanism of the dynamical breaking of chiral symmetry (due to the quark-antiquark condensate). The model has a good tool to introduce finite temperature suggested by Matsubara and is able to describe the matter properties at finite temperature and density. Nevertheless, the calculation of the $\pi\pi$-scattering amplitude in NJL model is difficult due to the appearing of four-point one-loop Feynman integrals, that make the using of Matsubara mechanism in the general kinematics complicated. That is why the problem was solved only for limiting cases, for example, for the case with $p_1 = p_2 = p_3 = p_4 = p$ [2]. This limit allows to estimate the scattering lengths a_0, a_2, but does not make it possible to evaluate the cross section, the pion damping width or the lifetime. This work focuses on the evaluation of the scattering amplitude in general kinematics but due to the use of the dimensional regularization scheme, without the finite temperature.

The evaluation of the scattering amplitude can be made in two steps: writing down the amplitude using the Feynman rules, evaluating traces and then integrating over the phase space, applying the chosen kinematics. Many packages allow to evaluate Dirac traces, for example, Form [3] or Cadabra [4]. Obtained results usually require a lot of additional analytical work for writing down the amplitude in appropriate form and for numerical calculation. To evaluate one-loop integrals that appear in higher order calculations of perturbative quantum field theory, there are exist, for example, the Mathematica packages FeynCalc [5], FormCalc [6] and the Fortran program Golem95 [7]. These packages compute the one-loop tensor integrals using the Passarino–Veltman reduction algorithm [8]. In this work we use the *Package*-X for Mathematica, developed by Hiren H. Patel [9]. The *Package*-X runs all steps for amplitude evaluation: performing traces over products of

Dirac matrices, giving the result in the term of Passarino–Veltman functions, computation of the one-loop integrals. *Package*-X provides analytic expressions for UV-divergent, IR-divergent and finite parts either separately or all together. Output expressions can be readily evaluated numerically and manipulated symbolically with built-in Mathematica functions.

2. Using the Package-X for the evaluation of $\pi - \pi$ scattering amplitude

In this work the meson-meson scattering amplitude in the frame of effective QCD models is considered. The work focuses on the NJL model [1], the Lagrangian of the model can consist of scalar, pseudo-scalar, vector, and axial-vector four-quark interactions. The expressions for the total amplitude $\mathcal{T}(s,t,u)$ depend on the number of interactions taken into account. For this work the Lagrangian with two flavours of quarks and scalar and pseudo-scalar four-quark interactions is chosen:

$$\mathcal{L}_{\text{NJL}} = \bar{q}\left(i\gamma_\mu \partial^\mu - \hat{m}_0\right) q + G\left[(\bar{q}q)^2 + (\bar{q}i\gamma_5\vec{\tau}q)^2\right], \tag{1}$$

where G is the scalar coupling constant, $\bar{q}, q$ are the quark fields, $\hat{m}_0$ is the diagonal matrix of the current quark mass, $\hat{m}_0 = \text{diag}(m_u^0, m_d^0)$ with $m_u^0 = m_d^0 = m_0$, and $\vec{\tau}$ are the Pauli matrices in space SU(2), $\tau^a (a = 1, 2, 3)$.

In the mean field approximation the constituent mass of the quark is provided by the gap equation:

$$m = m_0 + 2iG \int \frac{dp}{(2\pi)^4} \text{Tr}\{S(p)\}, \tag{2}$$

where $S(p) = (\hat{p} - m)^{-1}$ is the quark propagator and trace is taken over Dirac, flavour and colour indexes.

A meson is considered as a quark-antiquark couple forming a loop, and in the framework of the RPA approximation it leads to the Bethe–Salpeter equation:

$$1 - 2G\ \Pi_M(k^2)|_{k^2=M^2} = 0, \tag{3}$$

with the polarization operator $\Pi_M(k^2)$, which defines the meson properties:

$$\Pi_M(k^2) = i \int \frac{d^4p}{(2\pi)^4}\ \text{Tr}\left[\Gamma_M S(p+k)\Gamma_M S(p)\right], \tag{4}$$

where the vertex factor Γ_M depends on the sort of meson. $\Gamma_M = i\gamma_5\tau^a$ for the pseudo-scalar meson and $\Gamma_M = \mathbf{1}\tau^a$ for scalar meson. The meson propagator is defined as

$$D_M(k^2) = \frac{2iG}{1 - 2G\ \Pi_M(k^2)}. \tag{5}$$

For simplicity, in this work the parametrization suggested in the work [10] is used. The set of equations for fixing masses and coupling constants can be written as:

$$M_s^2 = M_\pi^2 Z + 4m^2, \quad g_{\sigma qq} = g_{\pi qq}\sqrt{Z}, \tag{6}$$

where $Z = 1 - 6m^2/M_{a_1}^2$, $M_{a_1} = 1.2$ GeV is the mass of a_1-meson, $M_\pi = 0.14$ GeV is the pion mass and m is the constituent quark mass. The coupling constant $g_{\pi qq}$ can be obtained from the Goldberger–Treiman relation [11]:

$$g_{\pi qq} f_\pi = m + \mathcal{O}(m),$$

where $f_\pi = 0.0924$ GeV is the pion decay constant.

On the lowest order $1/N_c$ there are two types of Feynman diagrams, contributed to the $\pi\pi$-scattering amplitude: four-vertex "box "-diagrams and the meson-exchange diagrams [2], [12]. The set of "box"-diagram is presented in the Figure 1. Here p_1, p_2 are the momenta of incoming particles, p_3, p_4 are the momenta of scattered particles, k is the integration variable.

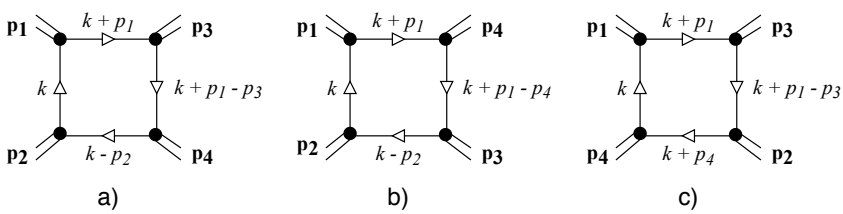


Figure 1. Feynman diagrams contributing to the $\pi\pi$-scattering

The amplitudes corresponding to each diagram in Figure 1 can be written as:

$$i\mathcal{T} = -g_{\pi qq}^4 \mu^{2\epsilon} \int \frac{d^d k}{(2\pi)^d} \frac{\mathrm{Tr}\{\gamma_5(\hat{q_1}+m)\gamma_5(\hat{q_2}+m)\gamma_5(\hat{q_3}+m)\gamma_5(\hat{q_4}+m)\}}{[{q_1}^2 - m^2][{q_2}^2 - m^2][{q_3}^2 - m^2][{q_4}^2 - m^2]}. \tag{7}$$

The prefactor $-g_{\pi qq}^4$ appears as the vertex factor in the diagrams are $\Gamma_\pi = i g_{\pi qq}\gamma_5$. The notation q_i, $i = 1, ..., 4$ was introduced for the simplicity and the values of q_i, corresponding to diagrams in Figure 1 a), b) c) accordingly are listed in Table 1.

Table 1

The q_i for the "box"-diagrams in Figure 1

	T_s^{box} (a)	T_u^{box} (b)	T_t^{box} (c)
q_1	k	k	k
q_2	$k - p_2$	$k - p_2$	$k + p_4$
q_3	$k + p_1 - p_3$	$k + p_1 - p_4$	$k + p_1 - p_3$
q_4	$k + p_1$	$k + p_1$	$k + p_1$

To compute traces of Dirac matrices in denominator of equation 7 the function `Spur` is used. The `LoopIntegrate` function initiates the evaluation

of integral and carries out its covariant tensor decomposition in term of Passarino–Veltman functions (PVA, PVB, PVC, PVD). For diagrams in Figure 1, keeping the notation for s-, t-, u- channels, it should be written:

In[2]:=
sChannel = LoopIntegrate[Spur[γ.k + m_1, γ_5, γ.(k - p_2) + m_1], γ_5, γ.(k + p_1 - p_3) + m_1, γ_5, γ.(k + p_1) + m_1, γ_5], k, {k, m}, {k - p_2, m}, {k + (p_1 - p_3), m}, {k + p_1, m}];
uChannel = LoopIntegrate[Spur[γ.k + m_1, γ_5, γ.(k - p_2) + m_1], γ_5, γ.(k + p_1 - p_4) + m_1, γ_5, γ.(k + p_1) + m_1, γ_5], k, {k, m}, {k - p_2, m}, {k + p_1 - p_4, m}, {k + p_1, m}];
tChannel = LoopIntegrate[Spur[γ.k + m_1, γ_5, γ.(k + p_1 + p_2 - p_3) + m_1], γ_5, γ.(k + p_1 - p_3) + m_1, γ_5, γ.(k + p_1) + m_1, γ_5], k, {k, m}, {k + p_1+ p_2 - p_3, m}, {k + p_1 - p_3, m}, {k + p_1, m}]

The output of the `LoopIntegrate` function contains a number of dot-products of the external momenta. It is possible to define on-shell conditions expressing scalar products in terms of Mandelstam invariants with the function `MandelstamRelations` and eliminate one of variables using additional command `Eliminate`.

In[1]:=
onShell = MandelstamRelations[p_1, p_2, p_3, p_4, M, M, M, M $\to$ s, t, u, Eliminate $\to$ u]
Out[1]:=
$\{\mathrm{p1}^2 \to M^2, \mathrm{p2}^2 \to M^2, \mathrm{p3}^2 \to M^2, \mathrm{p4}^2 \to M^2, \mathrm{p1.p2} \to \frac{1}{2}(s - 2M^2), \mathrm{p3.p4} \to \frac{1}{2}(s - 2M^2), \mathrm{p1.p3} \to \frac{1}{2}(2M^2 - t), \mathrm{p2.p4} \to \frac{1}{2}(2M^2 - t), \mathrm{p1.p4} \to \frac{1}{2}(-2M^2 + s + t), \mathrm{p2.p3} \to \frac{1}{2}(-2M^2 + s + t), \varepsilon^{\{\mathrm{p1}\}\{\mathrm{p2}\}\{\mathrm{p3}\}\{\mathrm{p4}\}} \to 0\}$

After covariant decomposition and on-shell or kinematic conditions are applied, the result in term of the coefficient functions is obtained. At the final step `LoopRefine` is run to reduce the obtained result in terms of analytic expressions DiscB, ScalarC0, ScalarD0, that are the in-built Mathematica functions and are suitable for numerical calculation. Actually, these functions are an abbreviation for a more complicated expression and the function `DiscExpand` displays them in terms of elementary functions.

In[5]:=
sChannelInt = LoopRefine[sChannel /. onShell]
uChannelInt = LoopRefine[tChannel /. onShell];
tChannelInt = LoopRefine[uChannel /. onShell];
Out[5]:=
$8 + 4\left(\frac{1}{\epsilon} + \mathrm{Log}\left[\frac{^2}{\mathrm{m}^2}\right]\right) + 2\mathrm{DiscB}[\mathrm{s}, \mathrm{m}, \mathrm{m}] + 2\mathrm{DiscB}[\mathrm{t}, \mathrm{m}, \mathrm{m}] -$
$2(2M^2 - s)\,\mathrm{ScalarC0}[\mathrm{M}^2, \mathrm{M}^2, \mathrm{s}, \mathrm{m}, \mathrm{m}, \mathrm{m}] - 2(2M^2 - t)\,\mathrm{ScalarC0}[\mathrm{M}^2, \mathrm{M}^2, \mathrm{t}; \mathrm{m}, \mathrm{m}, \mathrm{m}] +$
$(2\mathrm{M}^4 - \mathrm{st})\,\mathrm{ScalarD0}[\mathrm{M}^2, \mathrm{M}^2, \mathrm{M}^2, \mathrm{M}^2; \mathrm{s}, \mathrm{t}; \mathrm{m}, \mathrm{m}, \mathrm{m}, \mathrm{m}]$

There are a few notes concerning the outputs: in the outputs an overall factor $i/(16\pi^2)$ is omitted for brevity, and should be restored during analysis of the result. The result can contain the term $1/\epsilon$ that always explicitly displays logarithmic UV and/or IR divergences. During the analysis of the

results, it should be kept in mind that the term $1/\epsilon$ is equal to $(1/\epsilon - \gamma + \ln 4\pi)$. The discussion about the renormalization in QED and QCD can be found, for example, in the work [13]. The UV and/or IR divergence can be displayed separately using `Part → UVDivergent`.

In[8]:=
LoopRefine[sChannel, Part → UVDivergent]
Out[8]:= $\dfrac{1}{4\epsilon\pi^2}$

The scattering amplitude, expressed in variable s, t, u, is invariant and does not change when replacing $s \leftrightarrow t$, $s \leftrightarrow u$, $t \leftrightarrow u$. Therefore, the first diagram in Figure 1 a) can be obtained from the second one b) by replacing $t \leftrightarrow u$, and the third c) from the second b) — by replacing $s \leftrightarrow t$. Using this property, the simple check of result can be done:

In[9]:=
sChannelf[s_,t_,u_] = sChannel /. onShell;
uChannelf[s_, t_, u_] = uChannel /. onShell;
tChannelf[s_, t_, u_] = tChannel /. onShell;
FullSimplify[LoopRefine[sChannelf[s, t, u] - uChannelf[s, u, t]]]
FullSimplify[LoopRefine[uChannelf[s, t, u] - tChannelf[t, s, u]]]
Out[12]:= 0
Out[13]:= 0

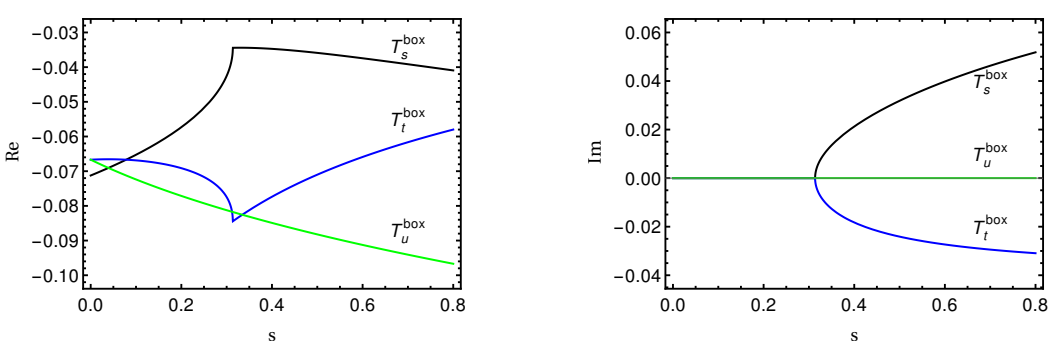


Figure 2. The real (left panel) and imaginary (right panel) of the "box"-diagrams for the case $t = 0$

The real and imaginary parts of the integral (7) for all "box"-diagrams as function of s are shown in Figure 2 for the case $t = 0$.

The second type of Feynman diagrams contributed to the $\pi\pi$-scattering amplitude is the diagram with the meson as intermediate state. As the intermediate state there can be scalar, vector, axial-vector mesons if they appear in the Lagrangian of the model. The diagrams with intermediate meson propagator are shown in Figure 3, where triangle vertexes correspond to $M \to \pi\pi$ decay and d) e) and f) will be denoted as s-, u-, t- channels accordingly. According to the Lagrangian (1), in the model only scalar and

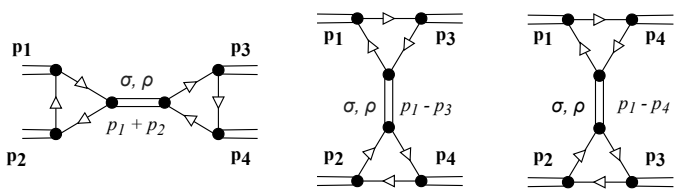
pseudo-scalar quark-antiquark states are present and as the intermediate state the scalar σ-meson appears. Accordingly, for this case, the triangle vertexes correspond to $\sigma \to \pi\pi$ decay. The total amplitude for the meson-exchange diagram is written as:

$$i\mathcal{T}^{\sigma} = i\Gamma^{\sigma qq} D_{\sigma}(p) i\Gamma^{\sigma\pi\pi}, \tag{8}$$

where D_{σ} is the meson propagator. As it was noticed above, the meson propagator in the NJL model has the form (5), but in the $1/N_c$ consideration at $T = 0$ it is reasonable to consider the meson propagator in the pole approximation:

$$D_M(x) = \frac{g_{Mqq}^2}{M_M^2 - x - i\Gamma_M M_M}, \tag{9}$$

where M_M is the meson mass, g_{Mqq} is the meson-quark coupling constant and Γ_M is the meson width.



d) e) f)

Figure 3. The meson-exchange diagrams for $\pi\pi$ scattering

The $\sigma \to \pi\pi$ triangle amplitude is written as:

$$i\Gamma^{\sigma\pi\pi} = -g_{\sigma\pi\pi} g_{\pi qq}^2 \mu^{2\epsilon} \int \frac{d^d k}{(2\pi)^d} \frac{\mathrm{Tr}\{\Gamma_1(\hat{q_1} + m)\Gamma_2(\hat{q_2} + m)\Gamma_3(\hat{q_3} + m)\}}{[{q_1}^2 - m^2][{q_2}^2 - m^2][{q_3}^2 - m^2]}, \tag{10}$$

where vertex factors Γ_i are $\Gamma_i = \Gamma_{\pi} = i\gamma_5 g_{\pi qq}$ for pion and $\Gamma_i = \Gamma_{\sigma} = \mathbf{1} g_{\sigma qq}$ — for σ-meson, the momenta q_i depend on the diagram.

In[14]:=
triags = LoopIntegrate[Spur[γ.k + m_1, γ_5, γ.(k - p_2) + m_1, **1**, γ.(k + p_1) + m_1, γ_5],k, k, m, (k - p_2), m, k + p_1, m];
triagu = LoopIntegrate[Spur[γ.k + m_1, γ_5, γ.(k - p_3) + m_1, **1**, γ.(k - p_1) + m_1, γ_5], k, k, m, (k - p_3), m, k - p_1, m];
triagt = LoopIntegrate[Spur[γ.k + m_1, γ_5 γ.(k - p_4) + m_1, **1**, γ.(k - p_1) + m_1, γ_5], k, k, m, (k - p_4), m, k - p_1, m];
In[17]:=
sTriagInt = LoopRefine[triags /. onShell]
uTriaglInt = LoopRefine[triagt /. onShell];
tTriagInt = LoopRefine[triagu /. onShell];
Out[17]:=
-8m - 4m DiscB[s, m, m] - 4m $\left(\frac{1}{\epsilon} + \mathrm{Log}\left[\frac{2}{\mathrm{m}^2}\right]\right)$ + 2m (2 M^2 - s) ScalarC0[M^2, M^2, s, m, m, m]

Combining the result for triangle diagrams and the propagator (9) according to equation (8), the final result for the meson-exchange diagram can be obtained. The real and imaginary parts of the amplitudes as a function s are shown in Figure 4 for the case $t = 0$. It is clearly seen in Figures 2, 4 that all results at $t = 0$ have the threshold at $s \sim M_\sigma$.

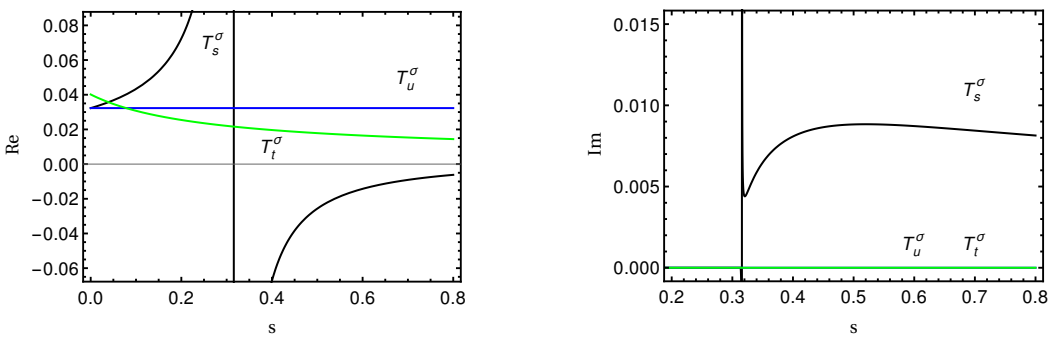


Figure 4. The real (left panel) and imaginary (right panel) parts of the sigma-exchange $\pi\pi$ scattering amplitudes for the case $t = 0$

3. The scattering lengths and the cross section

The invariant scattering amplitude in common view has the form [14]:

$$\langle cp_c; dp_d|\mathcal{T}|ap_a; bp_b\rangle = \\ = \delta_{ab}\delta_{cd}A(s,t,u) + \delta_{ac}\delta_{bd}B(s,t,u) + \delta_{ad}\delta_{bc}C(s,t,u), \quad (11)$$

where s, t, u are the Mandelstam variables and $s + t + u = 4M_\pi^2$ for the $\pi\pi$-scattering. The amplitude of definite total isospin I ($I = 0, 1, 2$) defined by A_I , can be projected out from equation (11):

$$A_0 = 3A + B + C, \quad A_1 = B - C, \quad A_2 = B + C. \quad (12)$$

The functions $A(s,t,u)$, $B(s,t,u)$, $C(s,t,u)$ are combined taking into account the isospin factors in the amplitudes in equations (7) (see Table 2).

Some practical results can be obtained after combining the functions $A(s,t,u)$, $B(s,t,u)$, $C(s,t,u)$ and restoring factors $(g^4_{\pi qq})$ in integrals $\mathcal{T}^{box}_{s,t,u}, \mathcal{T}^{\sigma}_{s,t,u}$. When the scattering is at the kinematic threshold, the scattering lengths can be obtained as $a_i = \frac{1}{32\pi}A_i$. At the conditions $s = 4M_\pi^2, u = t = 0$, the length $a_1 = 0$ as the a_1 has the meaning of the scattering "volume" [15].

In this work the parameters from the equations (6) were used with $M_\pi = 0.14$, $M_\sigma = 0.562$, $m = 0.28$, $g_{\pi qq} = 3.66$, $g_{\sigma qq} = 2.66$. For these parameters the values $a_0 = 0.147$ $a_2 = -0.0475$ were obtained.

As the general kinematics was used to write the amplitude $\mathcal{T}$, the total cross section can be evaluated. According to the charge and isospin conservation law, the following reaction for $\pi\pi$-scattering can exist: $\pi^0\pi^0 \to \pi^0\pi^0$,$\pi^0\pi^0 \to \pi^+\pi^-$,

$\pi^{\pm}\pi^{\pm} \to \pi^{\pm}\pi^{\pm}$, $\pi^{+}\pi^{-} \to \pi^{+}\pi^{-}$. In this work for analysis the reaction $\pi^{+}\pi^{-} \to \pi^{+}\pi^{-}$ was chosen as the most complete set of experimental data can be found for this reaction. The total amplitude for this case with taking into account the Clebsch–Gordan coefficients and isospin amplitudes is:

$$\mathcal{T}^{\pi^{+}\pi^{-}\to\pi^{+}\pi^{-}} = \frac{1}{6}A_2 + \frac{1}{2}A_1 + \frac{1}{3}A_0. \tag{13}$$

Table 2

The isospin factors

Diagram	Isospin factor
$\mathcal{T}_s^{box}$	$2(\delta^{ab}\delta^{cd} + \delta^{ac}\delta^{bd} - \delta^{ad}\delta^{cb})$
$\mathcal{T}_t^{box}$	$2(\delta^{ab}\delta^{cd} - \delta^{ac}\delta^{bd} + \delta^{ad}\delta^{cb})$
$\mathcal{T}_u^{box}$	$2(-\delta^{ab}\delta^{cd} + \delta^{ac}\delta^{bd} + \delta^{ad}\delta^{cb})$
$\mathcal{T}_s^{\sigma}$	$4\delta^{ab}\delta^{cd}$
$\mathcal{T}_t^{\sigma}$	$4\delta^{ac}\delta^{bd}$
$\mathcal{T}_u^{\sigma}$	$4\delta^{ad}\delta^{cb}$

In Figure 5 (left panel) the real, imaginary parts and the absolute value of the scattering amplitude are shown for the case $t = 0$.

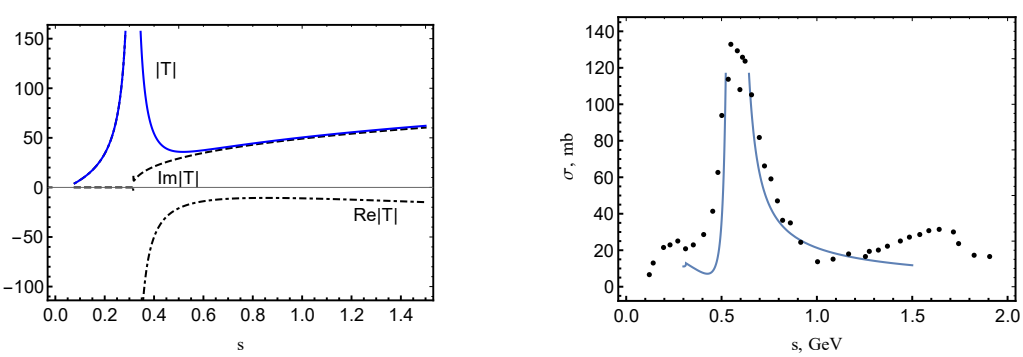


Figure 5. Left panel: the real, imaginary parts and absolute value for the scattering amplitude for the reaction $\pi^{+}\pi^{-} \to \pi^{+}\pi^{-}$ at $t = 0$. Right panel: total cross section

The total cross section in the center of mass of the system is defined using the standard expression:

$$\sigma_{\text{el}} = \frac{1}{16\pi\lambda(s, m^2)} \int_{t-}^{t^{+}} dt \; |\mathcal{T}^{\pi^{+}\pi^{-}\to\pi^{+}\pi^{-}}|^2, \tag{14}$$

where $\lambda(s, M_\pi^2) = (s - 4M_\pi^2)s$, $t^+ = 0$ and $t^- = 4M_\pi^2 - s$. It is clearly seen, that in the center of mass of the system there exists the kinematic threshold for the reaction: $s > 4M_\pi^2$.

In literature there is a wide range for the σ-meson mass and its width $M_\sigma(400 \div 1000)$, $\Gamma_\sigma(600 \div 1000)$ can be found. In Fig. 5 (right panel) the total cross section for the reaction $\pi^+\pi^- \to \pi^+\pi^-$ is shown with experimental data taken from [16], [17]. The result was obtained for $M_\sigma = 0.75$ GeV, $\Gamma_\sigma = 0.05$ GeV, $g_{\pi qq} = 4$.

4. Conclusion

The pions are involved in many physical processes in a wide energy range. For instance, during the heavy ion collision the pions are the final state for many hadronic decays and moreover, the pion annihilation contributes to the dilepton spectra. The electroweak pion decays ($\pi^\pm \to \mu^\pm + \nu_\mu$ or $\pi^0 \to 2\gamma$) are involved into a star cooling, etc. That is why the pion pion scattering attracts the special interest.

In this work the $\pi\pi$-scattering amplitude is calculated in the frame SU(2) NJL model based on the QCD Lagrangian. The model reproduces the most important low-energy theorems, describes the mechanism of spontaneous chiral symmetry breaking, vector dominance, mass spectra for light mesons and strong and electroweak decays of the ground meson states. When to the model the Polyakov-loop dynamics is added, which as a classical field couples to quarks, the model describes the confinement properties [18]. The main advantage of the NJL-like models is the possibility to include the temperature as a parameter using the Matsubara mechanism, that makes the model applicable to the description of matter under critical condition.

Nevertheless, the calculation of the pion-pion scattering amplitude within the framework of this model meets difficulties when the general kinematics and finite temperature are used (see [1], [2], [12]). Nowadays the finite temperature amplitude was obtained in the kinematic limit $s = 4M_\pi^2, u = t = 0$. This limit leads to the correct values of the scattering lengths a_0, a_1, a_2, but does not allows to calculate the total cross section, lifetime or width of the pion. Other models, for example, sigma-model gives the simple expression for the scattering amplitude [19], but does not take into account the quark structure of mesons.

In this work the pion-pion scattering amplitude was obtained in the frame of the NJL model at $T = 0$ using the dimensional regularization of the integrals, which is used in *Package*-X [9]. To make a simple check of the program, the scattering lengths a_0 and a_2 were obtained. At zero temperature, the results are $a_0 = 0.147$, $a_2 = -0.0475$, which are consistent with the Weinberg values $a_0^W = 7M_\pi^2/32\pi f_\pi^2 = 0.158$, $a_1^W = M_\pi^2/24\pi f_\pi^2 = 0.03$ $a_2^W = -2M_\pi^2/32\pi f_\pi^2 = -0.045$ [20] and other NJL results [2], [12]. At the threshold $s = 4M_\pi^2, u = t = 0$ the length $a_1 = 0$, as it plays the role of a volume of the reaction. Besides that, the most important contribution to a_1 is made by the diagrams with ρ-meson, which is not included in the model with Lagrangian (1).

The total cross section for the reaction $\pi^+\pi^- \to \pi^+\pi^-$ is shown in Figure 5 with experimental data from [16], [17]. The difference in experimental and model results is due to the fact that the simplest model with pseudo-scalar and scalar meson was used. The scattering amplitude involved only "box"- and σ- exchange diagrams, skipping more high-mass mesons. At the same time for model the $M_\sigma \sim 0.7$ GeV was used instead of 0.4-0.55 GeV according to PDG. It is obviously that including the vector ρ-meson with the mass ~ 0.77 GeV would lead to the shift of the maximum to the correct point with $s \sim 0.7$ GeV. The axial-vector a_1-meson with higher mass is a reason for the second maximum at $s > 1.5$ GeV. To take into account ρ-meson and other heavy mesons, the Lagrangian (1) should be changed and the set of equations (6) should be self-consistently extended for additional mesons.

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References

[1] S. P. Klevansky, "The Nambu—Jona-Lasinio model of quantum chromodynamics," *Reviews of Modern Physics*, vol. 64, pp. 649–708, 3 Jul. 1992. DOI: 10.1103/RevModPhys.64.649.

[2] Wei-jie Fu and Yu-xin Liu, "Mesonic excitations and pi–pi scattering lengths at finite temperature in the two-flavor Polyakov–Nambu–Jona-Lasinio model," 2009. arXiv: 0904.2914 [hep-ph].

[3] V. Jos. (1989). "FORM (symbolic manipulation system)," [Online]. Available: https://www.nikhef.nl/~form/.

[4] P. Kasper. (2020). "Cadabra," [Online]. Available: https://cadabra.science/.

[5] R. Mertig, M. Bohm, and A. Denner, "FEYN CALC: Computer algebraic calculation of Feynman amplitudes," *Computer Physics Communications*, vol. 64, pp. 345–359, 1991. DOI: 10.1016/0010-4655(91)90130-D.

[6] T. Hahn and M. Perez-Victoria, "Automatized one loop calculations in four-dimensions and D-dimensions," *Computer Physics Communications*, vol. 118, pp. 153–165, 1999. DOI: 10.1016/S0010-4655(98)00173-8. arXiv: hep-ph/9807565.

[7] T. Binoth, J.-P. Guillet, G. Heinrich, E. Pilon, and T. Reiter, "Golem95: A Numerical program to calculate one-loop tensor integrals with up to six external legs," *Computer Physics Communications*, vol. 180, pp. 2317–2330, 2009. DOI: 10.1016/j.cpc.2009.06.024. arXiv: 0810.0992 [hep-ph].

[8] G. Passarino and M. Veltman, "One-loop corrections for e^+e^- annihilation into $\mu^+\mu^-$ in the Weinberg model," *Nuclear Physics B*, vol. 160, no. 1, pp. 151–207, 1979. DOI: 10.1016/0550-3213(79)90234-7.

[9] H. H. Patel, "Package-X: A Mathematica package for the analytic calculation of one-loop integrals," *Computer Physics Communications*, vol. 197, pp. 276–290, Dec. 2015. DOI: 10.1016/j.cpc.2015.08.017.

[10] D. Ebert, Y. L. Kalinovsky, L. Munchow, and M. K. Volkov, "Mesons and diquarks in a NJL model at finite temperature and chemical potential," *International Journal of Modern Physics A*, vol. 8, pp. 1295–1312, 1993. DOI: 10.1142/S0217751X93000539.

[11] M. L. Goldberger and S. B. Treiman, "Decay of the pi meson," *Physical Review*, vol. 110, pp. 1178–1184, 1958. DOI: 10.1103/PhysRev.110.1178.

[12] E.Quack, P. Zhuang, Y. L. Kalinovsky, S. P. Klevansky, and J.Hufner, "$\pi\pi$ scattering lengths at finite temperature," *Physics Letters B*, vol. 348, pp. 1–6, 1995.

[13] S. Narison, "Techniques of dimensional regularization and the two-point functions of QCD and QED," *Physics Reports*, vol. 84, no. 4, pp. 263–399, 1982. DOI: 10.1016/0370-1573(82)90023-0.

[14] J. D. Bjorken and S. D. Drell, *Relativistic quantum mechanics*, ser. International series in pure and applied physics. New York, NY: McGraw-Hill, 1964.

[15] H. J. Schulze, "Pion pion scattering lengths in the SU(2) Nambu-Jona-Lasinio model," *Journal of Physics G*, vol. 21, pp. 185–191, 1995. DOI: 10.1088/0954-3899/21/2/006.

[16] V. Srinivasan *et al.*, "$\pi^-\pi^+ \to \pi^-\pi^+$ interactions below 0.7 GeV from $\pi^- p \to \pi^-\pi^+ n$ data at 5 GeV/c," *Physical Review D*, vol. 12, pp. 681–692, 3 Aug. 1975. DOI: 10.1103/PhysRevD.12.681.

[17] S. D. Protopopescu, M. Alston-Garnjost, A. Barbaro-Galtieri, S. M. Flatté, J. H. Friedman, T. A. Lasinski, G. R. Lynch, M. S. Rabin, and F. T. Solmitz, "$\pi\pi$ Partial-Wave Analysis from Reactions $\pi^+ p \to \pi^+\pi^-\Delta^{++}$ and $\pi^+ p \to K^+K^-\Delta^{++}$ at 7.1 GeV/c," *PPhysical Review D*, vol. 7, pp. 1279–1309, 5 Mar. 1973. DOI: 10.1103/PhysRevD.7.1279.

[18] Y. L. Kalinovsky, V. D. Toneev, and A. V. Friesen, "Phase diagram of baryon matter in the SU(2) Nambu – Jona-Lasinio model with a Polyakov loop," *Physics-Uspekhi*, vol. 59, no. 4, pp. 367–382, 2016. DOI: 10.3367/UFNe.0186.201604b.0387.

[19] S. R. Cotanch and P. Maris, "QCD based quark description of pi pi scattering up to the sigma and rho region," *Physical Review D*, vol. 66, p. 116 010, 2002. DOI: 10.1103/PhysRevD.66.116010. arXiv: hep-ph/0210151.

[20] V. Bernard, U. G. Meissner, A. Blin, and B. Hiller, "Four point functions in quark flavor dynamics: Meson meson scattering," *Physics Letters B*, vol. 253, pp. 443–450, 1991. DOI: 10.1016/0370-2693(91)91749-L.

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Применение средств компьютерной алгебры к вычислению амплитуды $\pi\pi$-рассеяния

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Целью данной работы является разработка программ для расчёта амплитуды рассеяния элементарных частиц, а также автоматизация таких расчётов с использованием систем компьютерной алгебры (Mathematica, Form, Cadabra). В статье рассматривается процесс рассеяния пиона на пионе в рамках эффективной КХД-мотивированной модели Намбу–Иона–Лазинио с двумя ароматами кварков. Для расчёта амплитуды рассеяния (начиная с расчёта Фейнмановских диаграмм и заканчивая вычислением Фейнмановских интегралов в однопетлевом приближении) использовался пакет *Package*-X для Mathematica. Интегралы Фейнмана в однопетлевом приближении вычислялись для случая общей кинематики. В *Package*-X в основе вычисления интегралов лежит метод Фейнмановской параметризации с последующей пространственной регуляризацией. Для проверки корректности вычислений был произведён расчёт длин рассеяния $a_0 = 0{,}147$ и $a_2 = -0{,}0475$ для случая нулевой температуры, и было построено полное сечение рассеяния как функции s. Полученные результаты сравнивались с другими моделями и экспериментальными данными.

Ключевые слова: Фейнмановские интегралы, однопетлевое приближение, полное сечение рассеяния, длины рассеяния, системы компьютерной алгебры, Package-X

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Asymptotic solution of Sturm–Liouville problem with periodic boundary conditions for relativistic finite-difference Schrödinger equation

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The quasi-potential approach is very famous in modern relativistic particles physics. This approach is based on the so-called covariant single-time formulation of quantum field theory in which the dynamics of fields and particles is described on a space-like three-dimensional hypersurface in the Minkowski space. Special attention in this approach is paid to methods for constructing various quasi-potentials. The quasi-potentials allow to describe the characteristics of relativistic particles interactions in quark models such as amplitudes of hadron elastic scatterings, mass spectra, widths of meson decays and cross sections of deep inelastic scatterings of leptons on hadrons.

In this paper Sturm–Liouville problems with periodic boundary conditions on a segment and a positive half-line for the $2m$-order truncated relativistic finite-difference Schrödinger equation (Logunov–Tavkhelidze–Kadyshevsky equation, LTKT-equation) with a small parameter are considered. A method for constructing of asymptotic eigenfunctions and eigenvalues in the form of asymptotic series for singularly perturbed Sturm–Liouville problems with periodic boundary conditions is proposed. It is assumed that eigenfunctions have regular and boundary-layer components. This method is a generalization of asymptotic methods that were proposed in the works of A. N. Tikhonov, A. B. Vasilyeva, and V. F Butuzov. We present proof of theorems that can be used to evaluate the asymptotic convergence for singularly perturbed problems solutions to solutions of degenerate problems when $\varepsilon \to 0$ and the asymptotic convergence of truncation equation solutions in the case $m \to \infty$. In addition, the Sturm–Liouville problem on the positive half-line with a periodic boundary conditions for the quantum harmonic oscillator is considered. Eigenfunctions and eigenvalues are constructed for this problem as asymptotic solutions for 4-order LTKT-equation.

Key words and phrases: asymptotic analysis, singularly perturbed differential equation, Sturm–Liouville problem, relativistic finite-difference Schrödinger equation, periodic boundary conditions, quasi-potential approach

1. Introduction

The relativistic finite-difference analog of the Schrödinger equation (Logunov–Tavkhelidze–Kadyshevsky equation, LTK-equation) with the quasi-potential in the relativistic configurational space for the radial wave functions of bound states for two identical elementary particles without spin has the form [1]–[13]:

$$\left[H_0^{\mathrm{rad}} + V(r) - 2c\sqrt{q^2 + m^2c^2}\right]\psi(r,l) = 0, \tag{1}$$

$$H_0^{\mathrm{rad}} = 2mc^2 \operatorname{ch}\left(\frac{i\hbar}{mc}D\right) + \frac{\hbar^2 l(l+1)}{mr(r+\frac{i\hbar}{mc})} \exp\left(\frac{i\hbar}{mc}D\right),$$

where m is a mass, q is a momentum, l is an angular momentum of each elementary particle and $V(r)$ is a quasi-potential (a piecewise continuous function).

Asymptotic solutions in the form of regular and boundary layer parts of boundary value problems for LTK-equation with the quasi-potential on a segment and on a positive half-line were constructed in the works [14]–[16], and the question of the asymptotic behavior of the solutions was investigated when a small parameter $\varepsilon \to 0$. Also in these works the truncation method was applied to LTK-equation. Thus, LTK-equation of infinite order was reduced to the equation of finite $2m$-order. Boundary value problems on a segment and on a positive half-line were formulated for this "truncated" equation (Logunov–Tavkhelidze–Kadyshevsky truncated equation, LTKT-equation). Eigenfunctions and eigenvalues in the form of asymptotic series were constructed for these problems and the solution behavior was studied when the order of LTKT-equation tends to infinity $2m \to \infty$.

In the paper [17] mass spectra and probabilities of radiative decays of heavy quarkonia were obtained in the framework of the constituent quark model of hadrons based on the relativistic Logunov–Tavkhelidze–Kadyshevsky equation.

Researchers pay a lot of attention to the description of quantum systems that consist of one-dimensional linear chains of n identical harmonic oscillators with a nearest neighbor interaction. Periodic boundary conditions, where the n-th oscillator is coupled back to the first oscillator, and fixed wall boundary conditions, where the first oscillator and the n-th oscillator are coupled to a fixed wall, was considered in the paper [18], [19].

In this paper Sturm–Liouville problems with periodic boundary conditions on a segment and a positive half-line are formulated for the truncated to order $2m$ relativistic finite-difference Schrödinger equation (Logunov–Tavkhelidze–Kadyshevsky equation, LTKT-equation) with a small parameter.

For these singularly perturbed problems a method is proposed for constructing eigenfunctions and eigenvalues in the form of asymptotic series. This method allows to obtain asymptotic solutions in the form of regular and boundary-layer parts. It is also possible to investigate the question of asymptotic solutions behavior when $\varepsilon \to 0$ and $2m \to \infty$. The Sturm–Liouville problem for 4-order LTKT-equation on a positive half-line with periodic

boundary conditions is formulated for the quantum harmonic oscillator quasi-potential and eigenfunctions and eigenvalues in the form of asymptotic series are constructed.

2. The Sturm–Liouville problems for the LTKT-equation

We consider the quasi-potential equation [3]–[5] in a relativistic configuration space for the radial wave functions of bounded states for two identical elementary particles

$$[H_0^{\rm rad} + V(r) - 2c\sqrt{q^2 + m^2c^2}]\psi(r,l) = 0, \tag{2}$$

$$H_0^{\rm rad} = 2mc^2\ {\rm ch}\left(\frac{i\hbar}{mc}D\right) + \frac{\hbar^2 l(l+1)}{mr(r+\frac{i\hbar}{mc})}\ \exp\left(\frac{i\hbar}{mc}D\right) =$$

$$= \sum_{p=0}^{\infty}\frac{(-1)^p 2mc^2}{(2p)!!}\left(\frac{\hbar}{mc}\right)^{2p}D^{2p} + \frac{\hbar^2 l(l+1)}{mr(r+\frac{i\hbar}{mc})}\sum_{p=0}^{\infty}\frac{1}{p!}\left(\frac{i\hbar}{mc}\right)^{p}D^p,$$

$$D^p = \frac{d^p}{dr^p},$$

where m is a mass, q is a momentum, l is a moment of elementary particles and $V(r)$ is a quasi-potential.

We can limit the speed of light to the infinity ($c \to \infty$) formally. In this case, the equation (1) becomes the non-relativistic Schrödinger equation [20]

$$\left[-\hbar^2 D^2 + \hbar^2 l(l+1)/r^2 + mV(r) - q^2\right]\psi(r) = 0. \tag{3}$$

Let physical parameter be $\hbar = 1$, $m = 1$, $\varepsilon = \frac{1}{c}$ and $l = 0$ (case of S-wave) in (1) where

$$\lambda_{\varepsilon,\infty} = 2q^2/\sqrt{1+\varepsilon^2 q^2} + 1, v = V(r), \quad q^2 = (1 + 0.25\varepsilon^2\lambda_{\varepsilon,\infty})\lambda_{\varepsilon,\infty}.$$

We can rewrite the equation (1) in the form as under

$$[\widetilde{L}_\infty^\varepsilon - \lambda_{\varepsilon,\infty}]\psi_{\varepsilon,\infty}(r) = 0, \tag{4}$$

$$\widetilde{L}_\infty^\varepsilon = L_2 + \varepsilon^2$$

$$L_\infty^\varepsilon = \sum_{p=1}^{\infty}\varepsilon^{2p-2}L_{2p} + v(r), \quad L_{2p} = \frac{2(-1)^p}{(2p)!!}D^{2p}, \quad \varepsilon \in (0,1],$$

$$L_2 = L_2 + v(r) = -D^2 + v(r),$$

$$L_\infty^\varepsilon = \sum_{p=1}^{\infty}\varepsilon^{2p-2}L_{2p+2} = \sum_{p=1}^{\infty}\frac{2(-1)^{p+1}}{(2p+2)!!}\varepsilon^{2p-2}D^{2p+2}.$$

The equation (1) is an infinite order differential equation with a small parameter ($\varepsilon \ll 1$) at higher derivatives and we can classify it as singularly perturbed equations.

We can truncate the equation (4) to a finite equation of $2m$-order with $m > 1$ and it can be rewritten as follows

$$[\widetilde{L}^{\varepsilon}_{2m} - \lambda_{\varepsilon,2m}]\psi_{\varepsilon,2m}(r) = 0,$$

$$\widetilde{L}^{\varepsilon}_{2m} = L_2 + \varepsilon^2 L^{\varepsilon}_{2m} = \sum_{p=1}^{m} \varepsilon^{2p-2} L_{2p} + v(r),$$

$$L^{\varepsilon}_{2m} = \sum_{p=1}^{m-1} \varepsilon^{2p-2} L_{2p+2} = \sum_{p=1}^{m-1} \frac{2(-1)^{p+1}}{(2p+2)!!} \varepsilon^{2p-2} D^{2p+2},$$

where L_2 is the self-adjoint 2-order elliptic operator, $\widetilde{L}^{\varepsilon}_{2m}$ is the self-adjoint $2m$-order elliptic operator, $\psi_{\varepsilon,2m}(r)$ is the solution of the $2m$-order equation.

We can formulate the boundary value problem A^{2m}_{ε} on a segment $[0, r_0]$ and the boundary value problem B^{2m}_{ε} on a positive half-line $[0, +\infty)$ for defining the eigenfunctions $[\psi_{\varepsilon,2m,\gamma}]^{\infty}_{\gamma=1}$ and the eigenvalues $[\lambda_{\varepsilon,2m,\gamma}]^{\infty}_{\gamma=1}$ for this differential equation as follows

$$\left[\widetilde{L}_{2m} - \lambda_{\varepsilon,2m}\right] \psi_{\varepsilon,2m}(r) = 0, \tag{5}$$

where

$$D^i \psi_{\varepsilon,2m}(0) = D^i \psi_{\varepsilon,2m}(r_0), \quad i = 0, 1, \ldots, 2m-1, \tag{6}$$

are the periodic boundary conditions of the problem A^{2m}_{ε}, and

$$D^i \psi_{\varepsilon,2m}(0) = D^i \psi_{\varepsilon,2m}(+\infty), \quad i = 0, 1, \ldots, 2m-1, \tag{7}$$

are the periodic boundary conditions of the problem B^{2m}_{ε}.

If we assume $\varepsilon = 0$, we can get the degenerate problems A_0 and B_0 for defining the eigenfunctions $[\psi_{0,\gamma}]^{\infty}_{\gamma=1}$ and the eigenvalues $[\lambda_{0,\gamma}]^{\infty}_{\gamma=1}$ of following type as under

$$[L_2 - \lambda_0]\psi_0(r) = 0, \tag{8}$$

where

$$D^i \psi_0(0) = D^i \psi_0(r_0), \quad i = 0, 1, \tag{9}$$

is the periodic boundary conditions of the problem A_0, and

$$D^i \psi_0(0) = D^i \psi_0(+\infty), \quad i = 0, 1, \tag{10}$$

is the periodic boundary conditions of the problem B_0.

We can consider the question of the behavior of the eigenfunctions $[\psi_{\varepsilon,2m,\gamma}]^{\infty}_{\gamma=1}$ and the eigenvalues $[\lambda_{\varepsilon,2m,\gamma}]^{\infty}_{\gamma=1}$ of the problems A^{2m}_{ε} and B^{2m}_{ε} in the case when a small parameter tends to zero ($\varepsilon \to 0$) but fixed order $2m$ of the operator $\widetilde{L}_{2m}$, and in the case when the order m is increased but a small parameter ε is fixed.

The eigenfunctions $[\psi_{\varepsilon,2m,\gamma}]_{\gamma=1}^{\infty}$ and $[\psi_{0,\gamma}]_{\gamma=1}^{\infty}$ are the solutions of the corresponding problems A_ε^{2m}, A_0 and B_ε^{2m}, B_0. These solutions are elements of a Hilbert space $H(\Omega_\Gamma)$ with an inner product $(\psi,\varphi)_{H(\Omega_\Gamma)} = \int_{\Omega_\Gamma} \psi(r)\,\varphi(r)\,dr$ $(\psi,\varphi \in H(\Omega_\Gamma))$, in which there is a set of a linear continuous self-adjoint operators $A(\Omega_\Gamma) : H(\Omega_\Gamma) \to H(\Omega_\Gamma)$ of problems A_ε^{2m}, B_ε^{2m}, A_0, B_0 ($\widetilde{L}_{2m}^{\varepsilon}, L_2 \in A$, $m > 2$), where Ω_Γ $(\Gamma = A, B)$ is a domain of the operator (a subscript A corresponds to a segment $[0, r_0]$ and a subscript B is a positive half-line $[0, +\infty)$).

Let $\|A(\Omega_\Gamma)\|_H$ denotes the norm of operators $A(\Omega_\Gamma)$ and we can write

$$\|A(\Omega_\Gamma)\|_H = \sup_{\psi\in H,\psi\neq 0} \frac{\|A\psi\|_H}{\|\psi\|_H}, \quad \|\psi\|_H = (\psi,\psi)_H^{1/2}.$$

We can give the sufficient conditions for the solvability of the problems A_0, B_0 and A_ε^{2m}, B_ε^{2m}.

Condition 1. *The operator L_2 for the periodic boundary conditions of the problems A_0 or B_0 must be positively defined, i.e.*

$$(L_2(\psi_0),\psi_0)_{H(\Omega_\Gamma)} = \int_{\Omega_\Gamma} L_2(\psi_0)\psi_0\,dr = \int_{\Omega_\Gamma} |D\psi_0|^2\,dr + \int_{\Omega_\Gamma} v(r)\psi_0^2\,dr \geqslant 0,$$

for any functions $v(r) \in C^\infty(\Gamma)$ and $\psi_0 \in H(\Omega_\Gamma)$ from domain Ω_Γ, and it must satisfy the boundary conditions of the corresponding degenerate problems (A_0 or B_0).

Condition 2. *The operator L_{2m}^{ε} under boundary conditions of problems A_ε^{2m} or B_ε^{2m} must be positive, i.e.*

$$\begin{aligned}(L_{2m}^{\varepsilon}\psi_{\varepsilon,2m},\psi_{\varepsilon,2m})_{H(\Omega_\Gamma)} &= \sum_{p=1}^{m-1} \frac{2(-1)^{p+1}}{(2p+2)!!}\varepsilon^{2p-2} \int_{\Omega_\Gamma} (D^{2p+2}\psi_{\varepsilon,2m})\,\psi_{\varepsilon,2m}\,dr = \\ &= \sum_{p=1}^{m-1} \frac{2}{(2p+2)!!}\varepsilon^{2p-2} \int_{\Omega_\Gamma} |D^{p+1}\psi_{\varepsilon,2m}|^2 dr \geqslant 0,\end{aligned}$$

for any functions $\psi_{\varepsilon,2m} \in H(\Omega_\Gamma)$ from domain Ω_Γ, and it must satisfy the boundary conditions of the corresponding singularly perturbed problem (A_ε^{2m} or B_ε^{2m}).

It is known that the degeneration of the problems $A_\varepsilon^{2m}, B_\varepsilon^{2m}$ into the problems A_0, B_0 are *regular* if the number of roots with negative real parts and positive real parts *of an additional characteristic equation*, which in our case has the form

$$P(\alpha^{2m}) = \sum_{p=1}^{m} \frac{(-1)^p}{(2p)!!}(\alpha^{2m})^{2p-2} = 0,$$

coincide with the number of boundary conditions that drop down on the left and, respectively, on the right when we replace the consideration problems A_ε^{2m}, B_ε^{2m} to problems A_0, B_0.

Let's now consider the generalized characteristic form of the operator $\sum\limits_{p=1}^{m} \varepsilon^{2p-2} L_{2p}$, which is obtained by replacing D^{2p} with $(i\xi)^{2p}$

$$\pi_\varepsilon(\xi) = \sum_{p=1}^{m} \frac{2(-1)^p}{(2p)!!} \varepsilon^{2p-2} (i\xi)^{2p}.$$

The regular degeneration of the problems A_ε^{2m}, B_ε^{2m} to A_0, B_0 is fulfilled if the following condition is true.

Condition 3. *If the following inequality take place for the real part of the sum* $\pi_\varepsilon(\xi)$

$$\mathbf{Re}\,(\pi_\varepsilon(\xi)) = \sum_{p=1}^{m} \frac{2}{(2p)!!} \varepsilon^{2p-2} \xi^{2p} \geqslant C \sum_{p=1}^{m} \varepsilon^{2p-2} |\xi|^{2p} \geqslant 0,$$

where C *is not depended on* ξ*, then problems* A_ε^{2m} *and* B_ε^{2m} *degenerate into problems* A_0 *and* B_0 *regularly.*

Let's assume that a set of eigenvalues $\lambda_{\varepsilon,2m,1} \leqslant \lambda_{\varepsilon,2m,2} \leqslant ... \leqslant \lambda_{\varepsilon,2m,n} \leqslant ...$ and $\lambda_{0,1} \leqslant \lambda_{0,2} \leqslant ... \leqslant \lambda_{0,n} \leqslant ...$ is ordered in ascending order $[\lambda_{\varepsilon,2m,\gamma}]_{\gamma=1}^{\infty}$, $[\lambda_{0,\gamma}]_{i=1}^{\infty}$, and this set of eigenvalues corresponds to a complete orthonormal set of eigenfunctions $[\psi_{\varepsilon,2m,\gamma}]_{\gamma=1}^{\infty}$, $[\psi_{0,\gamma}]_{\gamma=1}^{\infty}$.

Since existence domains Ω_A of operators $\widetilde{L}_{2m}$ and L_2 coincide for the problems A_ε^{2m} and A_0 and also for any function $\psi_{\varepsilon,2m} \in \Omega_A$, that satisfies the boundary conditions of the problem A_ε^{2m}, the following inequality from *Condition 2*

$$(L_{2m}^{\varepsilon} \psi_{\varepsilon,2m}, \psi_{\varepsilon,2m})_{H(\Omega_A)} \geqslant (L_2 \psi_{\varepsilon,2m}, \psi_{\varepsilon,2m})_{H(\Omega_A)},$$

holds true, then the following estimate inequality occurs $\lambda_{\varepsilon,2m,\gamma} \geqslant \lambda_{0,\gamma}$, $\gamma = 1, 2, ...$

A similar estimate takes place for the problems B_ε^{2m} and B_0.

3. Constructing of asymptotic solutions for boundary value problems

3.1. General scheme for constructing of the asymptotics. Regular and boundary series

We can use methods of the singular perturbations theory of differential equations and find solutions to problems A_ε^{2m} and B_ε^{2m}.

Let's search for a formal solution $\psi_{\varepsilon,2m}(r)$ of the problems A_ε^{2m} and B_ε^{2m} in the form of asymptotic series

$$\Theta\psi_{\varepsilon,2m}(r) = \bar{\psi}_{2m}(r,\varepsilon) + \Pi_{2m}\psi(\rho_1,\varepsilon) + Q_{2m}\psi(\rho_2,\varepsilon) = \\ = \sum_{k=0}^{\infty} \varepsilon^k(\bar{\psi}_{2m,k}(r) + \Pi_{2m,k}\psi(\rho_1) + Q_{2m,k}\psi(\rho_2)), \quad (11)$$

where a partial sum

$$\Theta_j\psi_{\varepsilon,2m}(r) = \sum_{k=0}^{j} \varepsilon^k(\bar{\psi}_{2m,k}(r) + \Pi_{2m,k}\psi(\rho_1) + Q_{2m,k}\psi(\rho_2)),$$

satisfies inequalities for solutions of the problem A_ε^{2m}

$$\max_{r\in[\delta_A, r_0-\delta_A]} |\psi_{\varepsilon,2m} - \Theta_j\psi_{\varepsilon,2m}| < M_A\,\varepsilon^{j+1},$$

and the problem B_ε^{2m}

$$\max_{r\in[\delta_B, \infty+)} |\psi_{\varepsilon,2m} - \Theta_j\psi_{\varepsilon,2m}| < M_B\,\varepsilon^{j+1},$$

and similar inequalities for the boundary conditions of these problems, where M_A, M_B and $\delta_A \ll 1$, $\delta_B \ll 1$ are positive constants that are independent of r and ε.

The asymptotic solution for $\psi_{\varepsilon,2m}$ have the form as under

$$\psi_{\varepsilon,2m}(r) = \sum_{k=0}^{j} \varepsilon^k(\bar{\psi}_{2m,k}(r) + \Pi_{2m,k}\psi(\rho_1) + Q_{2m,k}\psi(\rho_2)) + \bar{z}_j^{2m}(r),$$

$$\bar{z}_j^{2m}(r) = \psi_{\varepsilon,2m} - \Theta_j\psi_{\varepsilon,2m},$$

where $\bar{z}_j^{2m}(r) = \varepsilon^{j+1}z_j^{2m}(r)$ is error of the asymptotic approximation of the solution $\psi_{\varepsilon,2m}$ by a partial sum $\Theta_j\psi_{\varepsilon,2m}$.

We can write the regular part of the asymptotic expansion in the form

$$\bar{\psi}_{2m}(r,\varepsilon) \equiv \bar{\psi}_{2m,0}(r) + \varepsilon\bar{\psi}_{2m,1}(r) + \varepsilon^2\bar{\psi}_{2m,2}(r) + \dots,$$

and the singular parts of the asymptotic expansion have the forms as under

$$\Pi_{2m}\psi(\rho_1,\varepsilon) \equiv \Pi_{2m,0}\psi(\rho_1) + \varepsilon\Pi_{2m,1}\psi(\rho_1) + \varepsilon^2\Pi_{2m,2}\psi(\rho_1) + \dots,$$

for describing the behavior of the solution on the left edge of a segment $[0, r_0]$ or a positive half-line $[0, +\infty)$,

$$Q_{2m}\psi(\rho_2,\varepsilon) \equiv Q_{2m,0}\psi(\rho_2) + \varepsilon Q_{2m,1}\psi(\rho_2) + \varepsilon^2 Q_{2m,2}\psi(\rho_2) + \dots,$$

for describing the behavior of the solution of the problem A_ε^{2m} on the right edge of a segment $[0, r_0]$.

It is known that the function $Q_{2m}\psi(\rho_2,\varepsilon) = 0$ for the problem B_ε^{2m}, since the solution of the problem B_0 is chosen so that it tends to zero when $r \to +\infty$ together with all its derivatives. Here we use new independent (stretched)

variables $\rho_1 = r/\varepsilon$ and $\rho_2 = (r_0 - r)/\varepsilon$ for the boundary functions $\Pi_{2m,k}\psi$, $Q_{2m,k}\psi$.

Similarly, we can present the simple eigenvalue of $\lambda_{\varepsilon,2m}$ in the form of the asymptotic series in powers of the small parameter ε in the form as under

$$\lambda_{\varepsilon,2m} \equiv \lambda_{2m,0} + \varepsilon\lambda_{2m,1} + \varepsilon^2\lambda_{2m,2} + \dots, \tag{12}$$

where the partial sum

$$\Theta_j\lambda_{\varepsilon,2m} = \sum_{k=0}^{j} \varepsilon^k \lambda_{2m,k},$$

satisfies the condition $|\lambda_{\varepsilon,2m} - \Theta_j\lambda_{\varepsilon,2m}| < \tilde{M}\,\varepsilon^{j+1}$, where $\tilde{M} > 0$ is a positive constant that is independent of r and ε.

So an asymptotic approximation of the eigenvalue $\lambda_{\varepsilon,2m}$ has the form as under

$$\lambda_{\varepsilon,2m} = \sum_{k=0}^{j} \varepsilon^k \lambda_{2m,k} + \bar{\Delta}_j^{2m},$$

where $\bar{\Delta}_j^{2m} = \varepsilon^{j+1}\Delta_j^{2m}$, $bar\Delta_j^{2m} = \lambda_{\varepsilon,2m} - \Theta_j\lambda_{\varepsilon,2m}$ is an error of the asymptotic approximation of the eigenvalue $\lambda_{\varepsilon,2m}$ for this partial sum.

In addition, we assume that the function $v(r)$ can be decomposed as a convergent series in the neighborhood of the points $r = 0$ and $r = r_0$

$$v(r) = \sum_{s=-1}^{\infty} v_s^1 r^s, \quad v(r) = \sum_{s=-1}^{\infty} v_s^2 (r - r_0)^s,$$

and

$$v(\rho_1) = \sum_{s=-1}^{\infty} v_s^1 \varepsilon^s \rho_1^s, \quad v(\rho_2) = \sum_{s=-1}^{\infty} (-1)^{|s|} v_s^2 \varepsilon^s \rho_2^s, \tag{13}$$

where $\rho_1 = r/\varepsilon$ and $\rho_2 = (r_0 - r)/\varepsilon$ are the stretched variables.

3.2. The main terms of the asymptotic series

We can determine the terms of the asymptotic series of the decomposition $\bar{\psi}_{2m,k}$, $\Pi_{2m,k}\psi$, $Q_{2m,k}\psi$ and $\lambda_{2m,k}$ of the problems A_ε^{2m} and B_ε^{2m} if we substitute the decomposition (11), (12) and (13) in the equation (5) and the boundary conditions (6) of the problem A_ε^{2m} and the equation (5) and the boundary conditions (7) of the problem B_ε^{2m}, and then we equate all members of the series that stand at equal powers of a small parameter ε.

We should use additional requirements for the boundary functions

$$\Pi_{2m,k}\psi(\rho_1) \to 0, \quad Q_{2m,k}\psi(\rho_2) \to 0, \quad k = 0, 1, 2, \dots,$$

where $\varepsilon \to 0$ and a fixed r. These requirements allows to select the solutions $\Pi_{2m,k}\psi$ and $Q_{2m,k}\psi$ that tend to zero outside the boundary layer only.

3.2.1. Building a zero approximation of the asymptotic expansion

We can get the systems of equations and determine the solutions $\bar{\psi}_{2m,0}$, $\Pi_{2m,0}\psi$, $Q_{2m,0}\psi$ and $\lambda_{2m,0}$ of the problems A_ε^{2m} and B_ε^{2m} in a zero approximation in the form

$$\left[L_2 - \lambda_{2m,0}\right]\bar{\psi}_{2m,0} = 0, \quad L_2 = -D^2 + v(r),$$

$$L_{2m}^1 \Pi_{2m,0}\psi = 0, \quad L_{2m}^1 = \sum_{p=1}^{m} \frac{2(-1)^p}{(2p)!!}\frac{d^{2p}}{d\rho_1^{2p}},$$

$$L_{2m}^2 Q_{2m,0}\psi = 0, \quad L_{2m}^2 = \sum_{p=1}^{m} \frac{2(-1)^p}{(2p)!!}\frac{d^{2p}}{d\rho_2^{2p}},$$

$$D^i\left(\bar{\psi}_{2m,0}(0) + \Pi_{2m,0}\psi(0)\right) = D^i\left(\bar{\psi}_{2m,0}(\bar{r}) + Q_{2m,0}\psi(\bar{r})\right),$$

$$\Pi_{2m,0}\psi(\rho_1) \to 0, \quad Q_{2m,0}\psi(\rho_2) \to 0, \quad \varepsilon \to 0, \quad i = 0, 1, 2, \dots, 2m-1,$$

where $\bar{r} = r_0$ for A_ε^{2m} and $\bar{r} \to +\infty$ for B_ε^{2m}.

The eigenfunctions $[\bar{\psi}_{2m,0,\gamma}]_{\gamma=1}^{\infty}$ and the eigenvalues $[\lambda_{2m,0,\gamma}]_{\gamma=1}^{\infty}$ coincide with the solutions of the corresponding degenerate problems A_0 or B_0.

Thus, we can determine the boundary functions $\Pi_{2m,0}\psi(\rho_1)$, $Q_{2m,0}\psi(\rho_2)$ if we find the solutions of the boundary value problems as under

$$L_{2m}^1 \Pi_{2m,0}\psi = 0, \quad L_{2m}^2 Q_{2m,0}\psi = 0,$$

$$D^i\Pi_{2m,0}\psi(0) + D^i\bar{\psi}_{2m,0}(0) = D^i Q_{2m,0}\psi(\bar{r}) + D^i\bar{\psi}_{2m,0}(\bar{r}),$$

$$\Pi_{2m,0}\psi(\rho_1) \to 0, \quad Q_{2m,0}\psi(\rho_2) \to 0, \quad \varepsilon \to 0, \quad i = 0, 1, 2, \dots, 2m-1.$$

We can write the functions $\Pi_{2m,0}\psi(\rho_1)$ and $Q_{2m,0}\psi(\rho_2)$ in the forms

$$\Pi_{2m,0}\psi(\rho_1) = \sum_{\zeta=1}^{m-1} C_{\zeta,0}^{2m,1}\, \exp\left(-\alpha_\zeta^{2m}\rho_1\right),$$

$$Q_{2m,0}\psi(\rho_2) = \sum_{\zeta=1}^{m-1} C_{\zeta,0}^{2m,2}\, \exp\left(-\alpha_\zeta^{2m}\rho_2\right).$$

Hence, the number of arbitrary constants $C_{\zeta,0}^{2m,1}$ and $C_{\zeta,0}^{2m,2}$ equals the number of disappearing boundary conditions of problems A_ε^{2m} or B_ε^{2m} when we try formulate the degenerate problems A_0 or B_0.

Let the values α_ζ^{2m} $(\zeta = 1, \dots, 2m-2)$ be the roots *of the additional characteristic equation*

$$P(\alpha^{2m}) = \sum_{p=1}^{m} \frac{(-1)^p}{(2p)!!}(\alpha^{2m})^{2p-2} = 0.$$

Since an algebraic equation

$$\mathbf{Re}\,(\alpha_\zeta^{2m}) > 0, \quad \zeta = \overline{1, m-1}, \quad \mathbf{Re}\,(\alpha_\zeta^{2m}) < 0, \quad \zeta = \overline{m, 2m-2},$$

is biquadrate; thus, it has the same number of roots with positive and negative real parts.

We can get the following relations from the boundary conditions

$$D^i \Pi_{2m,0}\psi(0) - D^i Q_{2m,0}\psi(\bar{r}) = -D^i \bar{\psi}_{2m,0}(0) + D^i \bar{\psi}_{2m,0}(\bar{r}),$$

where $i = 0, 1, 2, \dots, 2m-1$, and we can derive a system of $2m$ linear equations like that

$$\mathbf{D}^{2m}\vec{\mathbf{C}}^{2m} = \vec{\mathbf{b}}^{2m}, \tag{14}$$

for finding coefficients $C_{\zeta,0}^{2m,1}$, $C_{\zeta,0}^{2m,2}$ $(\zeta = 1, 2, \dots, m-1)$, where a system has form as under

$$\mathbf{D}^{2m} = \begin{pmatrix} \mathbf{D}_{11}^{2m} & \mathbf{0} \\ \mathbf{0} & \mathbf{D}_{22}^{2m} \end{pmatrix},$$

and where

$$\mathbf{D}_{11}^{2m} = (d_{1,r\zeta})_{r,\zeta=1}^{m-1}, \quad d_{1,r\zeta} = (-\alpha_\zeta^{2m})^{r-1},$$
$$\mathbf{D}_{22}^{2m} = (d_{2,r\zeta})_{r,\zeta=1}^{m-1}, \quad d_{2,r\zeta} = -(\alpha_\zeta^{2m})^{r-1},$$
$$\vec{\mathbf{C}}^{2m\top} = (C_{1,0}^{2m,1}, ..., C_{m-1,0}^{2m,1}, C_{1,0}^{2m,2}, ..., C_{m-1,0}^{2m,2}),$$
$$\vec{\mathbf{b}}^{2m\top} = (p_1^{2m}, \dots, p_{m-1}^{2m}, q_1^{2m}, \dots, q_{m-1}^{2m}),$$
$$p_i^{2m} = -D^i \bar{\psi}_{2m,0}(0), \quad q_i^{2m} = D^i \bar{\psi}_{2m,0}(\bar{r}), \quad i = 0, 1, \dots, 2m-1,$$

are block matrices.

Since the values of $\alpha_\zeta^{2m} (\zeta = \overline{1, 2m-2})$ are pairwise different and the matrices $\mathbf{D}_{11}^{2m}$, $\mathbf{D}_{22}^{2m}$, $\mathbf{D}^{2m}$ are non-degenerate and there is an inverse of $\mathbf{D}^{2m}$ matrix $(\mathbf{D}^{2m})^{-1}$, so then the only solution of the algebraic system (14) exists and it has the form: $\vec{\mathbf{C}}^{2m} = (\mathbf{D}^{2m})^{-1}\vec{\mathbf{b}}^{2m}$.

Thus, a zero approximation of $\bar{\psi}_{2m,0}$, $\Pi_{2m,0}\psi$, $Q_{2m,0}\psi$, $\lambda_{2m,0}$ of the problems A_ε^{2m} and B_ε^{2m} could be constructed completely.

3.2.2. Further construction of the asymptotic series

We can get the systems of the equations for the problems A_ε^{2m} and B_ε^{2m} and use the additional conditions for finding the solutions $\bar{\psi}_{2m,k}$, $\Pi_{2m,k}\psi$, $Q_{2m,k}\psi$ and $\lambda_{2m,k}$ in the case $k > 0$ in this form

$$[L_2 - \lambda_{2m,0}]\bar{\psi}_{2m,k} = \lambda_{2m,k}\bar{\psi}_{2m,0} - h_k^{2m}(r),$$

$$L_{2m}^1 \Pi_{2m,k}\psi = g_{1k}^{2m}(\rho_1), \quad L_{2m}^2 Q_{2m,k}\psi = g_{2k}^{2m}(\rho_2),$$
$$D^i(\bar{\psi}_{2m,k}(0) + \Pi_{2m,k}\psi(0)) = D^i(\bar{\psi}_{2m,k}(\bar{r}) + Q_{2m,k}\psi(\bar{r})),$$

$$\Pi_{2m,k}\psi(\rho_1)\to 0,\ \ Q_{2m,k}\psi(\rho_2)\to 0,\ \ \varepsilon\to 0,\ \ k=1,2,\dots,\ \ i=0,1,\dots,2m-1,$$

$$h_k^{2m}(r)=\sum_{p=1}^{[k/2]\leqslant 2m}\frac{2(-1)^{p+1}}{(2p+2)!!}D^{2p+2}\bar{\psi}_{2m,k-2p}-\sum_{p=1}^{k-1}\lambda_{2m,p}\bar{\psi}_{2m,k-p},$$

$$g_{1k}^{2m}(\rho_1)=-\frac{v_{-1}^1}{\rho_1}\Pi_{2m,k-1}\psi+\sum_{p=0}^{k-2}\left(\lambda_{2m,p}-v_p^1\rho_1^p\right)\Pi_{2m,k-p-2}\psi,$$

$$g_{2k}^{2m}(\rho_2)=\frac{v_{-1}^2}{\rho_2}Q_{2m,k-1}\psi+\sum_{p=0}^{k-2}\left(\lambda_{2m,p}-(-1)^p v_p^2\rho_2^p\right)Q_{2m,k-p-2}\psi.$$

If the parameter λ is a simple proper value of the self-adjoint operator A that acting in the Hilbert space $H(\Omega_\Gamma)$ and if the function $\psi\in H(\Omega_\Gamma)$ is the corresponding normalized eigenfunction $\|\psi\|_{H(\Omega_\Gamma)}=1$ then in the space $H_1(\Omega_\Gamma)$ ($H_1(\Omega_\Gamma)$ is an orthogonal complement to the function ψ in the space $H(\Omega_\Gamma)$) and then there is the operator $A-\lambda I$ that has a bounded inverse operator $(A-\lambda I)^{-1}_{H_1(\Omega_\Gamma)}$ (pseudo-resolvent).

Hence, the equation $A\varphi-\lambda\varphi=\omega\psi-h$, $h\in H(\Omega_\Gamma)$ can be solved and the solution of this equation could be presented as under

$$\omega=(h,\psi)_{H(\Omega_\Gamma)},\varphi=(A-\lambda I)^{-1}_{H_1(\Omega_\Gamma)}(\omega\psi-h),$$

where $(\omega\psi-h)\in H_1(\Omega_\Gamma)$.

Thus, we can get the solutions $\bar{\psi}_{2m,k,n}$ and $\lambda_{2m,k,n}$ for any $k>0$

$$\lambda_{2m,k,n}=\left(h_k^{2m},\psi_{0,n}\right)_{H(\Omega_\Gamma)}=\int_{\Omega_\Gamma}h_k^{2m}(r)\,\psi_{0,n}(r)dr,\quad n=1,2,\dots,$$

$$\bar{\psi}_{2m,k,n}=(L_2-\lambda_{2m,0,n})^{-1}_{H_1(\Omega_\Gamma)}h_k^{2m},$$

where $H_1(\Omega_\Gamma)$ is the orthogonal complement to eigenfunctions $\psi_{0,n}\in H(\Omega_\Gamma)$, $(\Gamma=A,B)$ of the degenerate boundary value problem A_0 or B_0, where $\|\psi_{0,n}\|_{H(\Omega_\Gamma)}=1$.

We can find the boundary functions $\Pi_{2m,k}\psi(\rho_1)$, $Q_{2m,k}\psi(\rho_2)$ for $k>0$ from the boundary value problems in the form

$$L_{2m}^1\Pi_{2m,k}\psi=g_{1k}^{2m},\quad L_{2m}^2Q_{2m,k}\psi=g_{2k}^{2m},\tag{15}$$

$$D^i\Pi_{2m,k}\psi(0)-D^iQ_{2m,k}\psi(\bar{r})=-D^i\bar{\psi}_{2m,k}(0)+D^i\bar{\psi}_{2m,k}(\bar{r}),\tag{16}$$

$$\Pi_{2m,k}\psi(\rho_1)\to 0,\quad Q_{2m,k}\psi(\rho_2)\to 0,\ \varepsilon\to 0,\quad i=0,1,\dots,2m-1.\tag{17}$$

We can write the functions $\Pi_{2m,k}\psi$ and $Q_{2m,k}\psi$ as under

$$\Pi_{2m,k}\psi(\rho_1)=\Pi_{2m,k}\tilde{\psi}(\rho_1)+\Pi_{2m,k}\psi^*(\rho_1),\tag{18}$$

$$Q_{2m,k}\psi(\rho_2)=Q_{2m,k}\tilde{\psi}(\rho_2)+Q_{2m,k}\psi^*(\rho_2),\tag{19}$$

where

$$\Pi_{2m,k}\tilde{\psi}(\rho_1) = \sum_{\zeta=1}^{m-1} C_{\zeta,k}^{2m,1} \exp\left(-\alpha_\zeta^{2m}\rho_1\right),$$

$$Q_{2m,k}\tilde{\psi}(\rho_2) = \sum_{\zeta=1}^{m-1} C_{\zeta,k}^{2m,2} \exp\left(-\alpha_\zeta^{2m}\rho_2\right)$$

are the general solutions of the homogeneous equations (15), (17), and

$$\Pi_{2m,k}\psi^*(\rho_1) = \sum_{\zeta=1}^{m-1} \bar{C}_{\zeta,k}^{2m,1}(\rho_1) \exp\left(-\alpha_\zeta^{2m}\rho_1\right),$$

$$Q_{2m,k}\psi^*(\rho_2) = \sum_{\zeta=1}^{m-1} \bar{C}_{\zeta,k}^{2m,2}(\rho_2) \exp\left(-\alpha_\zeta^{2m}\rho_2\right),$$

are the partial solutions of these inhomogeneous equations.

Since, the roots α_i^{2m} are pairwise distinct, then the Vronsky determinants

$$W\left[e^{-\alpha_1^{2m}\rho_1}, \dots, e^{-\alpha_{m-1}^{2m}\rho_1}\right], \; W\left[e^{-\alpha_1^{2m}\rho_2}, \dots, e^{-\alpha_{m-1}^{2m}\rho_2}\right],$$

that are composed of the function systems $\left[\exp\left(-\alpha_\zeta^{2m}\rho_1\right)\right]_{\zeta=1}^{m-1}$ and $\left[\exp\left(-\alpha_\zeta^{2m}\rho_2\right)\right]_{\zeta=1}^{m-1}$, are non-zero.

Using the method of constant variation, we can find the partial solutions of the inhomogeneous equations (15), (17), i.e.

$$\mathbf{D}_{11}^{2m}\vec{\Omega}_1 = \mathbf{F}_1, \quad \mathbf{D}_{22}^{2m}\vec{\Omega}_2 = \mathbf{F}_2,$$

$$\vec{\Omega}_1^\top = \left(\frac{d\bar{C}_{\zeta,1}^{2m,1}(\rho_1)}{d\rho_1}, \dots, \frac{d\bar{C}_{\zeta,m-1}^{2m,1}(\rho_1)}{d\rho_1}\right),$$

$$\vec{\Omega}_2^\top = \left(\frac{d\bar{C}_{\zeta,1}^{2m,2}(\rho_2)}{d\rho_2}, \dots, \frac{d\bar{C}_{\zeta,m-1}^{2m,2}(\rho_2)}{d\rho_2}\right),$$

$$\mathbf{F}_1^\top = (0, \dots, 0, g_{1k}^{2m}), \quad \mathbf{F}_2^\top = (0, \dots, 0, g_{2k}^{2m}),$$

where $\det|\mathbf{D}_{11}^{2m}| \neq 0$, $\det|\mathbf{D}_{22}^{2m}| \neq 0$.

We can find the functions $\bar{C}_{\zeta,k}^{2m,1}(\rho_1)$ and $\bar{C}_{\zeta,k}^{2m,2}(\rho_2)$ from the systems as under $\vec{\Omega}_1 = (\mathbf{D}_{11}^{2m})^{-1}\mathbf{F}_1$, $\vec{\Omega}_2 = (\mathbf{D}_{22}^{2m})^{-1}\mathbf{F}_2$.

After integrating and substituting the solutions in (18), (19), we can find as many arbitrary constants as the boundary conditions of the problems A_ε^{2m} or B_ε^{2m} fall out when we proceed to analysis of the degenerate problems A_0 or B_0.

Thus, this algorithm allows us to find the asymptotic solutions of the problems A_ε^{2m} and B_ε^{2m} with any desired degree of accuracy of a small parameter ε^j.

4. Asymptotic analysis of the solutions

We can formulate the following theorem for the justification of the asymptotic solutions of the problems A_ε^{2m} and B_ε^{2m}.

Theorem 1. *If the self-adjoint elliptic operators L_2, L_{2m} satisfy Conditions 1-3 for the problems A_ε^{2m}, B_ε^{2m}, A_0, B_0 and the function $v(r) \in C^\infty$ is represented as the uniformly converging series in the neighborhood of the point $r = 0$ and the neighborhood of the point $r = r_0$*

$$v(r) = \sum_{s=-1}^{\infty} v_s^1 r^s, \quad v(r) = \sum_{s=-1}^{\infty} v_s^2 (r - r_0)^s,$$

the asymptotic solutions of boundary value problems A_ε^{2m} and B_ε^{2m} exist.

The corresponding n eigenvalue $\lambda_{\varepsilon,2m,n}$ and the corresponding n eigenfunction $\psi_{\varepsilon,2m,n}(r)$ of the operator $\widetilde{L}_{2m}$ have the following asymptotic representations

$$\lambda_{\varepsilon,2m,n} \equiv \lambda_{2m,0,n} + \varepsilon\lambda_{2m,1,n} + \varepsilon^2\lambda_{2m,2,n} + ... + \varepsilon^{j+1}\Delta_j^{2m},$$

$$\psi_{\varepsilon,2m,n}(r) = \sum_{k=0}^{\infty} \varepsilon^j (\bar{\psi}_{2m,k,n}(r) + \Pi_{2m,k,n}\psi(\rho_1) + Q_{2m,k,n}\psi(\rho_2)) + \varepsilon^{j+1} z_j^{2m}(r),$$

where $\lambda_{2m,0,n} = \lambda_{0,n}$ is n-th simple eigenvalue and $\bar{\psi}_{2m,0,n}(r) = \psi_{0,n}$ is the n-th function of the operator L_2 for boundary value problems A_0 and B_0; the functions $\bar{\psi}_{2m,k,n}(r)$, $\Pi_{2m,k,n}\psi$, $Q_{2m,k,n}\psi$ and the values of $\lambda_{2m,k,n}$ for $k > 0$ are determined from the systems of the equations and the boundary conditions given in Paragraph 2.

The estimations for the residual members $\bar{z}_j^{2m}(r)$ and Δ_j^{2m} have form as under $\|D\bar{z}_j^{2m}\|_H + \|\bar{z}_j^{2m}\|_H = O(\varepsilon^{j+1})$, $\Delta_j^{2m} = O(1)$, for p-order derivative of the partial sum $\Theta_j\psi_{\varepsilon,2m,n}$ is $\|D^{q+2}\bar{z}_j^{2m}\|_H = O(\varepsilon^{j-q+1})$, $1 \leqslant q \leqslant s$, $s \geqslant 2m-2$, in the inner subdomain $[\delta, r_0 - \delta]$ is $\|D^{q+2}\bar{z}_j^{2m}\|_H = O(\varepsilon^{j+1})$, $|q| \leqslant s$, in border regions $(0, \delta]$ and $[r_0 - \delta, r_0)$ is $\|D^{q+2}\bar{z}_j^{2m}\|_H = O(\varepsilon^{j-q+1})$, $1 \leqslant |q| \leqslant s$.

Proof. It is assumed that the function $\Theta_j\psi_{\varepsilon,2m,n}(r)$ satisfies the boundary conditions of the problems A_ε^{2m} and B_ε^{2m} and

$$\|\psi_0\|_H = \|\bar{\psi}_{2m,0}\|_H = 1, \quad \|\psi_{\varepsilon,2m}\|_H = 1 + O(\varepsilon).$$

Using series for the constructions of a solution, we can get

$$\left[\widetilde{L}_{2m}^\varepsilon - \Theta_j\lambda_{\varepsilon,2m}\right]\Theta_j\psi_{\varepsilon,2m}(r) = \varepsilon^{j+1}\bar{f}_j^{2m},$$

where $\bar{f}_j^{2m}$ is the restricted function $\left(\|\bar{f}_j^{2m}\|_H = O(1)\right)$.

According to the estimate, we have the evaluation in the form as under

$$\inf_n |\lambda - \lambda_{\varepsilon,2m,n}| \leqslant ||\widetilde{L}_{2m}^\varepsilon\psi - \lambda\psi\|_H / \|\psi\|_H,$$

where $\psi \in \Omega_\Gamma$ is an arbitrary function from the scope of the operator $\widetilde{L}^{\varepsilon}_{2m}$ and $\lambda > 0$ is an arbitrary real number.

Using the evaluation $\|\psi_{\varepsilon,2m}\|_H = 1 + O(\varepsilon)$, we can get that

$$\lambda_{\varepsilon,2m,n} - \Theta_j \lambda_{\varepsilon,2m} = \varepsilon^{j+1} \Delta_j^{2m},$$

where $|\Delta_j^{2m}| \leqslant \|\bar{f}_j\|_H / \|\Theta_j \psi_{\varepsilon,2m}\|_h$. Hence, we can get the estimate $\Delta_j^{2m} = O(1)$.

Let T_d^0 be a closed linear shell consisting of eigenfunctions $\Theta_j \psi_{\varepsilon,2m,n}(r)$, corresponding to the corresponding eigenvalues $\Theta_j \lambda_{\varepsilon,2m,n}$, that are lying on a segment $[\lambda_{0,n} - d, \lambda_{0,n} + d]$, where d is a number $d > \Sigma$ ($\|\tilde{l}^{\varepsilon}_{2m} \theta_j \psi_{\varepsilon,2m} - \Theta_j \lambda_{\varepsilon,2m} \Theta_j \psi_{\varepsilon,2m}\|_H \leqslant \sigma$), then there is such a function $\tilde{\psi}_T \in T_d^0$, $\|\tilde{\psi}_T\|_H = 1$, for which the following inequality $\|\Theta_j \psi_{\varepsilon,2m} - \tilde{\psi}_t\|_h \leqslant 2\Sigma/d$ is satisfied.

If ε is sufficiently small, then the following inequalities occur

$$\lambda_{\varepsilon,2m,n-1} - \lambda_{0,n-1} \leqslant d, \quad \lambda_{\varepsilon,2m,n} - \lambda_{0,n} \leqslant d, \quad \lambda_{\varepsilon,2m,n+1} - \lambda_{0,n+1} \leqslant d,$$

where $3d = \min[\lambda_{0,n} - \lambda_{0,n-1}; \lambda_{0,n+1} - \lambda_{0,n}]$.

Thus, a segment $[\lambda_{0,n} - d, \lambda_{0,n} + d]$ contains the single eigenvalue $\lambda_{\varepsilon,2m,n}$ of the operator $\widetilde{L}^{\varepsilon}_{2m}$, which is relevant to the single normalized eigenfunction $\psi_{\varepsilon,2m,n}(r)$, which coinciding with the normalized function $\tilde{\psi}_T$, and there is the estimation

$$\|\psi_{\varepsilon,2m,n} - \Theta_j \psi_{\varepsilon,2m,n} / \|\Theta_j \psi_{\varepsilon,2m,n}\|_H\|_H \leqslant O(\varepsilon^{j+1}).$$

Thus, we can get the estimation $\|z_j^{2m}\|_H = o(1)$, where $\bar{z}_j^{2m} = \varepsilon^{j+1} z_j^{2m} = \bar{\psi}_{\varepsilon,2m,n} - \theta_j \psi_{\varepsilon,2m,n}$, and $\bar{\psi}_{\varepsilon,2m,n} = \|\Theta_j \psi_{\varepsilon,2m,n}\|_H \, \psi_{\varepsilon,2m,n}$.

Since the inequality $\lambda_{\varepsilon,2m,\gamma} \geqslant \lambda_{0,\gamma}$, $\gamma = 1, 2, ...$ is true and there is the ratio

$$[\widetilde{L}^{\varepsilon}_{2m} - \Theta_j \lambda_{\varepsilon,2m}] \Theta_j \psi_{\varepsilon,2m}(r) = \varepsilon^{j+1} \bar{f}_j^{2m}, \quad \|\bar{f}_j^{2m}\|_H = o(1),$$

we can get the following estimations

$$\|[\widetilde{L}^{\varepsilon}_{2m} - \lambda_{\varepsilon,2m}] \bar{z}_j^{2m}\|_H = O(\varepsilon^{j+1})$$

and $\|\widetilde{L}^{\varepsilon}_{2m} \bar{z}_j^{2m}\|_H \leqslant \|[\widetilde{L}^{\varepsilon}_{2m} - \lambda_{\varepsilon,2m}] \bar{z}_j^{2m}\|_H + |\lambda_{\varepsilon,2m}| \, \|\bar{z}_j^{2m}\|_h = o(\varepsilon^{j+1})$.

Using *Conditions 1–3* and assuming that the function $\bar{z}_j^{2m}$ satisfies the boundary conditions of the problems A_ε^{2m} and B_ε^{2m}, we can get the following estimations

$$\|\bar{z}_j^{2m}\|_H^2 \leqslant \sum_{p=1}^{m-1} \varepsilon^{2p} \|D^p \bar{z}_j^{2m}\|_H^2 + \|D \bar{z}_j^{2m}\|_H^2 + \|\bar{z}_j^{2m}\|_h^2 \leqslant \bar{C} \, \varepsilon^{2(j+1)} \, \|\bar{W}_j^{2m}\|_h^2,$$

where the constant $\bar{C} > 0$ which is independent of r and ε and the function $\bar{w}_j^{2m}$ is the restricted function for which the estimation $\|\bar{w}_j^{2m}\|_H = O(1)$ takes place.

This implies the estimate for $\bar{z}_j^{2m}$ that is in the conditions of the theorem.□

5. Solutions behavior analysis of the problems A_ε^{2m} and B_ε^{2m} in the case $m \to \infty$

Here we investigate the question about the behavior of the eigenfunctions and the eigenvalues of A_ε^{2m} and B_ε^{2m} problems in the case of unlimited increasing of $2m$-order LTKT-equation.

Let's consider the problems of $A_\varepsilon^{2m}, B_\varepsilon^{2m}$ and $A_\varepsilon^{2m+2}, B_\varepsilon^{2m+2}$ for finding $[\psi_{\varepsilon,2m,\gamma}]_{\gamma=1}^{\infty}$, $[\lambda_{\varepsilon,2m,\gamma}]_{\gamma=1}^{\infty}$ and $[\psi_{\varepsilon,2m+2,\gamma}]_{\gamma=1}^{\infty}$, $[\lambda_{\varepsilon,2m+2,\gamma}]_{\gamma=1}^{\infty}$. Here we assume that the eigenvalues are arranged in order of monotonic increase.

Let the relations

$$\Delta_{2m}^{2m+2}\psi_{\varepsilon,n} = \psi_{\varepsilon,2m+2,n} - \psi_{\varepsilon,2m,n}, \quad \Delta_{2m}^{2m+2}\lambda_{\varepsilon,n} = \lambda_{\varepsilon,2m+2,n} - \lambda_{\varepsilon,2m,n},$$

take place, where $\|\psi_{\varepsilon,2m+2}\|_H = 1$, $\|\psi_{\varepsilon,2m}\|_H = 1$.

We can formulate the following

Theorem 2. *If the positive self-adjoint elliptic operators act in the space $H(\Omega_\Gamma)$, L_2, L_{2m} and satisfy Conditions 1–3 for the problems A_ε^{2m}, B_ε^{2m}, A_0, B_0, then we have the following estimates for $m \to \infty$*

$$|\Delta_{2m}^{2m+2}\lambda_{\varepsilon,n}| \leqslant \|\widetilde{L}_{2m+2}^{\varepsilon} - \widetilde{L}_{2m}^{\varepsilon}\|_H \leqslant \frac{2\varepsilon^{2m}}{(2m+2)!!},$$

$$\|\Delta_{2m}^{2m+2}\psi_{\varepsilon,n}\|_H \leqslant \frac{2\varepsilon^{2m}}{(2m+2)!!}.$$

Proof. We can get the ratios

$$\Delta_{2m}^{2m+2}L = \widetilde{L}_{2m+2}^{\varepsilon} - \widetilde{L}_{2m}^{\varepsilon} = \frac{2(-1)^{m+1}\varepsilon^{2m}}{(2m+2)!!}D^{2m+2},$$

$$\lambda_{\varepsilon,2m+2,n} \leqslant \sup_{\varphi}[((\Delta_{2m}^{2m+2}L + \widetilde{L}_{2m}^{\varepsilon})\varphi,\varphi)_H] \leqslant \lambda_{\varepsilon,2m,n} + \bar{\lambda},$$

$$\|\varphi\|_H = 1, (\varphi,\psi_{\varepsilon,2m,\gamma})_H = 0, \quad \gamma = \overline{1,n-1},$$

where $\bar{\lambda}$ is the largest positive eigenvalue of the operator $\Delta_{2m}^{2m+2}L$, and there is the following inequality $\bar{\lambda} \leqslant \|\Delta_{2m}^{2m+2}L\|_H$.

We get the inequalities $|\Delta_{2m}^{2m+2}\lambda_{\varepsilon,n}| \leqslant \|\widetilde{L}_{2m+2}^{\varepsilon} - \widetilde{L}_{2m}^{\varepsilon}\|_H$, where $|\Delta_{2m}^{2m+2}\lambda_{\varepsilon,n}| \leqslant 2\varepsilon^{2m}/(2m+2)!!$.

Thus, there is the equality

$$[\widetilde{L}^{\varepsilon}_{2m+2} - \lambda_{\varepsilon,2m+2}]\Delta^{2m+2}_{2m}\psi_{\varepsilon} = \frac{2\varepsilon^{2m}}{(2m+2)!!}\bar{v}_{2m},$$

where $\bar{v}_{2m}$ is the restricted function, $\|\bar{v}_{2m}\|_H = O(1)$, $(\bar{v}_{2m}, \Delta^{2m+2}_{2m}\psi_{\varepsilon})_H = 0$.

We can assume that the operator $(\widetilde{L}^{\varepsilon}_{2m+2} - \lambda_{\varepsilon,2m+2})$ has a limited inverse operator $(\widetilde{L}^{\varepsilon}_{2m+2} - \lambda_{\varepsilon,2m+2})^{-1}_{h_1}$ (a pseudo-resolvent) and there are the ratios

$$\Delta^{2m+2}_{2m}\psi_{\varepsilon} = \frac{2\varepsilon^{2m}}{(2m+2)!!}(\widetilde{L}^{\varepsilon}_{2m+2} - \lambda_{\varepsilon,2m+2})^{-1}_{H_1}\bar{v}_{2m},$$

and $\|\Delta^{2m+2}_{2m}\psi_{\varepsilon,n}\|_H \leqslant \dfrac{2\varepsilon^{2m}}{(2m+2)!!}$. Thus, the theorem is proved. □

6. Construction of an asymptotic solution in the case of the oscillator potential

We can consider the boundary value problem B^{2m}_{ε} on the $[0, \infty+)$ axis with the quasi-potential of a linear harmonic oscillator in the form $v(r) = r^2$. Analysis of this problem allows to describe the behavior chains of harmonic oscillators with periodic boundary conditions when they are very far apart from each other.

The solution of the degenerate boundary value problem B_0 is an orthonormal system of Hermite functions

$$\psi_{0,n} = [n!2^n\sqrt{\pi}]^{-1/2}\exp(-r^2/2)H_n(r), \quad \lambda_n = 2n+1, \quad n = 1, 3, 5, \dots,$$

where

$$H_n(r) = n!\sum_{m=0}^{[n/2]}(-1)^m\frac{2r^{n-2m}}{m!(n-2m)!}.$$

We can show that the zero approximation has equality $\bar{\psi}_{2m,0,n} = \psi_{0,n}$.

We can find the functions $\Pi_{2m,0,n}\psi(\rho_1)$ and $Q_{2m,0,n}\psi(\rho_2)$ in the form

$$\Pi_{2m,0,n}\bar{\psi}(\rho_1) = \sum_{k=1}^{m-1} C_{0kn}\exp(-\alpha_k\rho_1), \quad Q_{2m,0,n}\psi(\rho_2) = 0,$$

$$C_{0kn} = \sum_{s=1}^{m-1}\varepsilon^{s-1}A_{k,s}\frac{d^s\bar{\psi}_{2m,0,n}(0)}{dr^s},$$

$$A_{1,s} = \frac{1}{\prod_{l\neq s}(\alpha_l - \alpha_s)}, \quad l, s = 1, \dots, m-1,$$

$$A_{2q,s} = A_{2q+1,s} = -\frac{\sum\limits_{r=1}^{2q} \frac{(-1)^r}{(2r)!}\alpha_s^{2r-2}}{\prod_{l\neq s}(\alpha_l - \alpha_s)},\ q = 1,2,\dots,(m-1)/2,\ l,s = 1,\dots,m-1,$$

$$D^i\bar{\psi}_{0,n}(0) = [n!2^n\sqrt{\pi}]^{-1/2} D^i\left[\exp(-r^2/2)H_n(r)\right]|_{(r=0)},\quad n = 1,3,5,\dots$$

The first approximation of the solution has the forms

$$\bar{\psi}_{2m,1,n} = \psi_{0,n},\quad \lambda_{2m,1,n} = 0,$$

$$\Pi_{2m,1,n}\bar{\psi}(\rho_1) = \sum_{k=1}^{m-1} C_{1kn}\,\exp(-\alpha_k\rho),\quad Q_{2m,1,n}\psi(\rho_2) = 0,$$

$$C_{1kn} = \sum_{s=1}^{m-1} \varepsilon^{s-1} A_{k,s}\frac{d^s\bar{\psi}_{2m,1,n}(0)}{dr^s}.$$

The next approximation has the following ratios

$$\bar{\psi}_{2m,2,n} = \psi_{0,n},\quad \lambda_{2m,2,n} = \varepsilon\frac{1}{4}(n^2 + (n+1)^2),\quad n = 1,3,5,\dots,$$

$$\Pi_{2m,1,n}\bar{\psi}(\rho_1) = \sum_{k=1}^{m-1} F_{kn}(r,\varepsilon)\,\exp(-\varepsilon^{-1}\alpha_k r),\quad Q_{2m,2,n}\psi(\rho_2) = 0,$$

$$F_{kn}(r,\varepsilon) = R_{kn} + \rho_1 T_{kn},\quad R_{kn} = C_{1kn} - \lambda_{2m,0,n}\sum_{p=0}^{m-1} C_{1pn}B_{p,k},$$

$$T_{kn} = -C_{1kn}\lambda_{2m,0,n}\bar{B}_{k,k},\quad \bar{B}_{k,k} = \frac{1}{\prod_{j\neq k}(\alpha_j - \alpha_k)},$$

$$B_{k,k} = \frac{\sum\limits_{j=1,j\neq k}^{m-1}(\alpha_k - \alpha_j)}{\prod_{j\neq k}(\alpha_j - \alpha_k)^2},\quad B_{p,k} = \frac{1}{(\alpha_p - \alpha_k)\prod_{j\neq k}(\alpha_j - \alpha_k)}.$$

Thus, we can continue the procedure for constructing the asymptotic series and building an asymptotic solution of the problem under consideration with accuracy up to any given order ε.

7. Conclusions

Recently, there is a great interest in studying properties of bound states of a quarkonium such as charmonium $c\bar{c}$ and bottomonium $b\bar{b}$. These states are similar to the properties of positronium (the bound state of an electron and a positron). Special attention of researchers who deal with bound states of quarks is paid to quasi-potential methods. The quasi-potential approach allows to describe the characteristics of relativistic elementary particles such as amplitudes of hadron elastic scattering, mass spectra and widths of meson decays, and the cross sections of deep inelastic scattering of leptons on

hadrons. Since experimental measurements of relativistic elementary particles are carried out with high accuracy, the quark systems models allow to use the precision calculation of various parameters. Experiment has amassed a wealth of high precision data on quarkonium production in relativistic heavy ion collisions at RHIC and LHC in different kinematical regimes that provides a challenging testing ground for theory and phenomenology.

We use a quasi-potential approach in our work. The quasi-potential method in the field theory is based on a two-time Green function for particle systems. The bounded states of such systems are described by a wave function that satisfies a quasi-potential Schrödinger-type equation that depends on energy and non-local potential. The main advantage of this quasi-potential equation is its three-dimensional character. We have shown the absence of a non-physical parameter of relative time for this equation. This quasi-potential wave equation can be obtained for any system numbers of particles with arbitrary spins. This approach was successfully applied to calculate corrections to the energy levels of hydrogen-like systems within the framework of quantum electrodynamics. The great number of properties of the elementary particles amplitude scattering at high energies is explained using a quasi-potential Lippman–Schwinger equation with a Gaussian potential. The quasi-potential method has a number of advantages among the methods of studying the relativistic two-body problem. The advantage of this approach is that quasi-potential equations are written out in three-dimensional space, which makes it possible to use the methods of non-relativistic quantum mechanics.

In this paper Sturm–Liouville problems with periodic boundary conditions on a segment and a positive half-line are formulated for the truncated to order $2m$ relativistic finite-difference Schrödinger equation (Logunov–Tavkhelidze–Kadyshevsky equation, LTKT-equation) with a small parameter. For these singularly perturbed problems a method is proposed for constructing asymptotic solutions with accuracy up to any given order ε. With the help of this method asymptotic solutions in the form of regular and boundary-layer parts are obtained and the question of asymptotic solutions behavior when $\varepsilon \to 0$ is investigated.

The behavior of solutions is investigated in the case $m \to \infty$ and estimation of this behavior is given. It makes possible to determine the convergence of solutions of the Sturm–Liouville problems for LTKT-equation with periodic boundary conditions in the case $m \to \infty$.

In non-relativistic quantum mechanics, the particle in a one-dimensional lattice is a problem that occurs in the model of a periodic crystal lattice. The potential is caused by ions in the periodic structure of the crystal creating an electromagnetic field, so electrons are subject to a regular potential inside the lattice. This is a generalization of the free electron model, which assumes zero potential inside the lattice.

In this work the Sturm–Liouville problem on the positive half-line with a periodic boundary conditions for the quantum harmonic oscillator is considered and eigenfunctions and eigenvalues are constructed as asymptotic solutions for $2m$-order LTKT-equation. Their solutions allow to describe the behavior chains of harmonic oscillators with periodic boundary conditions when they are very far apart from each other. We can use more complex quasi-potentials and describe the bounded states of the elementary particles in the quark-gluon plasma.

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References

[1] A. A. Atanasov and A. T. Marinov, "$\hbar$–Expansion for bound states described by the relativistic three-dimensional two-particle quasi-potential equation," *Theoretical and Mathematical Physics*, vol. 129, no. 1, pp. 1400–1407, 2001. DOI: 10.1023/A:1012423629038.

[2] Y. D. Chernichenko, "On a solution of the relativistic inverse problem for the sum of nonlocal separable quasipotentials," *Russian Physics Journal*, vol. 55, no. 6, pp. 699–711, 2012. DOI: 10.1007/s11182-012-9869-3.

[3] V. G. Kadyshevsky, R. M. Mir-Kasimov, and N. B. Skachkov, "Quasipotential Approach and the Expansion in Relativistic Spherical Functions," *Nuovo Cimento A*, vol. 55, no. 2, pp. 233–257, 1968. DOI: 10.1007/BF02759225.

[4] V. G. Kadyshevsky and M. Mateev, "On a Relativistic Quasipotential Equation in the Case of Particles with Spin," *Nuovo Cimento A*, vol. 55, no. 2, pp. 275–300, 1968. DOI: 10.1007/BF02759227.

[5] V. G. Kadyshevsky, "Quasipotential type equation for the relativistic scattering amplitude," *Nuclear Physics*, no. 1, pp. 125–148, 1968.

[6] A. A. Logunov and A. N. Tavkhelidze, "Quasi-optical approach in quantum field theory," *Nuovo Cimento*, vol. 29, pp. 380–399, 1963. DOI: 10.1007/BF02750359.

[7] A. A. Logunov and A. N. Tavkhelidze, "Quasi-potential character of the scattering amplitude," *Nuovo Cimento*, vol. 30, pp. 134–142, 1963. DOI: 10.1007/BF02750754.

[8] A. A. Logunov, A. N. Tavkhelidze, and O. A. Khrustalev, "Quasipotential character of the Mandelstam representation," *Physics Letters*, vol. 4, no. 6, pp. 325–326, 1963.

[9] V. A. Matveev, V. I. Savrin, A. N. Sissakian, and A. N. Tavkhelidze, "Relativistic Quark Models in the Quasipotential Approach," *Theoretical and Mathematical Physics*, vol. 132, no. 2, pp. 1119–1136, 2002. DOI: 10.1023/A:1019704709192.

[10] A. Pokraka and R. Dick, "Dimensional effects on the density of states in systems with quasi-relativistic dispersion relations and potential wells," *Canadian Journal of Physics*, vol. 94, no. 8, pp. 773–779, 2016. DOI: 10.1139/cjp-2015-0758.

[11] K. A. Sveshnikov and P. K. Silaev, "Quasi-exact solution of a relativistic finite-difference analogue of the Schrödinger equation for a rectangular potential well," *Theoretical and Mathematical Physics*, vol. 132, no. 3, pp. 408–433, 2002. DOI: 10.1023/A:1020220104534.

[12] K. A. Sveshnikov and P. K. Silaev, "Quasi-exact solution of the problem of relativistic bound states in the (1+1)-dimensional case," *Theoretical and Mathematical Physics*, vol. 149, no. 3, pp. 1665–1689, 2006. DOI: 10.1007/s11232-006-0150-1.

[13] V. S. Minh, E. P. Zhidkov, and V. G. Kadyshevsky, "Solutions of relativistic radial quasipotential equations," *Theoretical and Mathematical Physics*, vol. 63, no. 2, pp. 493–503, 1985. DOI: 10.1007/BF01017906.

[14] I. V. Amirkhanov, E. P. Zhidkov, I. E. Zhidkova, and S. A. Vasilyev, "Construction of an asymptotic approximation of eigenfunctions and eigenvalues of a boundary value problem for the singular perturbed relativistic analog of the Schrödinger equation with an arbitrary potential [Asimptotika sobstvennyh funkcij i sobstvennyh znachenij kraevoj zadachi dlya singulyarno vozmushchennogo relyativistskogo analoga uravneniya Schrödingera pri proizvol'nom potenciale]," *Mathematical Models and Computer Simulations [Matematicheskoe modelirovanie]*, vol. 15, no. 9, pp. 3–16, 2003, in Russian.

[15] I. V. Amirkhanov, E. P. Zhidkov, D. Z. Muzafarov, N. R. Sarker, I. Sarhadov, and Z. A. Sharipov, "Investigation of boundary-value problems for the singular perturbed differential equation of high order [Issledovanie kraevyh zadach dlya singulyarno-vozmushchennogo differencial'nogo uravneniya vysokogo poryadka]," *Mathematical Models and Computer Simulations [Matematicheskoe modelirovanie]*, vol. 19, no. 11, pp. 65–79, 2007, in Russian.

[16] I. V. Amirkhanov, N. R. Sarker, I. Sarhadov, Z. K. Tukhliev, and Z. A. Sharipov, "Analytical and Computational Investigations of Solutions of Boundary-Value Problems for the Quasipotential Equation [Analiticheskoe i chislennoe issledovaniya reshenij kraevyh zadach dlya kvazipotencial'nogo uravneniya]," *Bulletin of Peoples' Friendship University of Russia. Series Mathematics. Information Sciences. Physics [Vestnik Rossijskogo universiteta druzhby narodov. Seriya: Matematika, informatika, fizika]*, no. 4, pp. 44–52, 2012, in Russian.

[17] V. O. Galkin, R. N. Faustov, and D. Ebert, "Logunov–Tavkhelidze equation in the relativistic quark model," *Theoretical and Mathematical Physics*, vol. 191, no. 2, pp. 641–648, 2017. DOI: 10.1134/S0040577917050038.

[18] N. Alam and S. Mandal, "On the quantum phase fluctuations of coherent light in a chain of two anharmonic oscillators coupled through a linear one," *Optics Communications*, vol. 366, pp. 340–348, 2016. DOI: 10.1016/j.optcom.2016.01.019.

[19] Z. Chen, "Mapping quantum many-body system to decoupled harmonic oscillators: general discussions and examples," *Physics Letters A*, vol. 382, no. 37, pp. 2613–2617, 2018. DOI: 10.1016/j.physleta.2018.07.043.

[20] E. P. Zhidkov, V. G. Kadyshevsky, and Y. V. Katyshev, "Problem of the $c \to \infty$ limit in the relativistic Schrödinger equation," *Theoretical and Mathematical Physics*, vol. 3, no. 2, pp. 443–446, 1970. DOI: 10.1007/BF01046508.

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Асимптотическое решение задачи Штурма–Лиувилля с периодическими граничными условиями для релятивистского конечно-разностного уравнения Шрёдингера

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Описание взаимодействия релятивистских частиц в рамках квазипотенциального подхода широко применяется в современной физике. Этот подход основан на так называемой ковариантной формулировке квантовой теории поля, в которой эта теория рассматривается на пространственно-подобной трёхмерной гиперповерхности в пространстве Минковского. Особое внимание в этом подходе уделяется методам построения различных квазипотенциалов, а также использованию квазипотенциального подхода для описания характеристик связанных состояний в кварковых моделях, таких как амплитуды адронного упругого рассеяния, масс-спектры и ширины распадов мезонов, сечения глубокого неупругого рассеяния лептонов на адронах.

В настоящей работе сформулированы задачи Штурма–Лиувилля с периодическими граничными условиями на отрезке и на положительной полуприямой для усечённого релятивистского конечно-разностного уравнения Шрёдингера (уравнение Логунова–Тавхелидзе–Кадышевского, LTKT-уравнение) с малым параметром при старшей производной.

Целью работы является построение асимптотических решений (собственных функций и собственных значений) в виде регулярных и погранслойных частей решений для этой сингулярно возмущённой задачи Штурма–Лиувилля. Основная задача исследования состоит в асимптотическом анализе поведенческих решений рассматриваемой задачи в случае $\varepsilon \to 0$ и $m \to \infty$. Нами был предложен метод построения асимптотических решений (собственных функций и собственных значений), который является обобщением асимптотических методов решения сингулярно возмущённых задач, представленных в работах А. Н. Тихонова, А. Б. Васильевой и В. Ф. Бутузова. Основной результат данной работы — доказанные теоремы об асимптотической сходимости решений сингулярно возмущённой задачи к решениям вырожденной задач при $\varepsilon \to 0$ и сходимости решений усечённого LTKT-уравнения в случае $m \to \infty$. Кроме того, в статье нами рассматривается задача Штурма–Лиувилля на положительной полуоси для LTKT-уравнения 4-го порядка с периодическими граничными условиями для квантового гармонического осциллятора. Для этой задачи построены асимптотические приближения собственных функций и собственных значений и показана их сходимость к решению вырожденной задачи.

Ключевые слова: асимптотический анализ, сингулярно возмущённое дифференциальное уравнение, задача Штурма–Лиувилля, релятивистское конечно-разностное уравнение Шрёдингера, периодические краевые условия, квазипотенциальный подход

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Asymptotic method for constructing a model of adiabatic guided modes of smoothly irregular integrated optical waveguides

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The paper considers a class of smoothly irregular integrated optical multilayer waveguides, whose properties determine the characteristic features of guided propagation of monochromatic polarized light. An asymptotic approach to the description of such electromagnetic radiation is proposed, in which the solutions of Maxwell's equations are expressed in terms of the solutions of a system of four ordinary differential equations and two algebraic equations for six components of the electromagnetic field in the zero approximation. The gradient of the phase front of the adiabatic guided mode satisfies the eikonal equation with respect to the effective refractive index of the waveguide for the given mode.

The multilayer structure of waveguides allows one more stage of reducing the model to a homogeneous system of linear algebraic equations, the nontrivial solvability condition of which specifies the relationship between the gradient of the radiation phase front and the gradients of interfaces between thin homogeneous layers.

In the final part of the work, eigenvalue and eigenvector problems (differential and algebraic), describing adiabatic guided modes are formulated. The formulation of the problem of describing the single-mode propagation of adiabatic guided modes is also given, emphasizing the adiabatic nature of the described approximate solution of Maxwell's equations.

Key words and phrases: smoothly irregular integrated optical multilayer waveguides, eigenvalue and eigenvector problem, single-mode propagation of adiabatic guided modes

1. Introduction

Fundamental results in the theory of regular waveguides were obtained for closed (metallic) waveguides by A. N. Tikhonov and A. A. Samarskii [1], and for open (dielectric) waveguides by A. G. Sveshnikov [2] and V. V. Shevchenko [3]. Among the irregular waveguides, one can distinguish transversely irregular and longitudinally irregular waveguides. For transversely irregular waveguides, the equations and the corresponding solutions allow the separation of variables [4].

Here the incomplete Galerkin method developed by A. G. Sveshnikov [2], [5], [6] received the greatest recognition.

For closed longitudinally irregular waveguides, B. Z. Katsenelenbaum developed the method of cross sections [7], which was generalized for open longitudinally irregular waveguides by V. V. Shevchenko [8]. These models do not describe depolarization and hybridization of guided modes in irregular sections of waveguides. A. A. Egorov, L. A. Sevastyanov and A. L. Sevastyanov developed the foundations of the theory of smoothly irregular 3D dielectric and, in particular, integrated optical waveguides [9], [10], which was successfully applied to a number of three-dimensional integrated optical waveguides and smoothly irregular 3D waveguide devices based on them [11]–[13]. The mathematical basis of the model of adiabatic guided modes (AGMs) is the asymptotic method and the method of coupled modes. The asymptotic method for solving a boundary value problem for a system of differential equations with respect to a small parameter δ allows it to be reduced to a system of ordinary differential equations with special boundary conditions, the method of solving which is known. The coupling of two second-order equations for modes of two different polarizations when solving the original system of equations by the asymptotic method, manifests itself in the first approximation as a weak (of the order of δ) coupling of two linear oscillators. It reflects the violation of the structure regularity caused by a change in the phase constant of smoothly irregular dielectric waveguides.

In this paper, we consider an approach to the construction of a model of propagation of electromagnetic radiation in integrated optical smoothly irregular waveguide structures. Traditionally, such models are described using Maxwell's equations. The paper considers only monochromatic radiation, depending on time as $\exp(i\omega t)$. Such time dependence of the solution allows considering a model of steady-state guided propagation of electromagnetic radiation.

2. Basic concepts and notations

Guided propagation of monochromatic polarized electromagnetic radiation in integrated optical waveguides is described by Maxwell's equations. The electromagnetic field is described using complex amplitudes. A material medium is considered, consisting of dielectric subdomains that fill the entire three-dimensional space. The permittivities of the subdomains are different and real, and the permeability is everywhere equal to the permeability of vacuum. It follows that in the absence of foreign currents and charges, the induced currents and charges are equal to zero.

In the absence of foreign charges and currents, the scalar Maxwell's equations follow from the vector ones, and the boundary conditions for the normal components follow from the boundary conditions for the tangential components [14]. The constitutive equations are assumed to be linear. Thus, the electromagnetic field in a space filled with dielectrics in the Gaussian system of units is described by equations

$$\mathrm{rot}\mathbf{E} = -\frac{1}{c}\frac{\partial \mathbf{B}}{\partial t}, \quad \mathrm{rot}\mathbf{H} = -\frac{1}{c}\frac{\partial \mathbf{D}}{\partial t}, \quad \mathbf{D} = \varepsilon\mathbf{E}, \quad \mathbf{B} = \mu\mathbf{H}, \tag{1}$$

where $\mathbf{E}, \mathbf{H}$ are the electric and magnetic field strength vectors, $\mathbf{D}$ is the electric displacement vector, $\mathbf{B}$ is the magnetic flux density vector, c is the velocity of electromagnetic waves in vacuum.

At the interface between dielectric media 1 and 2, the tangential components of electric and magnetic field strengths satisfy the following boundary (matching) conditions:

$$\mathbf{H}_\tau|_1 = \mathbf{H}_\tau|_2, \quad \mathbf{E}_\tau|_1 = \mathbf{E}_\tau|_2. \tag{2}$$

The asymptotic boundary conditions for guided modes at infinity

$$\|\mathbf{E}\| \xrightarrow[|x|\to\infty]{} 0, \quad \|\mathbf{H}\| \xrightarrow[|x|\to\infty]{} 0, \tag{3}$$

ensure uniqueness of the solution of the problem (1)–(3).

In equations (1), ε is the medium permittivity, μ is the medium permeability. Let us denote by $n = \sqrt{\mu\varepsilon}$ the refractive index of the medium (hereinafter — of a dielectric layer of the considered multilayer dielectric structure).

3. The considered class of objects

The object of our consideration is the guided propagation of monochromatic electromagnetic radiation of the optical range in thin-film integrated optical structures. Such structures are complex waveguide structures formed by the deposition of additional waveguide layers of various (smoothly irregular) geometric configurations on the base waveguide. As a base waveguide, we consider a regular planar three-layer waveguide filling the entire three-dimensional space (open waveguide): a substrate layer (substrate) is located in the lower half-space, then a guiding layer of constant thickness is located, and a cladding layer is located in the upper half-space. In this case, the guiding layer (core) is optically denser compared to the substrate and the cladding. By a thin-film waveguide, we mean a waveguide whose core thickness is comparable to the wavelength of propagating radiation.

Integrated optical waveguide structures are formed by introducing into the three-layer planar dielectric waveguide additional layers of variable thickness $h(y, z)$. The additional waveguide layers are specified by the interface between the additional and waveguide layers $x = h(y, z)$ and directly affect phase distribution $\varphi(y, z)$ and effective refractive index $n_{\text{eff}}(y, z)$ of the composite waveguide system. The phase velocity is smaller and the effective refractive index $n_{\text{eff}}(y, z)$ is greater in the locations where the total thickness of the waveguide layers is greater.

In particular, it can be a few-mode integrated optical waveguide implemented in the form of a three-layer dielectric "plate". On this structure, a local but smoothly irregular optical inhomogeneity is deposited, i.e., an additional dielectric layer of variable thickness. A thin-film waveguide generalized lens (TFWGL) (see Figure 1) is an example [11], [12].

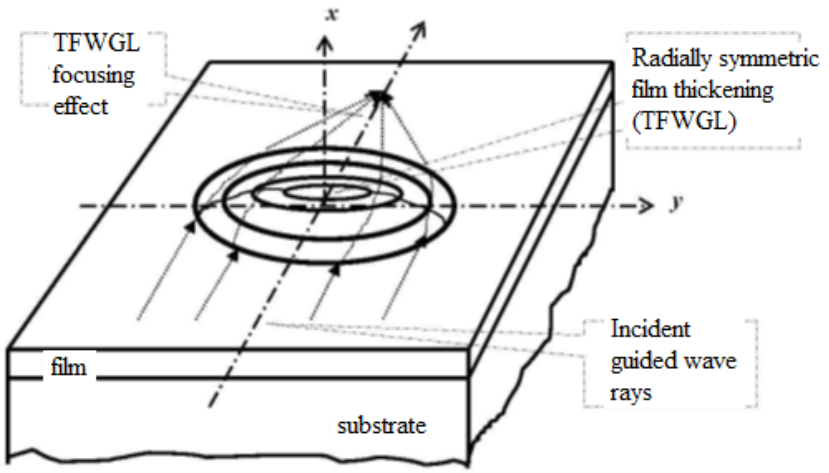

Figure 1. Schematic of Luneberg TFWGL with an additional waveguide layer having cylindrical symmetry

In such integrated optical waveguide, a normal mode of the planar waveguide (allowed by the structure[1], see Appendix) travelling from infinity (or from a point source in the plane of the planar waveguide) is deformed when meeting the localized irregularity (optical inhomogeneity). However, it preserves the structure of a 'transverse resonance', i.e., the structure of a standing wave in the 'transverse' (vertical) direction. Gorelyshev, Neishtadt et al. [20], [21] formulate this conditions as conservation of an adiabatic invariant.

After passing the irregularity region, the deformed "adiabatically invariant" guided (quasi)mode restores the initial (vertical) parameters of a normal mode of a regular waveguide (or transforms into a superposition of normal modes).

For convenience, let us define the Cartesian coordinate system so that all spatial subdomains corresponding to infinite dielectric layers be bounded by planes parallel to the yOz-plane and surfaces asymptotically parallel to the yOz-plane, so that hereafter $\varepsilon = \varepsilon(x)$, $\mu = 1$.

We will call smoothly irregular the optical structures satisfying the inequalities specified by the geometry of the additional waveguide layer:

$$\left|\frac{\partial h}{\partial y}\right|, \left|\frac{\partial h}{\partial z}\right| \ll 1.$$

In weakly inhomogeneous 3D media the electromagnetic radiation propagation is described by locally planar waves or adiabatic approximations to the solutions of the Maxwell's equations, obtained using the asymptotic method [22]. By analogy with locally plane and locally spherical 3D waves [22],

[1] From the theory of planar regular waveguides [15]–[19] it is known that an electromagnetic wave propagates through a regular waveguide in the form of a normal guided mode.

[23], we seek the guided propagation of electromagnetic monochromatic polarized radiation in a smoothly irregular integrated optical waveguide in the form of modified locally normal guided modes of reference waveguides[1].

The adiabatic approximation of the solution of Maxwell's equation obtained in this way will preserve the adiabatic invariants that reflect the guided character of light propagation (the so called transverse resonance condition [15], [26].

This work is devoted to the search for a model of adiabatic guided propagation of monochromatic electromagnetic radiation in smoothly irregular integrated optical structures. The technique for finding it is based on an asymptotic approach in the form of locally normal guided modes of a locally planar reference waveguide. The adiabatic approximation of the solution of Maxwell's equations obtained in this way will preserve adiabatic invariants reflecting the waveguide nature (the so-called transverse resonance condition) of light propagation.

4. Basic equations of the adiabatic guided mode model

Let us recall the earlier assumptions made for the considered integrated optical waveguides and the electromagnetic radiation propagating along them.

1. Electromagnetic radiation is optical and monochromatic with a fixed wavelength $\lambda \in [380; 780]$, *nm*.
2. The thickness of the guiding layer (core) of the base thin-film waveguide is comparable to the length of the propagating monochromatic electromagnetic radiation $d \sim \lambda$.
3. The surface of additional waveguide layer ($x = h(y, z)$) satisfies the limiting conditions $\left|\frac{\partial h}{\partial y}\right|, \left|\frac{\partial h}{\partial z}\right| \ll 1$.
4. The integrated optical waveguide is a material medium consisting of dielectric subdomains that fill the entire space.
5. The permittivities of the subdomains are different and real, and the permeability is everywhere equal to the magnetic permeability of vacuum.
6. There are no external currents and charges. It follows from this that in the absence of external currents and charges, the induced currents and charges are equal to zero.
7. A Cartesian coordinate system is introduced as follows: the interfaces between the dielectric media of the basic three-layer waveguide are parallel to the yOz-plane. In this case, the subdomains of space corresponding to the cladding and substrate layers are semi-infinite, the additional waveguide layers are asymptotically parallel to the yOz-plane, so that $\varepsilon = \varepsilon(x)$.

In Cartesian coordinates associated with the geometry of the substrate (or a three-layer planar dielectric waveguide), Maxwell's equations are written in the form

[1]The notion of reference waveguides (dielectric planar) is presented in papers by Katsenelenbaum and Shevchenko [7], [8], [24], [25].

$$\begin{aligned}
&\frac{\partial H_z}{\partial y}-\frac{\partial H_y}{\partial z}=\frac{\varepsilon}{c}\frac{\partial E_x}{\partial t}, \quad \frac{\partial E_z}{\partial y}-\frac{\partial E_y}{\partial z}=-\frac{\mu}{c}\frac{\partial H_x}{\partial t},\\
&\frac{\partial H_x}{\partial z}-\frac{\partial H_z}{\partial x}=\frac{\varepsilon}{c}\frac{\partial E_y}{\partial t}, \quad \frac{\partial E_x}{\partial z}-\frac{\partial E_z}{\partial x}=-\frac{\mu}{c}\frac{\partial H_y}{\partial t},\\
&\frac{\partial H_y}{\partial x}-\frac{\partial H_x}{\partial y}=\frac{\varepsilon}{c}\frac{\partial E_z}{\partial t}, \quad \frac{\partial E_y}{\partial x}-\frac{\partial E_x}{\partial y}=-\frac{\mu}{c}\frac{\partial H_z}{\partial t}.
\end{aligned} \tag{4}$$

To construct the model of adiabatic guided modes (AGMs) we represent the solutions of (4) in the form of locally normal guided modes of a locally planar reference waveguide (see [7], [8], [27]), which in the method of asymptotic expansion take the form

$$\vec{E}(x,y,z,t)=\sum_{s=0}^{\infty}\frac{\vec{E}_s(x,y,z)}{(-i\omega)^{\gamma+s}}\exp\left\{i\omega t-ik_0\varphi(y,z)\right\}, \tag{5}$$

$$\vec{H}(x,y,z,t)=\sum_{s=0}^{\infty}\frac{\vec{H}_s(x,y,z)}{(-i\omega)^{\gamma+s}}\exp\left\{i\omega t-ik_0\varphi(y,z)\right\}. \tag{6}$$

In the notation $\vec{E}_s(x,y,z,t)$, $\vec{H}_s(x,y,z,t)$ the separation of x with a semicolon means the following assumption

$$\left\|\frac{\partial\vec{E}_s(x,y,z)}{\partial y}\right\|,\left\|\frac{\partial\vec{E}_s(x,y,z)}{\partial z}\right\|\sim\frac{1}{\omega}\left\|\frac{\partial\vec{E}_s(x,y,z)}{\partial x}\right\|, \quad j=x,y,z \tag{7}$$

and

$$\left\|\frac{\partial\vec{H}_s(x,y,z)}{\partial y}\right\|,\left\|\frac{\partial\vec{H}_s(x,y,z)}{\partial z}\right\|\sim\frac{1}{\omega}\left\|\frac{\partial\vec{H}_s(x,y,z)}{\partial x}\right\|, \quad j=x,y,z, \tag{8}$$

where $\|\ \|$ is the Euclidean norm and ω is the circular frequency of the propagating monochromatic electromagnetic radiation.

Using the approach of the asymptotic expansion method with respect to the dimensional small parameter ω^{-1} [23], [28], [29], we substitute expressions (5), (6) into the system of equations (4) and equate the coefficients at equal powers of the small parameter ω^{-1}. As a result, with the relations (7) and (8) taken into account, in the zero approximation of the method of asymptotic expansion with respect to small parameter we arrive at a system of homogeneous equations:

$$-ik_0\frac{\partial\varphi}{\partial y}H_0^z+ik_0\frac{\partial\varphi}{\partial z}H_0^y=ik_0\varepsilon E_0^x, \tag{9}$$

$$-ik_0\frac{\partial\varphi}{\partial z}H_0^x-\frac{\partial H_0^z}{\partial x}=ik_0\varepsilon E_0^y, \tag{10}$$

$$\frac{\partial H_0^y}{\partial x} + ik_0 \frac{\partial \varphi}{\partial y} H_0^x = ik_0 \varepsilon E_0^z, \tag{11}$$

$$-ik_0 \frac{\partial \varphi}{\partial y} E_0^z + ik_0 \frac{\partial \varphi}{\partial z} E_0^y = ik_0 \mu H_0^x, \tag{12}$$

$$-ik_0 \frac{\partial \varphi}{\partial z} E_0^x - \frac{\partial E_0^z}{\partial x} = ik_0 \mu H_0^y, \tag{13}$$

$$\frac{\partial E_0^y}{\partial x} + ik_0 \frac{\partial \varphi}{\partial y} E_0^x = ik_0 \mu H_0^z. \tag{14}$$

By means of simple transformations, we reduce it to the form of interest to us. Namely, from the relation (12) we get the expression

$$E_0^x = -\frac{\partial \varphi}{\partial y} \frac{1}{\varepsilon} H_0^z + \frac{\partial \varphi}{\partial z} \frac{1}{\varepsilon} H_0^y,$$

which we substitute into equations (13)–(14) that take the form

$$-\frac{\partial E_0^z}{\partial x} = ik_0 \frac{\partial \varphi}{\partial z} \left(-\frac{\partial \varphi}{\partial y} \frac{1}{\varepsilon} H_0^z + \frac{\partial \varphi}{\partial z} \frac{1}{\varepsilon} H_0^y \right) - ik_0 \mu H_0^y, \tag{15}$$

$$\frac{\partial E_0^y}{\partial x} = -ik_0 \mu H_0^z - ik_0 \frac{\partial \varphi}{\partial y} \left(-\frac{\partial \varphi}{\partial y} \frac{1}{\varepsilon} H_0^z + \frac{\partial \varphi}{\partial z} \frac{1}{\varepsilon} H_0^y \right). \tag{16}$$

From relation (9) we get the expression

$$H_0^x = \frac{\partial \varphi}{\partial y} \frac{1}{\mu} E_0^z - \frac{\partial \varphi}{\partial z} \frac{1}{\mu} E_0^y,$$

and substitute it into equations (10)–(11), which take the form

$$-\frac{\partial H_0^z}{\partial x} = -ik_0 \varepsilon E_0^y + ik_0 \frac{\partial \varphi}{\partial z} \left(\frac{\partial \varphi}{\partial y} \frac{1}{\mu} E_0^z - \frac{\partial \varphi}{\partial z} \frac{1}{\mu} E_0^y \right), \tag{17}$$

$$\frac{\partial H_0^y}{\partial x} = ik_0 \varepsilon E_0^z - ik_0 \frac{\partial \varphi}{\partial y} \left(\frac{\partial \varphi}{\partial y} \frac{1}{\mu} E_0^z - \frac{\partial \varphi}{\partial z} \frac{1}{\mu} E_0^y \right). \tag{18}$$

Ultimately, Maxwell's equation reduced in the zero approximation to two algebraic equations and four differential equations of the first order.

At any fixed values of (y, z), equations (15)–(16), (17)–(18) take the form of a system of ordinary differential equations of the first order. Hereinafter, we deal with the zero approximation of the asymptotic expansion with respect to the small parameter; therefore, the index of the order of smallness is omitted:

$$\frac{dH^z}{dx} + \frac{ik_0}{\mu} \frac{\partial \varphi}{\partial z} \left(\frac{\partial \varphi}{\partial y} E^z - \frac{\partial \varphi}{\partial z} E^y \right) + ik_0 \varepsilon E^y = 0,$$

$$\frac{dH^y}{dx} + \frac{ik_0}{\mu} \frac{\partial \varphi}{\partial y} \left(\frac{\partial \varphi}{\partial y} E^z - \frac{\partial \varphi}{\partial z} E^y \right) - ik_0 \varepsilon E^z = 0,$$

$$\frac{dE^z}{dx} + \frac{ik_0}{\varepsilon}\frac{\partial\varphi}{\partial z}\left(\frac{\partial\varphi}{\partial z}H^y - \frac{\partial\varphi}{\partial y}H^z\right) - ik_0\mu H^y = 0,$$
$$\frac{dE^y}{dx} + \frac{ik_0}{\varepsilon}\frac{\partial\varphi}{\partial y}\left(\frac{\partial\varphi}{\partial z}H^y - \frac{\partial\varphi}{\partial y}H^z\right) + ik_0\mu H^z = 0.$$

In addition, for any fixed values of (y, z) the algebraic equations are valid

$$E_0^x = \frac{1}{\varepsilon}\left(\frac{\partial\varphi}{\partial z}H_0^y - \frac{\partial\varphi}{\partial y}H_0^z\right), \quad H_0^x = \frac{1}{\mu}\left(\frac{\partial\varphi}{\partial y}E_0^z - \frac{\partial\varphi}{\partial z}E_0^y\right).$$

Remark 1. In the proposed form (5)–(6) of the desired solutions of Maxwell's equations the quantities $\dfrac{\partial\varphi}{\partial y}$ and $\dfrac{\partial\varphi}{\partial z}$ have the meaning of phase constants of guided propagation of radiation in the directions Oy and Oz in all layers of the waveguide simultaneously, i.e., they determine the effective refractive index of the waveguide under study for the given adiabatic guided mode:

$$\left(\frac{\partial\varphi}{\partial y}(y,z)\right)^2 + \left(\frac{\partial\varphi}{\partial z}(y,z)\right)^2 = n_{\text{eff}}^2(y,z). \tag{19}$$

From the analysis carried out, we conclude that with the accepted assumptions the zero approximation to the guided solution of Maxwell's equations is given by the following relations:

$$\begin{Bmatrix}\vec{E}(x,y,z,t)\\ \vec{H}(x,y,z,t)\end{Bmatrix} = \begin{Bmatrix}\vec{E}_0(x;y,z)\\ \vec{H}_0(x;y,z)\end{Bmatrix}\exp\left\{i\omega t - i\varphi(y,z)\right\},$$

with

$$\begin{aligned}
\varepsilon\frac{\partial E_0^y}{\partial x} &= -ik_0\left(\frac{\partial\varphi}{\partial y}\right)\left(\frac{\partial\varphi}{\partial z}\right)H_0^y - ik_0\left(\varepsilon\mu - \left(\frac{\partial\varphi}{\partial y}\right)^2\right)H_0^z,\\
\varepsilon\frac{\partial E_0^z}{\partial x} &= ik_0\left(\varepsilon\mu - \left(\frac{\partial\varphi}{\partial z}\right)^2\right)H_0^y + ik_0\left(\frac{\partial\varphi}{\partial z}\right)\left(\frac{\partial\varphi}{\partial y}\right)H_0^z.\\
\mu\frac{\partial H_0^y}{\partial x} &= ik_0\left(\frac{\partial\varphi}{\partial y}\right)\left(\frac{\partial\varphi}{\partial z}\right)E_0^y + ik_0\left(\varepsilon\mu - \left(\frac{\partial\varphi}{\partial y}\right)^2\right)E_0^z,\\
\mu\frac{\partial H_0^z}{\partial x} &= -ik_0\left(\varepsilon\mu - \left(\frac{\partial\varphi}{\partial z}\right)^2\right)E_0^y - ik_0\left(\frac{\partial\varphi}{\partial z}\right)\left(\frac{\partial\varphi}{\partial y}\right)E_0^z.
\end{aligned} \tag{20}$$

and

$$E_0^x = -\frac{\partial\varphi}{\partial y}\frac{1}{\varepsilon}H_0^z + \frac{\partial\varphi}{\partial z}\frac{1}{\varepsilon}H_0^y, \quad H_0^x = \frac{\partial\varphi}{\partial y}\frac{1}{\mu}E_0^z - \frac{\partial\varphi}{\partial z}\frac{1}{\mu}E_0^y \tag{21}$$

as well as

$$\left(\frac{\partial\varphi}{\partial y}(y,z)\right)^2 + \left(\frac{\partial\varphi}{\partial z}(y,z)\right)^2 = n_{\text{eff}}^2(y,z).$$

For thin-film multilayer waveguide, consisting of optically homogeneous layers, from (2) the conditions of the electromagnetic field matching at the interfaces between the media follow:

$$\vec{n} \times \vec{E}^{-} + \vec{n} \times \vec{E}^{+} = 0, \tag{22}$$

$$\vec{n} \times \vec{H}^{-} + \vec{n} \times \vec{H}^{+} = 0. \tag{23}$$

From (3) the asymptotic conditions follow

$$E_y^0,\, E_z^0,\, H_y^0,\, H_z^0 \xrightarrow[x \to \pm\infty]{} 0. \tag{24}$$

The system of equations (20), (24) for any fixed (y, z) defines a problem of finding eigenvalues $\left(\vec{\nabla}\varphi\right)_j^2 (y, z)$ and eigenfunctions $(E_y^j, E_z^j, H_y^j, H_z^j)^T(y, z)$, normalized to unity:

$$\int_{-\infty}^{\infty} \left|E_y^j\right|^2 dx = 1, \quad \int_{-\infty}^{\infty} \left|H_y^j\right|^2 dx = 1.$$

5. Algebraic model of adiabatic guided modes

In the case of a multilayer integrated optical waveguide consisting of homogeneous dielectric layers (possible, with complex permittivities) the relations (20), (22)–(24) are valid with generally non-horizontal interfaces between the layers (see Figure 2).

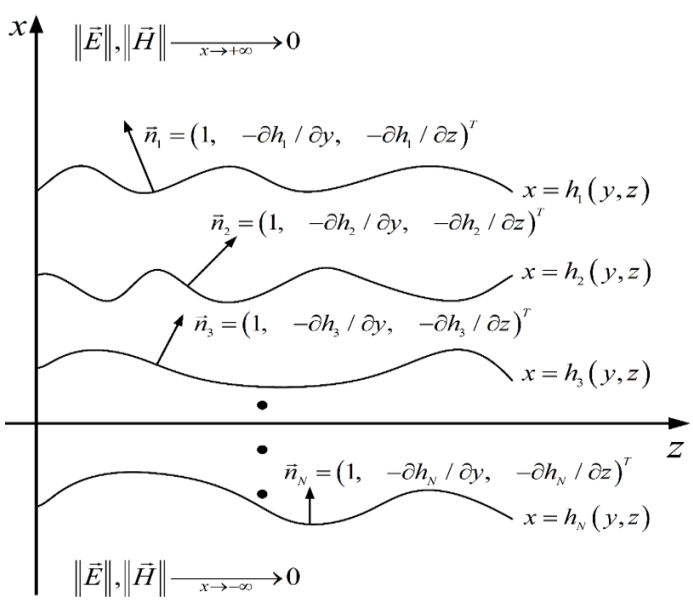

Figure 2. Structure of a multilayer thin-film waveguide

In this case, in each inner layer the four-dimensional system of ordinary differential equations with constant coefficients has a four-parameter system of fundamental solutions. Then the general solutions of equations (20) in the layers take the form

$$\vec{U}(x;y,z) = C_1\vec{\xi}_1 e^{\gamma_+ x} + C_2\vec{\xi}_2 e^{\gamma_- x} + C_3\vec{\xi}_3 e^{\gamma_+ x} + C_4\vec{\xi}_4 e^{\gamma_- x},$$

$$E_y(x) = \frac{-I(A_2 - A_4)\sqrt{-\mu\varepsilon + \frac{\partial\varphi^2}{\partial y} + \frac{\partial\varphi^2}{\partial z}}\mu \exp\left\{-k_0\sqrt{\frac{\partial\varphi^2}{\partial y} + \frac{\partial\varphi^2}{\partial z} - \mu\varepsilon x}\right\}}{\frac{\partial\varphi}{\partial y}\frac{\partial\varphi}{\partial z}} -$$
$$- \frac{\exp\left\{k_0\sqrt{\frac{\partial\varphi^2}{\partial y} + \frac{\partial\varphi^2}{\partial z} - \mu\varepsilon x}\right\}(A_1 + A_3)\left(\mu\varepsilon - \frac{\partial\varphi^2}{\partial y}\right)}{\frac{\partial\varphi}{\partial y}\frac{\partial\varphi}{\partial z}},$$

$$H_z(x) = \frac{-(A_2 + A_4)\left(\mu\varepsilon - \frac{\partial\varphi^2}{\partial z}\right)\exp\left\{-k_0\sqrt{\frac{\partial\varphi^2}{\partial y} + \frac{\partial\varphi^2}{\partial z} - \mu\varepsilon x}\right\}}{\frac{\partial\varphi}{\partial y}\frac{\partial\varphi}{\partial z}} -$$
$$- \frac{I(A_1 - A_4)\varepsilon \exp\left\{k_0\sqrt{\frac{\partial\varphi^2}{\partial y} + \frac{\partial\varphi^2}{\partial z} - \mu\varepsilon x}\right\}\sqrt{\frac{\partial\varphi^2}{\partial y}\frac{\partial\varphi^2}{\partial z} - \mu\varepsilon}}{\frac{\partial\varphi}{\partial y}\frac{\partial\varphi}{\partial z}},$$

$$H_y(x) = (A_2 + A_4)\exp\left\{-k_0\sqrt{\frac{\partial\varphi^2}{\partial y} + \frac{\partial\varphi^2}{\partial z} - \mu\varepsilon x}\right\},$$

$$E_z(x) = (A_1 + A_3)\exp\left\{k_0\sqrt{\frac{\partial\varphi^2}{\partial y} + \frac{\partial\varphi^2}{\partial z} - \mu\varepsilon x}\right\},$$

where

$$\vec{u} = \left(H^z(x;y,z); E^z(x;y,z); H^y(x;y,z); E^y(x;y,z)\right)^T$$

and $\gamma_\pm = \pm k_0\sqrt{-\varepsilon\mu + \varphi_y^2 + \varphi_z^2}$.

The rest components of the electromagnetic field are calculated using formulas (21), and all the six components enter the explicit form of relations (22), (23).

In the substrate and cladding layers due to asymptotic conditions the two-dimensional systems of ordinary differential equations with constant coefficients have two-parametric systems of fundamental solutions.

The solution unique for all layers satisfies the matching conditions at the interfaces between the layers, i.e., determines a system of linear algebraic equations for indefinite coefficients, which specify the expression of particular solutions in the layers in terms of the systems of fundamental solutions.

At an arbitrary smooth interface between two dielectric media, described by the equation $F(x,y,z) = x - h(y,z) = 0$ (see Figure 3), conditions (22) and (23) take the form

$$\left[\vec{n} \times \vec{E}\right] = \left(E_y \frac{\partial h}{\partial z} - E_z \frac{\partial h}{\partial y}; -E_z - E_x \frac{\partial h}{\partial z}; E_y - E_x \frac{\partial h}{\partial y}\right)^T, \qquad (25)$$

$$\left[\vec{n} \times \vec{H}\right] = \left(H_y \frac{\partial h}{\partial z} - H_z \frac{\partial h}{\partial y}; -H_z - H_x \frac{\partial h}{\partial z}; H_y - H_x \frac{\partial h}{\partial y}\right)^T. \qquad (26)$$

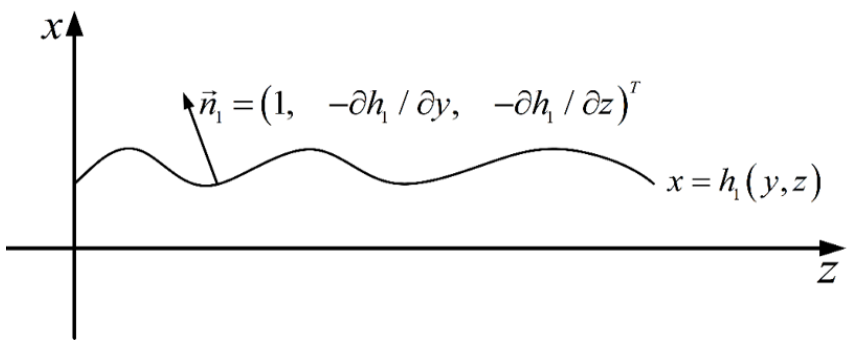

Figure 3. Equation of a normal to the interface between the layers

In the expressions (25) and (26) the denominator $\sqrt{1 + \left(\frac{\partial h}{\partial y}\right)^2 + \left(\frac{\partial h}{\partial z}\right)^2}$ in the expressions for the normal was omitted, since it is nonzero and coincides in both sides of equations (25), (26). It is worth noting that only two of three components of the obtained vectors (25) and (26) are linearly independent. Therefore, for writing the boundary conditions we will use the following expressions:

$$\left(A_z^1 + A_x^1 \frac{\partial h}{\partial z}\right)\Big|_{x=h(y,z)} = \left(A_z^2 + A_x^2 \frac{\partial h}{\partial z}\right)\Big|_{x=h(y,z)},$$

$$\left(A_y^1 - A_x^1 \frac{\partial h}{\partial y}\right)\Big|_{x=h(y,z)} = \left(A_y^2 - A_x^2 \frac{\partial h}{\partial y}\right)\Big|_{x=h(y,z)},$$

where $\vec{A} = \left\{\vec{E}, \vec{H}\right\}$. Moreover, for a planar boundary $F(x,y,z) = x - \text{const}$ the above expressions simplify to the following form:

$$A_y^1\big|_{x=\text{const}} = A_y^2\big|_{x=\text{const}}, \quad A_z^1\big|_{x=\text{const}} = A_z^2\big|_{x=\text{const}}.$$

The above relations should be completed with the asymptotic condition (24).

Thus, in each inner layer of a k-layer waveguide the four-dimensional general solution is parametrized by four indefinite coefficients, in the substrate and cladding layers at the expense of asymptotic conditions the number of coefficients is reduced by two in each layer. Therefore, there is a total of $4(k-2) + 2 + 2 = 4(k-1)$ coefficients. To each of $(k-1)$ interfaces four

equations correspond, making the total of $4(k-1)$. Thus, we have $4(k-1)$ linear homogeneous algebraic equations for $4(k-1)$ unknown coefficients.

Returning to the calculation of the electromagnetic field in the multilayer waveguide, we seek a nontrivial solution to the homogeneous system of linear algebraic equations with respect to the coefficient of expansion over the fundamental system of solutions in each dielectric layer:

$$M\left(h(y,z), \nabla h(y,z), \varphi(y,z), \nabla\varphi(y,z)\right)\vec{A} = \vec{0}. \tag{27}$$

To find nontrivial fields $\vec{E}$, $\vec{H}$ at an arbitrary point (y,z) the condition of solvability should be satisfied for the system of homogeneous linear algebraic equations

$$\det\left(M\left(h(y,z), \nabla h(y,z), \varphi(y,z), \nabla\varphi(y,z)\right)\right) = 0. \tag{28}$$

Thus the system of homogeneous linear algebraic equations (27), nontrivially solvable under the condition (28), is an algebraic model of adiabatic guided modes in a smoothly irregular multilayer integrated optical waveguide. The roots of equation (28) are a set of eigenvalues and the solution of the system of equations (27) after substitution of each particular root is the corresponding eigenvector normalized by the condition $\left\|\vec{A}\right\| = 1$.

6. Results

Thus, in the course of several stages of sequential reduction, we have formulated a number of problems of modeling the adiabatic guided modes in a smoothly irregular integrated optical multilayer waveguide.

Problem 1. *The problem of finding eigenvalues and eigenfunctions within the AGM model*

$$\begin{Bmatrix} \vec{E}(x,y,z,t) \\ \vec{H}(x,y,z,t) \end{Bmatrix} = \begin{Bmatrix} \vec{E}_0(x;y,z) \\ \vec{H}_0(x;y,z) \end{Bmatrix} \exp\left\{i\omega t - i\varphi(y,z)\right\}, \tag{29}$$

is formulated as follows:

$$\begin{aligned} \varepsilon\frac{\partial E_0^y}{\partial x} &= -ik_0\left(\frac{\partial\varphi}{\partial y}\right)\left(\frac{\partial\varphi}{\partial z}\right)H_0^y - ik_0\left(\varepsilon\mu - \left(\frac{\partial\varphi}{\partial y}\right)^2\right)H_0^z, \\ \varepsilon\frac{\partial E_0^z}{\partial x} &= ik_0\left(\varepsilon\mu - \left(\frac{\partial\varphi}{\partial z}\right)^2\right)H_0^y + ik_0\left(\frac{\partial\varphi}{\partial z}\right)\left(\frac{\partial\varphi}{\partial y}\right)H_0^z. \end{aligned} \tag{30}$$

$$\begin{aligned} \mu\frac{\partial H_0^y}{\partial x} &= ik_0\left(\frac{\partial\varphi}{\partial y}\right)\left(\frac{\partial\varphi}{\partial z}\right)E_0^y + ik_0\left(\varepsilon\mu - \left(\frac{\partial\varphi}{\partial y}\right)^2\right)E_0^z, \\ \mu\frac{\partial H_0^z}{\partial x} &= -ik_0\left(\varepsilon\mu - \left(\frac{\partial\varphi}{\partial z}\right)^2\right)E_0^y - ik_0\left(\frac{\partial\varphi}{\partial z}\right)\left(\frac{\partial\varphi}{\partial y}\right)E_0^z. \end{aligned} \tag{31}$$

Eigenfunctions $\left(E_y^0, E_z^0, H_y^0, H_z^0\right)_j^T \left(x; (\nabla\varphi)_j^2\right)$ *correspond to eigenvalues* $(\nabla\varphi)_j^2$.

The accompanying components of the electromagnetic field are calculated by the formulas:

$$E_0^x = -\frac{\partial\varphi}{\partial y}\frac{1}{\varepsilon}H_0^z + \frac{\partial\varphi}{\partial z}\frac{1}{\varepsilon}H_0^y, \quad H_0^x = \frac{\partial\varphi}{\partial y}\frac{1}{\mu}E_0^z - \frac{\partial\varphi}{\partial z}\frac{1}{\mu}E_0^y. \tag{32}$$

Problem 2. *The problem of finding eigenvalues of eigenfunctions within the AGM model*

$$\begin{Bmatrix} \vec{E}(x,y,z,t) \\ \vec{H}(x,y,z,t) \end{Bmatrix} = \begin{Bmatrix} \vec{E}_0(x;y,z) \\ \vec{H}_0(x;y,z) \end{Bmatrix} \exp\left\{i\omega t - i\varphi(y,z)\right\},$$

is formulated as follows:

$$\frac{\partial^2 E_0^y}{\partial x^2} + k_0^2\left(\varepsilon\mu - (\nabla\varphi)^2\right)E_0^y = 0, \quad \frac{\partial^2 H_0^y}{\partial x^2} + k_0^2\left(\varepsilon\mu - (\nabla\varphi)^2\right)H_0^y = 0. \tag{33}$$

Eigenfunctions $\left(E_y^0, H_y^0, \right)_j^T \left(x; (\nabla\varphi)_j^2\right)$ *correspond to eigenvalues* $(\nabla\varphi)_j^2$.

The accompanying components of the electromagnetic field are calculated by the formulas

$$\begin{aligned}
\varepsilon\frac{\partial E_0^y}{\partial x} &= -ik_0\left(\frac{\partial\varphi}{\partial y}\right)\left(\frac{\partial\varphi}{\partial z}\right)H_0^y - ik_0\left(\varepsilon\mu - \left(\frac{\partial\varphi}{\partial y}\right)^2\right)H_0^z, \\
\varepsilon\frac{\partial E_0^z}{\partial x} &= ik_0\left(\varepsilon\mu - \left(\frac{\partial\varphi}{\partial z}\right)^2\right)H_0^y + ik_0\left(\frac{\partial\varphi}{\partial z}\right)\left(\frac{\partial\varphi}{\partial y}\right)H_0^z. \\
\mu\frac{\partial H_0^y}{\partial x} &= ik_0\left(\frac{\partial\varphi}{\partial y}\right)\left(\frac{\partial\varphi}{\partial z}\right)E_0^y + ik_0\left(\varepsilon\mu - \left(\frac{\partial\varphi}{\partial y}\right)^2\right)E_0^z, \\
\mu\frac{\partial H_0^z}{\partial x} &= -ik_0\left(\varepsilon\mu - \left(\frac{\partial\varphi}{\partial z}\right)^2\right)E_0^y - ik_0\left(\frac{\partial\varphi}{\partial z}\right)\left(\frac{\partial\varphi}{\partial y}\right)E_0^z.
\end{aligned} \tag{34}$$

Problem 3. *Following the ideology of the cross section method, the steady-state regime of guided propagation of electromagnetic radiation within the frameworks of the AGM model, i.e., the solution of Maxwell's equations* $rot\vec{H} = ik\varepsilon\vec{E}$, $rot\vec{E} = -ik\mu\vec{H}$ *with asymptotic conditions* $\left(\vec{E},\vec{H}\right)^T(x) \xrightarrow[x\to\pm\infty]{} \vec{0}$ *is sought in the form of a sum*

$$\left(\vec{E},\vec{H}\right)^T(x,y,z) = \sum_j C_{\vec{\beta}_j}(y,z)\left(\vec{E},\vec{H}\right)^T(x,\vec{\beta}_j),$$

where $\left(\vec{E},\vec{H}\right)^T\left(x,\vec{\beta}_j\right)$ *are solutions to the equations* (30)–(31), (32) *with additional condition:*

$$\vec{\nabla}\left(\vec{E},\vec{H}\right)^T(x,y,z) = -\sum_j i\beta_j C_{\vec{\beta}_j}(y,z)\left(\vec{E},\vec{H}\right)^T(x,\vec{\beta}_j),$$

where $\vec{\beta}(y,z) = \vec{\nabla}\varphi(y,z)$.

Problem 4. *Following the ideology of the method of cross sections, the steady-state regime of guided propagation of electromagnetic radiation within the frameworks of the AGM model, i.e., the solution of Maxwell's equations* $rot(rot\vec{H}) = k_0^2\varepsilon\mu\vec{E}$, $rot(rot\vec{E}) = k_0^2\varepsilon\mu\vec{H}$ *with asymptotic conditions* $\left(\vec{E},\vec{H}\right)^T(x) \xrightarrow[x\to\pm\infty]{} \vec{0}$ *is sought in the form of a sum*

$$\left(\vec{E},\vec{H}\right)^T(x,y,z) = \sum_j C_{\vec{\beta}_j}(y,z)\left(\vec{E},\vec{H}\right)^T(x,\vec{\beta}_j),$$

where $\left(\vec{E},\vec{H}\right)^T\left(x,\vec{\beta}_j\right)$ *are solutions to the equations* (33), (34) *with additional condition:*

$$\vec{\nabla}\left(\vec{E},\vec{H}\right)^T(x,y,z) = -\sum_j i\beta_j C_{\vec{\beta}_j}(y,z)\left(\vec{E},\vec{H}\right)^T(x,\vec{\beta}_j),$$

where $\vec{\beta}(y,z) = \vec{\nabla}\varphi(y,z)$.

The single-mode regime is specified by ansatz

$$\left(\vec{E},\vec{H}\right)_j^T(x,y,z) = C_{\vec{\beta}_j}(y,z)\left(\vec{E},\vec{H}\right)^T(x,\vec{\beta}_j)$$

with the additional condition

$$\vec{\nabla}\left(\vec{E},\vec{H}\right)_j^T(x,y,z) = -i\vec{\beta}_j C_{\vec{\beta}_j}(y,z)\left(\vec{E},\vec{H}\right)^T(x,\vec{\beta}_j),$$

where $\vec{\beta}(y,z) = \vec{\nabla}\varphi(y,z)$.

Remark 2. Similar to the method of cross sections [24], [25], [30], the solution of the last equation has the form

$$C_{\vec{\beta}_j^2}(y,z) = \frac{1}{\beta(y,z)}\exp\left\{ik_0\int\limits_{y_0,z_0}^{y,z}\left(\beta_y(y,z)dy + \beta_z(y,z)dz\right)\right\},$$

which together with relations (29), (30)–(31), (32) concludes the description of the adiabatic character of the model under consideration.

7. Conclusion

The development of methods for the rigorous and approximate analysis of smoothly irregular integrated optical waveguides requires the development of new mathematical models of the corresponding objects, as well as the use of new methods for studying the problems arising in this case. The fundamental problem of electrodynamics of smoothly irregular waveguide three-dimensional (3D) structures is the development of stable methods and algorithms for solving the corresponding Maxwell's equations.

The paper considers an approach to the formulation of the problem of propagation of electromagnetic radiation in integrated optical smoothly irregular waveguide structures. Traditionally, similar problems are formulated based on Maxwell's equations. In this paper, only monochromatic radiation is considered, which is reflected in the dependence of solution on the frequency of propagating radiation. This type of time dependence of the solution allows considering a steady-state electrodynamic problem for electromagnetic radiation.

The problem of finding the eigenvectors (guided modes) and eigenvalues is considered using the model of adiabatic guided modes in the framework of the zero approximation of the asymptotic expansion for a planar regular three-layer optical waveguide. Considering that the permittivity and permeability are piecewise constant functions, the problem is solved in each subdomain with constant values of ε, μ with subsequent matching of solutions at the interfaces between the dielectric media. In each layer ε, μ have constant values, and the construction of the entire fields $\vec{E}, \vec{H}$ requires setting and solving the problem of finding $\varphi(y, z)$.

The paper considers a class of smoothly irregular integrated-optical multilayer waveguides, the properties of which determine the characteristic features of waveguide propagation of monochromatic polarized light in them. An asymptotic approach to the description of this type of electromagnetic radiation is proposed, reducing the solutions of the system of Maxwell's equations to a form, which is expressed in terms of the solutions of a system of four ordinary differential equations and two algebraic equations for six components of the electromagnetic field in the zero approximation.

The multilayer structure of waveguides allows one more stage of reducing the model to a homogeneous system of linear algebraic equations, the nontrivial solvability condition of which specifies the relationship between the gradient of the phase front of radiation and the gradients of interfaces between thin homogeneous layers.

In the final part of the work, eigenvalues and eigenvector problems (differential and algebraic) describing adiabatic guided modes are formulated. The problem of describing the single-mode propagation of adiabatic guided modes is also formulated with emphasis on the adiabatic nature of the described approximate solution of Maxwell's equations.

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Appendix. Normal modes of a regular planar optical waveguide

"Plane" guided modes

The monographic literature [15]–[19] widely describes normal modes of a regular planar dielectric waveguide propagating along the axis Oz from $-\infty$ to ∞ (and/or back). In the vertical direction (along the Ox axis) they have the structure of standing waves, while in the horizontal direction along the waveguide they are travelling waves and are considered (not quite correctly) steady-state ('invariant') in the direction transverse with respect to the propagation direction (along the axis Oy).

The vertical distribution of the electromagnetic field of a TE mode expressed in terms of the 'leading' transverse component of the electric field E_y is given by the equation

$$\frac{d^2 E_y}{dx^2}(x) + (\varepsilon\mu - \beta^2)E_y(x) = 0. \tag{35}$$

Two other components of the electromagnetic field of the TE mode are expressed in terms of the leading one by the formulas

$$H_x = -\frac{\beta}{\mu}E_y, \qquad H_z = \frac{1}{ik_0\mu}\frac{dE_y}{dx}. \tag{36}$$

These three relations can be derived from Maxwell's equations in the form (4).

For TM modes analogous relations that follow from Maxwell's equations have the form

$$\varepsilon\frac{d}{dx}\left(\frac{1}{\varepsilon}\frac{dH_y}{dx}\right)(x) + (\varepsilon\mu - \beta^2)\,H_y(x) = 0, \tag{37}$$

$$E_x = \frac{\beta}{\varepsilon}H_y, \quad E_z = -\frac{1}{ik_0\varepsilon}\frac{dH_y}{dx}. \tag{38}$$

Equations (35) and (37) in multilayer waveguides composed of uniform regular dielectric layers, in each subdomain of the real axis (at the intersection of each layer with the vertical axis) take the form of second-order linear ordinary differential equations with constant coefficients. Therefore, the most common form of solutions to these equations is obtained using a fundamental system of solutions. Consequently, the distributions of the corresponding leading components of the electromagnetic field are written in the form of expansions of general solutions in terms of $(\sin(\chi x), \cos(\chi x))$ or $(\exp\{\pm i(\chi x)\})$ and the expansion coefficients of the particular solution are determined from the boundary conditions (22)–(23).

These solutions, in particular, can be obtained according to the following algorithm.

For guided TE modes we get a homogeneous system of linear algebraic equations (SLAE) with matrix $\mathbf{M}_{TE}^{\downarrow 4}(\beta)$ with respect to variables $A_s^+, A_1^+, A_1^+, A_c^-$

$$\begin{gathered}
A_s^+ \exp\left\{\gamma_s^j a_1\right\} = A_1^+ \exp\left\{i\chi_1^j a_1\right\} + A_1^- \exp\left\{-i\chi_1^j a_1\right\}, \\
\frac{\gamma_s^j}{ik_0} A_s^+ \exp\left\{\gamma_s^j a_1\right\} = \frac{\chi_1^j}{k_0}\left(A_1^+ \exp\left\{i\chi_1^j a_1\right\} - A_1^- \exp\left\{-i\chi_1^j a_1\right\}\right), \\
A_1^+ \exp\left\{i\chi_1^j a_2\right\} + A_1^- \exp\left\{-i\chi_1^j a_2\right\} = A_c^- \exp\left\{-\gamma_c^j a_2\right\}, \\
\frac{\chi_1^j}{k_0}\left(A_1^+ \exp\left\{i\chi_1^j a_2\right\} - A_1^- \exp\left\{-i\chi_1^j a_2\right\}\right) = -\frac{\gamma_c^j}{ik_0} A_c^- \exp\left\{-\gamma_c^j a_2\right\}.
\end{gathered}$$

The homogeneous SLAE $\left(\widehat{M}_E\right)\vec{A} = \vec{0}$ is nontrivially solvable if and only if its determinant is zero,

$$\det\left(\widehat{M}_E\right) = 0. \tag{39}$$

For guided TM modes a system of homogeneous linear algebraic equations is obtained with the matrix $\mathbf{M}_{TM}^{\downarrow 4}(\beta)$ for unknowns B_s^+, B_1^+,B_1^+,B_c^-, the solutions of which yield the values of the unknown amplitude coefficients

$$\begin{gathered}
B_s^+ \exp\left\{\gamma_s^j a_1\right\} = B_1^+ \exp\left\{i\chi_1^j a_1\right\} + B_1^- \exp\left\{-i\chi_1^j a_1\right\}, \\
\frac{\gamma_s^j}{ik_0\varepsilon_s} B_s^+ \exp\left\{\gamma_s^j a_1\right\} = \frac{\chi_1^j}{k_0\varepsilon_1}\left(B_1^+ \exp\left\{i\chi_1^j a_1\right\} - B_1^- \exp\left\{-i\chi_1^j a_1\right\}\right), \\
B_1^+ \exp\left\{i\chi_1^j a_2\right\} + B_1^- \exp\left\{-i\chi_1^j a_2\right\} = B_c^- \exp\left\{-\gamma_c^j a_2\right\}, \\
\frac{\chi_1^j}{k_0\varepsilon_1}\left(B_1^+ \exp\left\{i\chi_1^j a_2\right\} - B_1^- \exp\left\{-i\chi_1^j a_2\right\}\right) = -\frac{\gamma_c^j}{ik_0\varepsilon_c} B_c^- \exp\left\{-\gamma_c^j a_2\right\}.
\end{gathered}$$

The homogeneous SLAE $\left(\widehat{M}_H\right)\vec{B} = \vec{0}$ is nontrivially solvable if its determinant equals zero

$$\det\left(\widehat{M}_H\right) = 0. \tag{40}$$

Here A and B are the coefficients of expansion of TE and TM modes in terms of the fundamental system of solutions, respectively.

Equations (39) and (40) are equivalent to the dispersion relations in the trigonometric form

$$\chi_f d = \operatorname{arctg}\left(\frac{\gamma_c^m}{\chi_1^m}\right) + \operatorname{arctg}\left(\frac{\gamma_s^m}{\chi_1^m}\right) + m\pi \tag{41}$$

for guided TE modes and

$$\chi_f d = \operatorname{arctg}\left(\frac{\varepsilon_1\gamma_c^m}{\varepsilon_c\chi_1^m}\right) + \operatorname{arctg}\left(\frac{\varepsilon_1\gamma_s^m}{\varepsilon_s\chi_1^m}\right) + m\pi \tag{42}$$

for guided TM modes.

If the expressions for the electromagnetic field strength are presented in complex form with the described dependence on the rest coordinates and time taken into account, i.e., in the form

$$\left(E_y, H_x, H_z\right)^T(x,y,z,t) = (A_1, A_2, A_3)^T(x,y,z)\exp\left\{i\omega t - i\varepsilon_E(x,y,z)\right\},$$
$$\left(H_y, E_x, E_z\right)^T(x,y,z,t) = (B_1, B_2, B_3)^T(x,y,z)\exp\left\{i\omega t - i\varepsilon_H(x,y,z)\right\}$$

with real-valued amplitude $A(B)$ and phase $\varphi_E(\varphi_H)$, then the phase remains constant in time along x, defines a travelling wave along z, and is constant along y. In other words, the phase front of the described solution to Maxwell's equations is "planar" (i.e., linear in the yOz-plane) and defines a "plane" (i.e., linear in the yOz-plane) wave. There exist "forward" and "backward" waves travelling in opposite directions along the z-axis. The can be identified with the "plane" (in the yOz-plane) waves emitted by infinitely remote sources.

"Cylindrical" guided modes

Now let us proceed to the guided modes of a regular planar dielectric waveguide, excited by a source linear along the Ox-axis and point-like in the yOz-plane, localized at the point $(0, z_0)$. The structure of the modes along the Ox-axis completely coincides with that of "plane" guided and leaky TE and TM modes. Let us analyze the structure of cylindrical guided modes propagating in the yOz-plane

$$\begin{pmatrix}\vec{E}\\ \vec{H}\end{pmatrix}(x,y,z,t) = \begin{pmatrix}\vec{E}\\ \vec{H}\end{pmatrix}_{\beta}^{E,H}(x)\exp\left\{i\omega t - ik_0\beta r\right\},$$

where $r^2 = y^2 + (z-z_0)^2$; $y = r\sin\theta$, $z = z_0 + r\cos\theta$. In the yOz-plane circular fronts propagate from the origin of polar coordinates $y = r\sin\theta$, $z = z_0 + r\cos\theta$.

Thus, in both cases the solutions for the normal modes are written as

$$\begin{pmatrix}\vec{E}\\ \vec{H}\end{pmatrix}(x,y,z,t) = \begin{pmatrix}\vec{E}\\ \vec{H}\end{pmatrix}_{\beta}^{E,H}(x)\frac{\exp\left\{i\omega t - ik_0\varphi(y,z)\right\}}{\sqrt{\beta^{E,H}}},$$

where:

— $\varphi(y,z) = \beta z$ for the modes from an infinitely remote source and

— $\varphi(y,z) = \beta\sqrt{y^2 + (z-z_0)^2}$ for the modes from a localized source.

References

[1] A. A. Samarskii and A. N. Tikhonov, "Representation of the field in a waveguide as the sum of the TE and TM fields [O predstavlenii polya v volnovode v vide summy polej TE i TM]," *Zhurnal tekhnicheskoy fiziki*, vol. 18, no. 7, pp. 959–970, 1948, in Russian.

[2] A. G. Sveshnikov, "A substantiation of a method for computing the propagation of electromagnetic oscillations in irregular waveguides," *USSR Computational Mathematics and Mathematical Physics*, vol. 3, no. 2, pp. 413–429, 1963. DOI: 10.1016/0041-5553(63)90027-2.

[3] V. V. Shevchenko, "Spectral decomposition in eigen- and associated functions of a nonselfadjoint problem of Sturm–Liouville type on the entire axis [O spektral'nom razlozhenii po sobstvennym i prisoedinennym funkciyam odnoj nesamosopryazhennoj zadachi tipa SHturma–Liuvillya na vsej osi]," *Differ. Uravn.*, vol. 15, no. 11, pp. 2004–2020, 1979, in Russian.

[4] L. N. Deryugin, A. N. Marchuk, and V. E. Sotin, "Properties of planar asymmetrical dielectric waveguides on a substrate of dielectric [Svojstva planarnogo asimmetrichnogo dielektricheskogo volnovoda na podlozhke iz dielektrika]," *Izv. Vyssh. Uchebn. Zaved., Ser. Radioelektron.*, vol. 10, no. 2, pp. 134–141, 1967, in Russian.

[5] A. G. Sveshnikov, "The incomplete Galerkin method [Nepolnyj metod Galerkina]," *Dokl. Akad. Nauk SSSR*, vol. 236, no. 5, pp. 1076–1079, 1977, in Russian.

[6] A. A. Bykov, A. G. Sveshnikov, and M. K. Trubetskov, "Reduced Galerkin's method application to calculations of eigenwaves in open waveguides [Primenenie nepolnogo metoda Galerkina dlya rascheta sobstvennyh voln otkrytyh volnovodov]," *Matem. Mod.*, vol. 3, no. 7, pp. 111–123, 1991, in Russian.

[7] B. Z. Katsenelenbaum, *Theory of Irregular Waveguides with Slowly Varying Parameters [Teoriya neregulyarnyh volnovodov s medlenno menyayushchimisya parametrami]*. Moscow: Akad. Nauk SSSR, 1961, in Russian.

[8] V. V. Shevchenko, *Continuous Transitions in Open Waveguides [Plavnye perekhody v otkrytyh volnovodah]*. Moscow: Nauka, 1969, in Russian.

[9] L. A. Sevastianov and A. A. Egorov, "Theoretical analysis of the waveguide propagation of electromagnetic waves in dielectric smoothly-irregular integrated structures," *Optics and Spectroscopy*, vol. 105, no. 4, pp. 576–584, 2008. DOI: 10.1134/S0030400X08100123.

[10] A. A. Egorov and L. A. Sevastianov, "Structure of modes of a smoothly irregular integrated optical four-layer three-dimensional waveguide," *Quantum Electronics*, vol. 39, no. 6, pp. 566–574, 2009. DOI: 10.1070/QE2009v039n06ABEH013966.

[11] A. A. Egorov, K. P. Lovetskiy, A. L. Sevastianov, and L. A. Sevastianov, "Simulation of guided modes (eigenmodes) and synthesis of a thin-film generalised waveguide Luneburg lens in the zero-order vector approximation," *Quantum Electronics*, vol. 40, no. 9, pp. 830–836, 2010. DOI: 10.1070/QE2010V040N09ABEH014332.

[12] A. A. Egorov, A. L. Sevast'yanov, and L. A. Sevast'yanov, "Stable computer modeling of thin-film generalized waveguide Luneburg lens," *Quantum Electronics*, vol. 44, no. 2, pp. 167–173, 2014. DOI: 10.1070/QE2014v044n02ABEH015303.

[13] A. A. Egorov, A. L. Sevastyanov, E. A. Ayryan, and L. A. Sevastyanov, "Stable computer modeling of thin-film generalized waveguide Luneburg lens [Ustojchivoe komp'yuternoe modelirovanie tonkoplenochnoj obobshchennoj volnovodnoj linzy Lyuneberga]," *Matem. Mod.*, vol. 26, no. 11, pp. 37–44, 2014, in Russian.

[14] A. S. Il'inskii, V. V. Kravtsov, and A. G. Sveshnikov, *Mathematical Models of Electrodynamics [Matematicheskie modeli elektrodinamiki]*. Moscow: Vyssh. Shkola, 1991, in Russian.

[15] M. J. Adams, *An Introduction to Optical Waveguides*. New York: Wiley, 1981.

[16] T. Tamir, "Guided-Wave Optoelectronics," in *Integrated Optics*, T. Tamir, Ed. Berlin: Springer-Verlag, 1990.

[17] A. W. Snyder and J. D. Love, *Optical Waveguide Theory*. New York: Chapman and Hall, 1983.

[18] D. Markuze, *Theory of Dielectric Optical Waveguides*. New York: Academic Press, 1974.

[19] M. Barnoski, *Introduction to Integrated Optics*. New York: Plenum Press, 1974.

[20] A. I. Neishtadt, "On the accuracy of conservation of the adiabatic invariant," *Journal of Applied Mathematics and Mechanics*, vol. 45, no. 1, pp. 58–63, 1981. DOI: 10.1016/0021-8928(81)90010-1.

[21] I. V. Gorelyshev and A. I. Neishtadt, "On the adiabatic perturbation theory for systems with impacts," *Journal of Applied Mathematics and Mechanics*, vol. 70, no. 1, pp. 4–17, 2006. DOI: 10.1016/j.jappmathmech.2006.03.015.

[22] V. M. Babich and V. S. Buldyrev, *Asymptotic Methods in Short-Wavelength Diffraction Theory, Alpha Science Series on Wave Phenomena*. Harrow, UK: Alpha Science International, 2009.

[23] Y. A. Kravtsov and Y. I. Orlov, *Geometrical Optics of Inhomogeneous Media*. Berlin: Springer-Verlag, 1990.

[24] B. Z. Katsenelenbaum, "Irregular waveguides with slowly varying parameters [Neregulyarnye volnovody s medlenno menyayushchimisya parametrami]," *Doklady Akademii Nauk SSSR*, vol. 102, no. 4, p. 711, 1955, in Russian.

[25] B. Z. Katsenelenbaum, "A contribution to the general theory of nonregular wave guides [K obshchej teorii neregulyarnyh volnovodov]," *Dokl. Akad. Nauk SSSR*, vol. 116, no. 2, pp. 203–206, 1957, in Russian.

[26] A. I. Neishtadt, "Propagation of rays in smoothly irregular waveguides and perturbation theory of Hamiltonian systems [Rasprostranenie luchej v plavno neregulyarnyh volnovodah i teoriya vozmushchenij gamil'tonovyh sistem]," *Izv. vuzov. Radiofizika*, vol. 25, no. 2, pp. 218–226, 1982, in Russian.

[27] A. L. Sevastyanov, "Single-mode waveguide spread of light in a smooth irregular integral optical waveguide [Komp'yuternoe modelirovanie polej napravlyaemyh mod tonkoplenochnoj obobshchennoj volnovodnoj linzy Lyuneberga]," in Russian, Ph.D. dissertation, Peoples' Friendship University of Russia, Moscow, 2010.

[28] S. Solimeno, B. Crosignani, and P. DiPorto, *Guiding, Diffraction, and Confinement of Optical Radiation*. Orlando, FL: Academic Press, 1986.

[29] M. Kline and I. W. Kay, *Electromagnenic Theory and Geometricak Optics*. New York: Wiley (Inter-science), 1965.

[30] M. V. Fedoryuk, "A justification of the method of transverse sections for an acoustic wave guide with nonhomogeneous content," *Mathematical Physics*, vol. 13, no. 1, pp. 162–173, 1973. DOI: 10.1016/0041-5553(74)90012-3.

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Асимптотический метод построения модели адиабатических волноводных мод плавно-нерегулярных интегрально-оптических волноводов

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В работе рассмотрен класс плавно нерегулярных интегрально-оптических многослойных волноводов, свойства которых определяют характерные черты волноводного распространения в них монохроматического поляризованного света. Предложен асимптотический подход к описанию данного вида электромагнитного излучения, в результате которого решения системы уравнений Максвелла редуцируется к такому виду, который выражается через решения системы четырёх обыкновенных дифференциальных уравнений и двух алгебраических уравнений для шести компонент электромагнитного поля в нулевом приближении. Градиент фазового фронта адиабатической волноводной моды удовлетворяет уравнению эйконала относительно эффективного показателя преломления волновода относительно данной моды.

Многослойная структура волноводов позволяет произвести ещё один этап редукции системы уравнений модели к однородной системе линейных алгебраических уравнений, условие нетривиальной разрешимости которой задаёт связь градиента фазового фронта излучения с градиентами поверхностей раздела между тонкими однородными слоями.

В завершающей части работы сформулированы задачи (дифференциальная и алгебраическая) на собственные значения и собственные векторы для описания адиабатических волноводных мод. Приведена также формулировка задачи описания одномодового режима распространения адиабатических волноводных мод, подчёркивающая адиабатический характер описываемого приближенного решения уравнений Максвелла.

Ключевые слова: плавно нерегулярные интегрально-оптические многослойные волноводы, задачи на собственные значения и собственные векторы, одномодовый режим распространения адиабатических волноводных мод

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Kuryshkin–Wodkiewicz quantum measurement model for alkaline metal atoms

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The constructive form of the Kuryshkin–Wodkiewicz model of quantum measurements was earlier developed in detail for the quantum Kepler problem. For more complex quantum objects, such a construction is unknown. At the same time, the standard (non-constructive) model of Holevo–Helstrom quantum measurements is suitable for any quantum object. In this work, the constructive model of quantum measurements is generalized to a wider class of quantum objects, i.e., the optical spectrum of atoms and ions with one valence electron. The analysis is based on experimental data on the energy ordering of electrons in an atom according to the Klechkovsky–Madelung rule and on the substantiation of a single-particle potential model for describing the energy spectrum of optical electrons in alkali metal atoms. A representation of the perturbation of a single-particle potential in the form of a convolution of the potential of an electron in a hydrogen atom with the Wigner function of a certain effective state of the core in an alkali metal atom representation allows reducing all calculation algorithms for alkali metals to the corresponding algorithms for the hydrogen atom.

Key words and phrases: models of quantum measurements, energy spectrum of alkali metal atoms, method of single-particle potential, perturbation of discrete spectrum of an observable

1. Introduction

The energy spectrum $E_n = -R/(2n^2)$ of a valence electron in a hydrogen atom is described by the discrete spectrum of Hamiltonian $\hat{H} = -\Delta/2 - 1/r$ of the quantum Kepler problem with Hamilton function $H(q,p) = \vec{p}^2/(2m) - e^2/|\vec{r}|$. In addition to operator $\hat{H}$, the measured spectrum of the valence electron also depends on the state $\hat{\rho}$ of the quantum probe of a measuring instrument, i.e., is described by the discrete spectrum of the measured observable $O_\rho(H) = O_W\left(H * W_\rho\right)$ [1].

The constructive form of the Kuryshkin–Wodkiewicz quantum measurement model is thoroughly developed for the quantum Kepler problem [2]

and quantum oscillator [3], [4]. For more complex quantum objects, such a construction is unknown. At the same time, the standard (nonconstructive) Holevo–Helstrom quantum measurement model is applicable to any quantum object, any quantum system [5], [6].

The goal of this paper is to generalize the constructive quantum measurement Kuryshkin–Wodkiewicz model to a wider class of quantum objects and to develop a quantum measurement model for optical spectrum of atoms and ions with one valence electron. We will consider the alkali metal atoms that consist of a core (atomic nucleus and electrons of all filled shells) and a valence (outer) electron, as well as ions with one valence electron.

2. Hydrogen atom

Quantum mechanics understands the description of the hydrogen atom as the description of the electron in this atom. Its energy spectrum has a very simple form

$$E_n = -\frac{R}{2n^2}, \tag{1}$$

when the atom is theoretically considered as an isolated quantum object. In the process of measurement, the quantum object is no more isolated, it becomes an open system incorporated in a more complex 'object + probe' quantum system [7]–[10].

The measured energy spectrum of an electron in a hydrogen atom is perturbed with respect to the spectrum (1): $\tilde{E}_n = E_n + \delta E_n$.

Thus, a problem of description (constructing a mathematical model) of the measured values of the hydrogen atom optical spectrum. This model incorporates the Weyl–Kuryshkin quantization rule and the rigging of the above mentioned model: $\{\varphi_k\}$ is the mixed state of the quantum probe, the smoothed (perturbed) classical observable is $A * W_{\{\varphi_k\}}(q,p)$, and the Weyl rule applied to it is $O_{\{\varphi_k\}}(A) = O_W(A)$. Theoretical study of the spectrum of this operator and the numerical calculation of the discrete spectrum parts affiliated with $\{\varphi_k\}$ are published in Ref. [11]. For the hydrogen atom the model is verified with the relative accuracy of $\sim 10^{-16}$.

Before discussing the dependence of the perturbation δE_n in the hydrogen atom induced by the action of the measuring instrument with a quantum probe in the state $\{\varphi_k\}$, we recall what is known about the discrete energy spectrum E^Z_{nl} of the valence electron in an isolated alkali metal atom with the atomic number Z.

3. Energy spectrum of a valence electron in alkali metal atoms

Quantum mechanical description of the valence electron in a hydrogen atom is provided by the Schrödinger equation

$$\hat{H}_0\psi(\vec{r}) = \varepsilon\psi(\vec{r}) \tag{2}$$

with the operator $\hat{H}_0 = O_W(H)$, where O_W is the Weyl quantization rule, transforming the Hamiltonian Kepler function $H = \vec{p}^2/2 - 1/|\vec{r}|$ into Hamiltonian operator $\hat{H}_0 = -\vec{\nabla}^2/2 - 1/|\vec{r}|$. Equation (2) for the eigenvalues (the energy spectrum of the electron in the hydrogen atom) and eigenfunctions (the discrete spectrum wave functions of the hydrogen atom) has exact solutions [12]:

$$\varepsilon_n = -\frac{1}{2n^2}, \quad \psi_{nlm}(\vec{r}) = R_{nl}(r)Y_{lm}(\theta, \varphi),$$

where $\vec{r} = (r, \theta, \varphi)$ are spherical coordinates and n, l, m are the principal, orbital, and azimuthal quantum number, respectively.

While in the hydrogen atom and hydrogen-like ions, the spectral lines are ordered according to the law

$$-\frac{1}{2n^2}, \tag{3}$$

i.e., the energy spectrum is degenerate with respect to the orbital and azimuthal quantum numbers, in the energy spectrum of valence (optical) electrons in the alkali metal atoms the orbital degeneracy is removed (see Eq. (4)). The degeneracy with respect to azimuthal quantum number remains in any potential having a spherical symmetry.

In the book by V. N. Kondratyev [13] in Table 9 on page 181 the following data are presented for the optical spectra of alkali metals (in Hartree atomic units):

$$\varepsilon_{nl} = -\frac{1}{2(n - \delta(l))^2}, \tag{4}$$

namely:

(3) Li:

$e20 = -0.1982754792$, $e21 = -0.1302870145$,
$e30 = -0.07465200225$, $e31 = -0.05710578080$, $e32 = -0.05562970375$,
$e40 = -0.03883874030$, $e41 = -0.03190061096$, $e42 = -0.03128127346$,
$e50 = -0.02375325800$, $e51 = -0.02033207896$, $e52 = -0.02001600960$,
$e60 = -0.01601242872$, $e61 = -0.01408066718$, $e62 = -0.03128127346$;

(11) Na:

$e30 = -0.1888838814$, $e31 = -0.1115650818$, $e32 = -0.05592778605$,
$e40 = -0.07245191330$, $e41 = -0.05146315410$, $e42 = -0.03140683790$,
$e50 = -0.03800798912$, $e51 = -0.02949906632$, $e52 = -0.02008024064$,
$e60 = -0.02335452320$, $e61 = -0.01909585773$, $e62 = -0.03140683790$;

(19) K:

$e40 = -0.1595965400$, $e41 = -0.1010881942$, $e42 = -0.03366251684$,
$e50 = -0.06516440980$, $e51 = -0.04810386124$, $e52 = -0.02122122550$,
$e60 = -0.03517930894$, $e61 = -0.02802348772$, $e62 = -0.03366251684$;

(37) Rb:

$$e50 = -0.1534672079, \quad e51 = -0.09542857065, \quad e52 = -0.03523536413,$$
$$e60 = -0.06354834915, \quad e61 = -0.04622131078, \quad e62 = -0.06530578980;$$

(55) Cs:

$$e60 = -0.1431368322, \quad e61 = -0.09046170025, \quad e62 = -0.2075805080,$$
$$e70 = -0.06074477220, \quad e71 = -0.04452676553.$$

As a result of splitting in the spectrum (4), the ordering of the spectral (energy) levels with increasing energy changes in comparison with the ordering in the hydrogen atom (3). This new ordering obeys the so-called Klechkovsky–Madelung rule [14]–[16]. The relation of this order with the pairs (n, l) of the principal and orbital quantum number is phenomenologically described by formula (4) and is determined by the increase of the pair $(n + l, l)$: 1s, 2s, 2p, 3s, 3p, 4s, 3d, 4p, 5s, 4d, 5p, 6s, 4f, 5d, 6p, 7s, 5f, 6d, 7p, 8s, 5g. Here the values $l = 0, 1, 2, 3, ...$ correspond to the indices $s, p, d, f, ...$

At the phenomenological level, the consideration of optical spectra of alkali metal atoms leads to a necessity of using potential function in the form [13]:

$$V(r) = -\frac{e^2}{r}\left(1 + c_1\left(\frac{r_a}{r}\right) + c_2\left(\frac{r_a}{r}\right)^2 + c_3\left(\frac{r_a}{r}\right)^3 + ...\right),$$

where $c_1, c_2, ...$ are constants determined by the distortion character of the Coulomb field of the nucleus, r_a being the Bohr radius (for hydrogen atom).

4. Pseudopotential method for description of multielectron atoms

For atoms having more than one electron, even the simplest ones, the Schrödinger equation can be solved directly neither analytically, nor by numerical methods. For this reason, the study of spectra of multielectron atoms is based on an approximate model. The approximation is based on the idea of self-consistent field that implies independent motion of each electron in a certain average field created by other electrons and atomic nucleus. A set of orbitals used for constructing the wave function is referred to as atomic configuration [11]. The most adequate scheme based on single-electron orbitals and atomic configuration is the Hartree–Fock approximation.

In fact the meaning of configuration is to assign to the entire atom a set of approximate integrals of motion, specified by set of labels $\{n_j, l_j, Z_j\}$, where the subscript j enumerates the filled orbitals, and Z_j is the occupation number, i.e., the number of electrons at the j-th orbital. The number of exact integrals of motion is typically insufficient for complete classification. Therefore, approximate but well-preserved integrals of motion are of primary importance [11]. To find out which orbitals in an atom are filled, the Aufbau rule should be used, namely, for ground state the distribution of electrons over the orbitals should correspond to the minimal energy compatible with

the Pauli principle. The result of applying the Aufbau rule directly depends on the ordering of energy levels in the single-electron effective potential $U_a(r)$.

Far from the nucleus, the electron is subjected to the attractive Coulomb potential of the atomic nucleus, shielded by all other electrons, so that

$$U_a(r) \sim -\frac{1}{r}, \quad r \gg r_a, \tag{5}$$

where r_a is the characteristic radius of the atom. Near the nucleus, the shielding effect vanishes and the electron is attracted by the Coulomb potential of a bare atomic nucleus

$$U_a(r) \sim -\frac{Z}{r}, \quad r \ll r_a.$$

Considering the outer (valence) electrons, it is possible to construct a model of effective potential $U_a(r)$ based on the approximate behavior (5).

If the deviation of the effective single-electron potential $U_a(r)$ from the dependence $-1/r$ can be considered a small perturbation, then the spectrum remains ordered like in a hydrogen atom. However, when considering the periodic law this is not true, which is an evidence of strong deviations of the effective potential from the Coulomb potential, leading to essential changes in the spectrum. An overlap of groups of energy levels with different principal quantum numbers n appears together with a new type of ordering according to $(n + l, n)$.

The notion of n-shell, i.e., states with the same principal quantum number n arises from the fact that for pure Coulomb potential in a hydrogen atom these states are energy degenerate. If the potential slightly differs from the Coulomb one, the degeneracy is removed, but the energy levels with the same n remain densely grouped in the energy scale. In this case, the notion of a shell remains physically significant. Otherwise, if the deviation from Coulomb potential is large, a complete regrouping of energy levels occurs and the hydrogen-like shells loose physical meaning, becoming merely formal entities. On the contrary, the notion of 'subshell' labelled by a pair of quantum numbers $\{n, l\}$ always remains significant for atoms, since the energy levels are degenerate with respect to azimuthal quantum number m in any spherically symmetric potential.

A valence electron in an atom of alkali metal allows approximate quantum mechanical description using a single-particle model:

$$\left[-\frac{\hbar^2}{2m}\vec{\nabla}^2 + V_{\text{eff}}(\vec{r})\right]\psi(\vec{r}) = \varepsilon_{nl}\psi(\vec{r}). \tag{6}$$

For the first-order approximation the effective single-particle potential in the Thomas–Fermi method can be expressed as

$$U_a^{TF}(r) = \frac{Z}{r}\chi(kr), \quad k = \left(\frac{8\sqrt{2}}{3\pi}\right)^{2/3} Z^{1/3}.$$

through a table-defined function $\chi(r)$.

Since the middle of the last century, researchers have been looking for a theoretical justification for the fact that in a many-electron atom the single-particle potential has a form that provides the "Aufbau rule" – the Klechkovsky–Madelung rule. In a number of articles and then in the book [15], Klechkovsky constructed this justification, starting from the Hartree–Fock approximation. The pseudopotential is expressed through the tabular function χ, which is approximated by the expression:

$$\chi(x) = (1 + ax)^{-2}.$$

At the same time, a number of researchers concluded that the desired pseudopotential has the form:

$$U_a^Z(r) = -\frac{Z}{r\left(1 + \frac{r}{R}\right)^2}, \quad R = \frac{1}{a\sqrt{Z}}\left(\frac{3\pi}{8\sqrt{2}}\right)^{2/3}.$$

Demkov and Ostrovsky [17], [18] substantiated the existence of such a single-particle potential proceeding from the geometric-symmetry model of the hydrogen atom by V.A. Fock [19].

$$U_\mu^{DO}(r) = -\frac{2\nu}{r^2R^2}\left[\left(\frac{r}{R}\right)^\mu + \left(\frac{R}{r}\right)^\mu\right]^{-2}. \tag{7}$$

In [17], [18] Demkov and Ostrovsky established that equation (7) provides the most precise description of Klechkovsky–Madelung rule at $\mu = 1/2$. In subsequent papers [20], [21] Demkov and Ostrovsky's proof was questioned, but the result was confirmed.

Remark 1. Subsequently, when considering the multielectron atom in the framework of the quantum field theory, Kholodenko et al. [22], [23] confirmed the correctness of the Demkov–Ostrovsky proof, and also generalized this result to such a degree that he began to describe not only the Klechkovsky–Madelung rule, but also exceptions to it (see also [24], [25]).

These potentials are in good agreement with the experimentally observed spectra:

$$\varepsilon_{nl} = -\frac{1}{2(n + \delta(l))^2} = -\frac{1}{2n_{\text{eff}}^2}.$$

in Hartree atomic units.

The solution obtained is not universal, since there are exceptions to the Madelung rule in transition metals, as well as among lanthanides and actinides. Quantum-mechanically, these exceptions, as well as the rule itself, are still considered using relativistic Hartree–Fock calculations. The results obtained do not yet detail the exceptions. Kholodenko and Kaufman [23], using quantum field theory, showed that the Demkov–Ostrovsky potential does indeed give the correct answer. In addition, thanks to work [26], it became possible to identify the Demkov–Ostrovsky potential $U_{1/2}^{DO}(r)$ with the Hartree–Fock potential.

Remark 2. It was shown in [22] that, confining oneself to quantum mechanical methods, it is impossible to derive Madelung's rule with exceptions. Madelung's rule and its exceptions contain much more information than is required for its use in chemistry. Recall that the invention of quantum mechanics in 1925–1926 was initially driven by the needs of atomic physics. Subsequently, quantum mechanics was extended to quantum field theory, which led to the development of the Standard Model of particle physics. Not surprisingly, particle physics methods have recently been applied to the periodic table of elements [25], [27]. In [22], it was demonstrated that the Madelung rule and its exceptions can be described within the framework of this model.

5. Modeling the measured energy spectrum of alkali metal atoms

So far, we have mainly dealt with the study of the quantum-measured energy state of the valence electron in the hydrogen atom. The energy spectrum of a non-measured (isolated) hydrogen atom has the form $\varepsilon_{nl} = -1/(2n^2)$, degenerate with respect to the orbital quantum number l. The measurement procedure slightly perturbs potential energy $V_0(\vec{r}) = -1/r$ of the isolated hydrogen atom to $V_\rho(\vec{r}) = -1/r + \delta V_\rho(\vec{r})$, so that the perturbed spectrum of the hydrogen atom subjected to measurement has the form $\varepsilon^\kappa_{nl} = -1/(2n^2) + \delta E^1_\kappa$. Under such weak perturbation, the ordering of spectral lines remains unchanged.

However, even in first spectral lines of alkali metals the Klechkovsky–Madelung ordering is observed.

In "hydrogen-like" alkali metal atoms the spectral terms have the form

$$E^Z_{nl} = -\frac{R}{2(n+\sigma^Z_l)^2}.$$

In the process of measurement, the "measured" energy spectrum takes the form

$$E^Z_{nl,\kappa} = -\frac{R}{2(n+\sigma^Z_l)^2} + \delta E^Z_\kappa,$$

where the contributions δE^1_κ and δE^Z_κ are obtained from convolution $V(r) * W_{\{\varphi_k\}}(q,p)$, where

$$V^1(r) = -\frac{1}{r};$$

$$U^Z_a(r) = -\frac{Z}{r\left(1+\frac{r}{R}\right)^2}, \quad R = \frac{1}{a\sqrt{Z}}\left(\frac{3\pi}{8\sqrt{2}}\right)^{\frac{2}{3}}. \tag{8}$$

Therefore, the Weyl–Kuryshkin quantization rule is adequate for alkali metals to the same degree as adequate is potential $V_\kappa(r,\vartheta)$ that takes into account small corrections to the centrally symmetric potential.

Ref. [23] shows the coincidence of the Demkov–Ostrovsky potential (7) with the Hartree–Fock potential (6). Similar to the potential $V_\rho(\vec{r})$ from the Kuryshkin–Wodkiewicz quantization rule [28], potential $V^Z(\vec{r})$ from equation (8) is an $\hat{H}_0$-compact perturbation of the potential $V^1(\vec{r})$ that equals zero at infinity (see the papers by B. Simon [29], [30] about Kato theorems). Thus, potential $U_\mu^{DO}(r)$ satisfies the conditions of the theorem from Ref. [31].

6. Kuryshkin–Wodkiewicz quantum measurement model for alkali metal atoms and ions with one valence electron

For valence electron in a hydrogen atom the potential has the form $V_1(r) = -1/r$ and the energy spectrum is $\varepsilon_n = -1/(2n^2)$. In the process of measurement with an instrument whose quantum part is in the state $\rho = \sum c_j \left|\psi_j\right\rangle\left\langle\psi_j\right|$ both the potential and the spectrum are perturbed:

$$\rho : V_1(r) \mapsto V_\rho(r) = V_1(r) + \delta V_\rho(r),$$

$$\rho : \varepsilon_n = -\frac{1}{2n^2} \mapsto \varepsilon_{nl}^\rho = -\frac{1}{2n^2} + \delta\varepsilon_{nl}^\rho.$$

In this case $V_\rho(r) = \left(V_1 * W_\rho\right)(r)$;

$$O_\rho(H) = O_W(H * W_\rho) = O_W\left(\left(\frac{p^2}{2} - \frac{1}{r}\right) * W_\rho\right) = \\ = -\frac{1}{2}\nabla^2 + C_\rho\hat{I} + \left(V_\rho = V_1 * W_\rho = V_1 + \delta V_\rho\right)\hat{I}.$$

For a valence electron in an atom of alkali metal, the potential has asymptotic expressions

$$-\frac{Z}{r} \underset{r\to 0}{\longleftarrow} V^Z(r) \underset{r\to\infty}{\longrightarrow} -\frac{1}{r},$$

approximately equals $V_{\text{eff}}(r)$ from the Hartree–Fock method and conventionally has the form

$$U_{1/2}^{D-O}(r) = -\frac{2\nu}{r^2R^2}\left[\sqrt{\frac{r}{R}} + \sqrt{\frac{R}{r}}\right]^{-2}. \tag{9}$$

Then the spectrum is traditionally presented in the form

$$\varepsilon_{nl}^Z = -\frac{1}{2\left(n_{\text{eff}}^Z\right)_{nl}^2} = -\frac{1}{2\left(n + \sigma_{\text{eff}}^Z\right)_{nl}^2}. \tag{10}$$

According to the theorem of Ref. [31], there exists such an abstract state $\rho_Z = \sum f_j \left|\psi_j\right\rangle\left\langle\psi_j\right|$, that

$$\rho_Z : V_1(r) \mapsto V_Z(r) = \left(V_1 * W_{\rho Z}\right)(r) = V_1(r) + \delta V_Z(r), \tag{11}$$

$$\rho_Z : \varepsilon_n = -\frac{1}{2n^2} \mapsto \varepsilon_{nl}^Z = -\frac{1}{2\left(n_{\text{eff}}^Z\right)_{nl}^2} = -\frac{1}{2\left(n+\sigma_{\text{eff}}^Z\right)_{nl}^2}. \tag{12}$$

Now let us apply the procedure of measuring the energy spectrum of the valence electron in an alkali metal atom with an instrument whose quantum part is in the state $\rho_{ap} = \sum c_j \left|\psi_j\right\rangle\left\langle\psi_j\right|$. As a result of the measurement the perturbation of the pseudopotential and the spectrum will occur:

$$\rho_{ap} : V_Z(r) \mapsto V_{\rho_{ap}}^Z(r) = \left(V_Z * W_{\rho_{ap}}\right)(r) = V_Z(r) + \delta V_{\rho_{ap}}^Z(r), \tag{13}$$

$$\rho_{ap} : \varepsilon_{nl}^Z = -\frac{1}{2\left(n_{\text{eff}}^Z\right)_{nl}^2} \mapsto \varepsilon_{nl}^Z + \left(\delta\varepsilon_{\rho_{ap}}^Z\right)_{nl}.$$

Let us rewrite relation (13) in more detail

$$V_{\rho_{ap}}^Z(r) = \left(V_z * W_{\rho_{ap}}\right)(r) = \left(\left(V_1 * W_{\rho z}\right) * W_{\rho_{ap}}\right)(r) =$$
$$= \left(\left(V_1 + \delta V_Z\right) * W_{\rho_{ap}}\right)(r) = V_1(r) + \delta V_\rho(r) + \left(\delta V_z * W_{\rho_{ap}}\right)(r).$$

In this case

$$H^Z * W_{\rho_{ap}} = \left(H_1 * W_{\rho_Z}\right) * W_{\rho_{ap}} = \left(\left(\frac{p^2}{2} - \frac{1}{r}\right) * W_{\rho_Z}\right) * W_{\rho_{ap}}$$

and

$$O_\rho(H) = O_W(H * W\rho) = O_W\left(\left(\frac{p^2}{2} - \frac{1}{r}\right) * W_\rho\right) =$$
$$= -\frac{1}{2}\nabla^2 + C_\rho\hat{I} + \left(V_\rho = V_1 * W_\rho = V_1 + \delta V_\rho\right)\hat{I}.$$

7. Discussion

Ref. [28] describes a program calculating elements of the Ritz matrix and storing them in external files. According to the Ritz method, the eigenvalues of the Ritz matrix are spectral values of the quantity under study, i.e., the energy. This algorithm consists in solving generalized eigenvalue problem $M\vec{x} = B\vec{x}$, where M is the Ritz matrix and B is the matrix of pair scalar products of auxiliary functions in the Kuryshkin quantum mechanics. The program allows calculating Ritz matrices of arbitrary dimension. However, there are hardware limitations. To date the calculations are possible for matrix dimension of 55 and 91. Parameter E_0 is the only one to be fitted to experimental data. For example, Figures 1 and 2 show the dependences of discrepancies on E_0 for first few energy levels of lithium atom and Figure 3 for sodium atom. The discrepancy functions are seen to have expressed minima that determine the effective fitted values of the parameters.

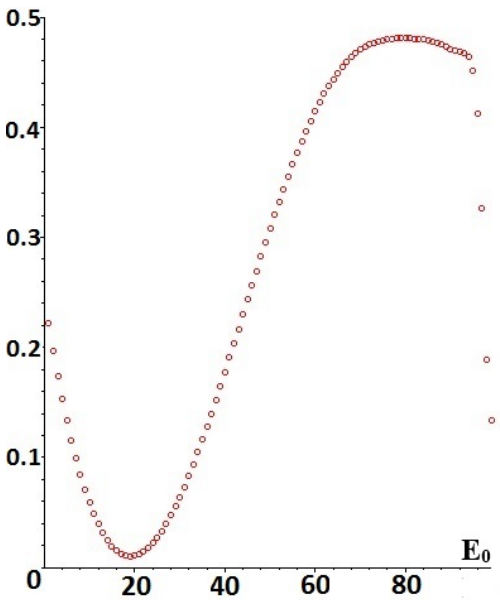

Figure 1. Quadratic discrepancy versus parameter E_0 for a group of first four energy levels of a lithium atom

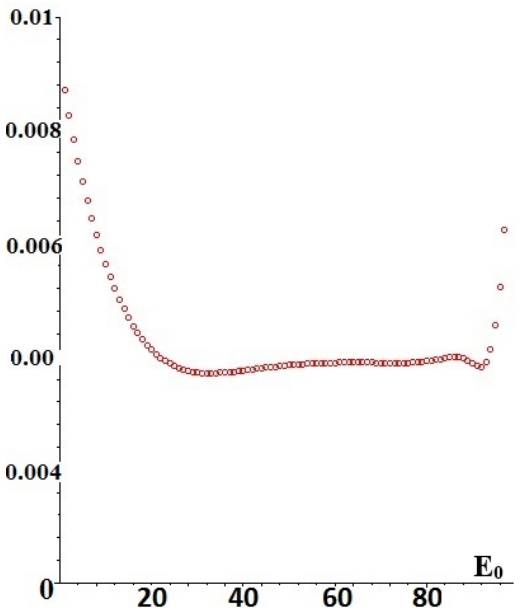

Figure 2. Quadratic discrepancy versus parameter E_0 for a group of first 8 energy levels of a lithium atom

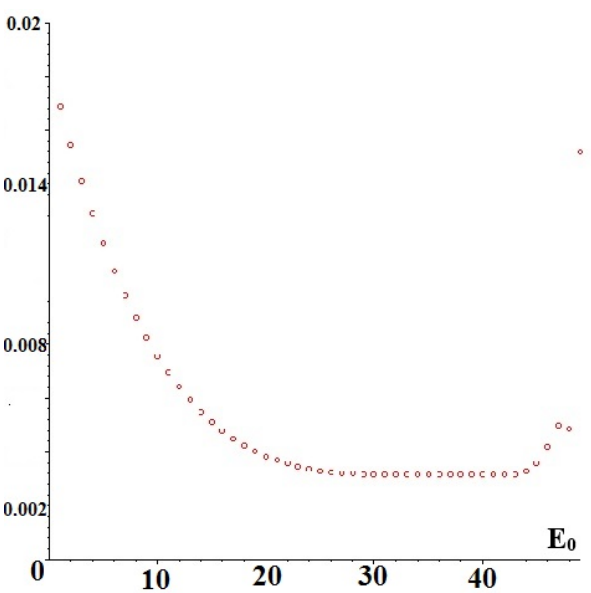

Figure 3. Quadratic discrepancy versus parameter E_0 for a group of first 4 energy levels of a sodium atom

Let us describe an algorithm for restoring the effective potential parameters for a valence electron in an alkali metal atom and the parameters of the energy spectrum perturbation of this valence electron in the process of measurement.

1. Known "theoretical" spectrum (10) and (12) of the valence electron in an alkali metal atom, we can restore $\rho_Z = \sum f_j \left|\psi_j\right\rangle\left\langle\psi_j\right|$ from (12):
   — for individual "segments" of the spectrum (10) and (12);
   — for the "initial part" of the spectrum (10) and (12) from the spectrum ordered according to the Klechkovsky–Madelung rule.
2. Restore $V_Z(r) = (V_1 * W_{\rho Z})(r)$ from (11).
3. Compare the restored pseudopotential with the effective pseudopotential (9) (current verification).
4. Restore $\rho_{ap} = \sum c_j \left|\psi_j\right\rangle\left\langle\psi_j\right|$ from individual segments of table-defined spectrum using the calculated $\left\{f_j^Z\right\}$ from item 1:

$$O_{\rho_{ap}}(H^Z) = O_W\left(H^Z * W_{\rho_{ap}}\right) = O_W\left(\left(H^1 * W_{\rho_Z}\right) * W_{\rho_{ap}}\right).$$

5. Check by means of the calculated probabilities of "optical transitions" and compare with the data from [32] (final verification).

8. Conclusion

In Refs. [2], [28] the Kuryshkin–Wodkiewicz model of quantum measurement was implemented in application to the quantum Kepler problem. Earlier the quantum measurement model in certain modifications has been implemented in application to the quantum oscillator problem [3], [4]. In the present paper the Kuryshkin–Wodkiewicz model, realizing the Weyl–Kuryshkin quantization rule [2], [28], is generalized to quantum systems with one valence electron, e.g., atoms of alkali metals. The analysis is based on experimental data on the energy ordering of electrons in an atom according to the Klechkovsky–Madelung rule and on the substantiation of a single-particle potential model for describing the energy spectrum of optical electrons in alkali metal atoms.

The author of Ref. [31] obtained a representation of the perturbation of a single-particle potential in the form of a convolution of the potential of an electron in a hydrogen atom with the Wigner function of a certain effective state of the core in an alkali metal atom. This representation allows reducing all calculation algorithms for alkali metals to the corresponding algorithms for the hydrogen atom. The proof of the model consistency is based on two Kato theorems [29], [30]. In the course of the proof, explicit formulas were obtained for the discrete spectrum of a valence electron for various spectral series, depending on the serial parameters of the disturbance of the spectrum of an isolated object in the process of quantum measurements.

References

[1] A. V. Zorin and L. A. Sevastianov, "Hydrogen-like atom with nonnegative quantum distribution function," *Physics of Atomic Nuclei*, no. 70, pp. 792–799, 2007. DOI: 10.1134/S1063778807040229.

[2] L. Sevastyanov, A. Zorin, and A. Gorbachev, "Pseudo-Differential Operators in an Operational Model of the Quantum Measurement of Observables," in *Mathematical Modeling and Computational Science*, G. Adam, J. Buša, and M. Hnatič, Eds., vol. 7125, Berlin, Heidelberg: Springer Berlin Heidelberg, 2012, pp. 174–181. DOI: 10.1007/978-3-642-28212-6_17.

[3] G. M. D'Ariano, U. Leonhardt, and H. Paul, "Homodyne detection of the density matrix of the radiation field," *Phys. Rev. A*, vol. 52, R1801–R1804, 1995. DOI: 10.1103/PhysRevA.52.R1801.

[4] G. M. D'Ariano, "Measuring Quantum States," in *Concepts and Advances in Quantum Optics and Spectroscopy of Solids*, T. Hakioglu and A. S. Shumovsky, Eds., Amsterdam: Kluwer Acad. Publishers, 1997, pp. 175–202.

[5] A. S. Holevo, *Statistical Structure of Quantum Theory*, ser. Lecture Notes in Physics Monographs. Berlin: Springer, 2001, vol. 67. DOI: 10.1007/3-540-44998-1.

[6] C. W. Helstrom, *Quantum Detection and Estimation Theory*. New York: Academic Press, 1976.

[7] G. Ludwig, *Attempt of an axiomatic foundation of quantum mechanics and more general theories, II*, ser. Commun. Math. Phys. 2001, vol. 4. DOI: 10.1007/BF01653647.

[8] E. B. Davies and J. T. Lewis, "An operational approach to quantum probability," *Communications in Mathematical Physics*, vol. 17, no. 3, pp. 239–260, 1970.

[9] M. Ozawa, *Quantum reality and measurement: A quantum logical approach*, ser. Foundations of Physics. 2011, vol. 41, pp. 592–607.

[10] M. Ozawa and Y. Kitajima, *Reconstructing Bohr's Reply to EPR in Algebraic Quantum Theory*, ser. Foundations of Physics. 2012, vol. 42, pp. 475–487. DOI: 10.1007/s10701-011-9615-7.

[11] A. V. Zorin, L. A. Sevastianov, and N. P. Tretyakov, "Computer modeling of hydrogen-like atoms in quantum mechanics with nonnegative distribution function," *Programming and Computer Software*, vol. 33, no. 2, pp. 94–104, 2007. DOI: 10.1134/S0361768807020077.

[12] V. A. Fock, *Foundations of quantum mechanics*. Mir Publishers, 1978.

[13] V. Kondratyev, *The Structure of Atoms and Molecules*. Univ Pr. of the Pacific, 2002.

[14] V. N. Ostrovsky, "What and How Physics Contributes to Understanding the Periodic Law," *Foundations of Chemistry*, no. 3, pp. 145–181, 2001. DOI: 10.1023/A:1011476405933.

[15] V. M. Klechkovskii, *The Distribution of Atomic Electrons and the Rule of Successive Filling of (n + l)-Groups [Raspredelenie atomnyh elektronov i pravilo posledovatel'nogo zapolneniya (n + l)-grupp]*. Moscow: Atomizdat, 1968, in Russian.

[16] E. Madelung, *Die Mathematischen Hilfsmittel des Physikers, 3rd edition*. Berlin: Springer, 1936. DOI: 10.1007/978-3-662-21800-6.

[17] Y. N. Demkov and V. N. Ostrovskii, "Internal Symmetry of the Maxwell "Fish-eye" Problem and the Fock Group for the Hydrogen Atom," *JETP*, vol. 33, no. 6, pp. 1083–1087, 1971.

[18] Y. N. Demkov and V. N. Ostrovsky, "n+l Filling Rule in the Periodic System and Focusing Potentials," *JETP*, vol. 35, no. 1, pp. 66–69, 1972.

[19] V. A. Fock, "Hydrogen atom and non-Euclidean geometry," *Zs. Phys.*, vol. 98, p. 145, 1935.

[20] Y. Kitagawara and A. O. Barut, "Period doubling in the n+l filling rule and dynamical symmetry of the Demkov–Ostrovsky atomic model," *Journal of Physics B: Atomic and Molecular Physics*, vol. 16, no. 18, pp. 3305–3327, 1983. DOI: 10.1088/0022-3700/16/18/006.

[21] Y. Kitagawara and A. O. Barut, "On the dynamical symmetry of the periodic table. II. Modified Demkov-Ostrovsky atomic model," *Journal of Physics B: Atomic and Molecular Physics*, vol. 17, no. 21, pp. 4251–4259, 1984. DOI: 10.1088/0022-3700/17/21/013.

[22] A. L. Kholodenko. (2020). "From Mendeleev to Seiberg-Witten via Madelung. Available from." accessed Jul 16 2020, [Online]. Available: https://www.researchgate.net/publication/341597880.

[23] A. L. Kholodenko and L. H. Kauffman, "How the modified Bertrand theorem explains regularities of the periodic table I. From conformal invariance to Hopf mapping," 2019. arXiv: 1906.05278.

[24] Y. B. Rumer and A. I. Fet, "The group Spin (4) the Mendeleev system," *Theor. Math. Phys*, vol. 9, pp. 1081–1085, 1971. DOI: 10.1007/BF01036944.

[25] V. V. Varlamov, "Group Theoretical Description of Periodic System of Elements [Teoretiko-gruppovoe opisanie periodicheskoj sistemy elementov]," *Mathematical Structures and Modelling*, vol. 46, no. 2, pp. 5–23, 2018, in Russian. DOI: 10.25513/2222-8772.2018.2.5-23.

[26] D. Kirzhnitz, Y. Lozovik, and G. Shpatkovskaya, "Statistical model of matter," *Sov. Phys. Uspekhi.*, vol. 18, no. 9, pp. 649–672, 1975. DOI: 10.1070/PU1975v018n09ABEH005199.

[27] A. Fet, *Group Theory of Chemical Elements*. Berlin: de Gryuter, 2016.

[28] L. Sevastianov, A. Zorin, and A. Gorbachev, "A Quantum Measurements Model of Hydrogen-Like Atoms in Maple," in *Computer Algebra in Scientific Computing*, V. P. Gerdt, W. Koepf, E. W. Mayr, and E. V. Vorozhtsov, Eds., vol. 8136, Cham: Springer International Publishing, 2013, pp. 369–380. DOI: 10.1007/978-3-319-02297-0_30.

[29] B. Simon, "Tosio Kato's work on non-relativistic quantum mechanics: Part 1," *Bulletin of Mathematical Sciences*, no. 8, pp. 121–232, 2018. DOI: 10.1007/s13373-018-0118-0.

[30] B. Simon, "Tosio Kato's work on non-relativistic quantum mechanics, Part 2," *Bulletin of Mathematical Sciences*, vol. 9, no. 1, p. 1 950 005, 2019. DOI: 10.1142/S166436071950005X.

[31] A. V. Zorin, "Approximate Computation of States with Minimal Dispersion in Kuryshkin–Wodkiewicz Quantum Mechanics," in *2019 11th International Congress on Ultra Modern Telecommunications and Control Systems and Workshops (ICUMT), Dublin, Ireland, 2019*, 2019, pp. 1–5. DOI: 10.1109/ICUMT48472.2019.8971007.

[32] (2020). "Physical reference data." accessed Jul 16 2020, [Online]. Available: https://www.nist.gov/pml/productsservices/physical-reference-data/.

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Модель квантовых измерений Курышкина–Вудкевича для атомов щелочных металлов

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Конструктивная форма модели квантовых измерений Курышкина–Водкевича ранее была подробно разработана для квантовой задачи Кеплера. Для более сложных квантовых объектов такая конструкция неизвестна. В то же время стандартная (неконструктивная) модель квантовых измерений Холево–Хелстрома подходит для любого квантового объекта. В данной работе конструктивная модель квантовых измерений обобщена на более широкий класс квантовых объектов, то есть на оптический спектр атомов и ионов с одним валентным электроном. Анализ основан на экспериментальных данных об энергетическом упорядочении электронов в атоме по правилу Клечковского–Маделунга и на обосновании одночастичной потенциальной модели для описания энергетического спектра оптических электронов в атомах щелочных металлов. Представление возмущения одночастичного потенциала в виде свертки потенциала электрона в атоме водорода с функцией Вигнера некоторого эффективного состояния остова в представлении атома щелочного металла позволяет редуцировать все алгоритмы расчета для щелочных металлов к соответствующим алгоритмам для атома водорода.

Ключевые слова: модели квантовых измерений, энергетический спектр атомов щелочных металлов, метод одночастичного потенциала, модель квантовых измерений, возмущение дискретного спектра наблюдаемой