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PERTURBATION THEORY FOR THE ONE-DIMENSIONAL SCHRÖDINGER SCATTERING PROBLEM

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1. Introduction

Perturbation theory [1,2] is one of the powerful mathematical methods of investigating quantum mechanical problems. Many versions [1-4] of this theory are realised by the uniform, from the mathematical viewpoint, scheme based on the iteration method known in the theory of differential equations [5]. In that scheme, one can, rather conditionally, distinguish five basic stages.

Stage 1. The initial problem for a set $\mathcal{F}$ of unknown functions is formulated in terms of new unknown functions forming some set $\mathcal{Y}$. This formulation should satisfy two basic requirements: first, the representation

$$f = f(\mathcal{Y}, \dots) \tag{1}$$

of each sought function f, connected with the initial problem ($f \in \mathcal{F}$), should be rather smooth and simple; second, the problem for new unknown functions should have a form most convenient for its investigation by the standard iteration method.

Stage 2. By this method, each function y of the set $\mathcal{Y}$ is put into correspondence with the iteration sequence $\{y^{(m)}\}_{m=-1}^{\infty}$. Usually, as its first element $y^{(-1)}$ one uses a known and easily calculable function having a simple physical meaning and the rest of the elements are constructed in the following recursive way. Index m successively ($m = 0, 1, \dots$) increases. At each step, the element $y^{(m)}$ is determined by the equality

$$y^{(m)} = y(\mathcal{Y}^{(m-1)}, \dots) \quad , \tag{2}$$

i.e., is assumed to be equal to the right-hand side of the relation

$$y = y(\mathcal{Y}, \dots) \tag{3}$$

determining the corresponding function y, in which all the functions of the set $\mathcal{Y}$ are replaced by (m-1) elements, found earlier, of the corresponding iteration sequences. This change generates a set $\mathcal{Y}^{(m)}$ from the set $\mathcal{Y}$.

Stage 3. First, the conditions are determined under which for any function y of the set $\mathcal{Y}$ in a predetermined sense (for instance, in the C^0-metric [6]) the following limiting relations hold:

$$y^{(m)} \to y \quad , \qquad {}^{(m)}y \equiv y - y^{(m)} \to 0 \quad , \qquad m \to \infty \tag{4}$$

due to which approximation $y \simeq y^{(m)}$ of the function y of the elements $y^{(m)}$ of its iteration sequence is valid at large enough m. Then, the accuracy ${}^{(m)}y$ of that approximation is estimated.

Stage 4. Each sought function f of the set $\mathcal{F}$ is put into correspondence to the sequence $\{f^{(m)}\}_{m=0}^{\infty}$. Each its element is determined as right-hand side of the corresponding representation (1) in which each function y is replaced by the function $y^{(m-1)}$ approximating it:

$$f^{(m)} = f(\mathcal{Y}^{(m-1)}, \dots) \quad , \qquad m = 0, 1, \dots \tag{5}$$

Then, it is proved that the limiting relations

$$f^{(m)} \to f \quad , \qquad {}^{(m)}f \equiv f - f^{(m)} \to 0 \quad , \qquad m \to \infty \quad , \tag{6}$$

hold in the same sense and under the same conditions as the relations (4).

Stage 5). It is analysed how sufficient conditions of perturbation theory and the relations (6) depend on parameters and functions containing in them. The main aim of that analysis are: to establish all the cases in which sufficient conditions hold; to indicate the additional conditions under which perturbation theory becomes more effective and to explain the meaning of the last conditions from intuitive-physical point of view.

Physical and mathematical intuition is the guarantee of successful realisation of the first and second stages of the above-described sheme. This intuition helps one to reformulate the initial problem and choose the zero approximation in a most appropriate way.

As a rule, the third and fourth stages of the above scheme are most difficult. However, they provide a mathematical correctness of perturbation theory developed, i.e. ensure that, first, the constructed function $f^{(m)}$ is really an approximation of the function f studied, and second, is an approximation being improved with increasing m. It is obvious that the use of $f^{(m)}$ instead of f without such an assurance is senseless. A rich and brilliant collection of instructive examples confirming this statement is available in the book [7] by Peierls.

The last stage is an urgent and interesting investigation which establishes the region of applicability of perturbation theory and, moreover, discoveres new possibilities for using of this theory.

The present paper is aimed at constructing, according to the above-described scheme, a peculiar perturbation theory for the one-dimensional Schrödinger scattering problem:

$$(\partial_x^2 - l(l+1)x^{-2} - V_c(x) - V(x) + q^2)u_l^{\pm}(x,q) = 0 \quad , \qquad x \in \mathcal{R}^+ \quad , \qquad (7a)$$

$$u_l^{\pm} = O(x^{\pm(l+1/2)+1/2}) \quad , \qquad x \to 0 \quad , \qquad (7b)$$

$$u_l^{\pm}(x,q) \to \sin(\rho - \eta ln 2\rho - (2l+1 \mp 1)\pi/4 + \delta_{cl}(q) + \delta_l(q)) \ , \quad x \to \infty \quad , \qquad (7c)$$

with really fixed parameters l and q ($l \in \mathcal{R}^+ \equiv l : 0 \le l \le \infty, \quad 0 < q < \infty$), Coulomb potential $V_c \equiv signR/x$ and the potential V obeying the only rather a general condition

$$I_l(b,x) \equiv (2\pi/(2l+1))^{1/2} \int_b^x t \, |V(t)| \, dt < \infty \quad , \qquad 0 \le b \le x \le \infty \quad . \qquad (8)$$

Here we have used the system of units, in which $\hbar = 2\mu = 1$, instead of the distance r and momentum k we have introduced the dimensionless independent variable $x \equiv r/|R|$ and dimensionless parameter $q \equiv k|R|$, the Bohr radius [1] $R \equiv \hbar^2/2\mu Z_1 Z_2 e^2$ is determined so that $signR = signV_c$, and the symbols $\rho \equiv kr = qx$, $\eta \equiv 1/2kR = signR/2q$, u_l^+, u_l^- and δ_l denote, respectively, the standard Coulomb variable, the Zommerfeld parameter, the sought regular and irregular wave functions and the scattering phase generated by the interference of the Coulomb potential and the potential V in addition to the pure Coulomb phase δ_{cl}.

Further, where possible, the index l is omitted; if not specified, it is assumed that $x \in \mathcal{R}^+$, $\rho = qx$, and the symbol b denotes a certain fixed value of the variable x.

2. Perturbation Theory

Stage 1. The Coulomb functions [8] $F_l(\rho,\eta)$ and $G_l(\rho,\eta)$ are thoroughly studied and coincide with the solutions $u^+(x,q)$ and $u^-(x,q)$ of the problem (7) in the trivial case ($V \equiv 0$). Therefore, it is reasonable to use F and G as known and , to a certain extent, standard functions. Moreover, to use them so as to reduce the initial problem to a simpler one. Just for this purpose, the method of varying constant coefficients [5] (in fact, equivalent to the linear version of the variable phase approach [9,10]) is applied as follows.

Instead of each sought function u^+ and u^- the couple new unknown functions c^+, s^+ and , respectively, c^-, s^- are introduced. By definition $c^\pm$ and $s^\pm$ are "constant" coefficients [5] or amplitude functions [10] satisfying the following Lagrange identities [11]:

$$F(\rho,\eta)\ \partial_x c^\pm(x,q) + G(\rho,\eta)\ \partial_x s^\pm(x,q) \equiv 0 \quad . \tag{9}$$

The solution u^+ and then u^- is sought for in the form

$$u^\pm(x,q) = N^\pm(q)\ U^\pm(x,q) + \left\{ \begin{array}{c} 0 \\ \alpha(q)\ u^+(x,q) \end{array} \right\} \quad , \tag{10a}$$

where

$$U^\pm(x,q) \equiv c^\pm(x,q)\ F(\rho,\eta) + s^\pm(x,q)\ G(\rho,\eta) \quad , \tag{10b}$$

and $N^\pm(q)$ and $\alpha(q)$ are determined as factors ensuring the normalisation (7c).

By the known method [5,10], based on the substitution of the functions $u^\pm$ in the form of (10a) into eq. (7a) and subsequent use of the Wronskian relation [8]

$$G(\rho,\eta)\ \partial_x F(\rho,\eta) - F(\rho,\eta)\ \partial_x G(\rho,\eta) \equiv q$$

and the identity (9), one can get two systems (the first for c^+ and s^+, and the second for c^- and s^-) of ordinary linear and homogeneous differential equations of the first order:

$$\partial_x \left\{ \begin{array}{c} c^\pm(x,q) \\ s^\pm(x,q) \end{array} \right\} = q^{-1}\ V(x)\ U^\pm(x,q) \left\{ \begin{array}{c} +G(\rho,\eta) \\ -F(\rho,\eta) \end{array} \right\} \quad . \tag{11a}$$

For the wave functions $u^\pm$ in the form of (10) to have the required asymptotics (7b), the systems of eqs. (11a) for c^+, s^+ and c^-, s^- are to be added by the corresponding boundary conditions:

$$\left\{ \begin{array}{c} c^+(x,q) \\ s^+(x,q) \end{array} \right\} \to \left\{ \begin{array}{c} 1 \\ 0 \end{array} \right\} + q^{-1} \int_0^x V(t)\ F(\rho,\eta) \left\{ \begin{array}{c} +G(\rho,\eta) \\ -F(\rho,\eta) \end{array} \right\} dt \tag{11b}$$

and

$$c^-(x,q) \to c^-(x_0,q) + q^{-1} \int_{x_0}^x V(t)\ G^2(\rho,\eta)\, dt \quad ,$$

$$s^-(x,q) \to -q^{-1} \int_0^x V(t)\ F(\rho,\eta)\ G(\rho,\eta)\, dt \quad . \tag{11c}$$

Here $x \to 0$, $\rho = tq$; if the product $V(x)\, G^2(\rho,\eta)$ is integrable in the vicinity of zero, then $x_0 = 0$ and $c^-(x,q) = 0$ otherwise x_0 is an arbitrary but fixed parameter satisfying the inequalities $x < x_0$ and $x_0 q \ll 1$; and the functions c^- and s^- are derived by the method described below. It is based on the displacement of boundary conditions from the point $x = 0$ to the point $x = x_0$ and on the identity

$$W(x,q) \equiv c^+(x,q)\ s^-(x,q) - c^-(x,q)\ s^+(x,q) \equiv 1 \quad , \tag{12a}$$

for the Wronskian relation [5] of the problem (11). The method consists in the following construction.

So let the function $V(x)\, G^2(\rho,\eta)$ be integrable in the vicinity of zero. Then, according to (11b) and (11c) the function c^-, unlike the functions c^+, s^+ and s^-, has asymptotics diverging as $x \to 0$. The values of $c^+(x_0,q)$, $s^+(x_0,q)$ and $s^-(x_0,q)$ are found by solving the problem (11) for the functions c^+ and s^+ in the interval $[0, x_0]$, and correspondingly, by formula (11c) for the asymptotics of s^-. These values are substituted into the identity (12a) written down at $x = x_0$. The equation derived is solved with respect to $c^-(x_0,q)$. Now, with the values of $c^-(x_0,q)$ and $s^-(x_0,q)$ being known, the sought functions c^- and s^- are given at $x \le x_0$ explicitly by their asymptotics (11c) and at $x \ge x_0$ they are determined as a solution of eqs. (11a) with the boundary conditions at the point $x = x_0$.

Using the construction described and the known theorems [5] one can easily prove, first, that under the condition (8) both the problems (11) are uniquely solvable in the class of functions having first derivatives on $\mathcal{R}^+$, and second, that the solutions of these problems satisfy the identity (12a) and the following inequalities:

$$|\,c^\pm(x,q)\,| + |\,s^\pm(x,q)\,| > 0 \quad ; \qquad |\,c^+(x,q)\,| \quad , \qquad |\,s^\pm(x,q)\,| < \infty \quad ; \tag{12b}$$

$$|\,c^-(x,q)\,| < \infty \quad , \qquad x > 0 \quad . \tag{12c}$$

For instance, the identity (12a) is valid because from eqs. (11a) and the asymptotics (11b) and (11c) it follows that $\partial_x W(x,q) \equiv 0$ for any $x > 0$ and $W(0,q) = 1$.

Since both the problems (11) are uniquely solvable and their solutions have the properties (11b), (11c) and (12), each of the functions $A(x,q) \equiv \delta(x,q)$, $N^\pm(x,q)$, $\alpha(x,q)$ given by the corresponding formulae

$$\delta(x,q) \equiv \arctan\big(\, s^+(x,q)/c^+(x,q)\,\big) \quad , \tag{13a}$$

$$N^\pm(x,q) \equiv \Big(\, \big(c^+(x,q)\big)^2 + \big(s^+(x,q)\big)^2 \,\Big)^{\mp 1/2} \quad , \tag{13b}$$

$$\alpha(x,q) \equiv -c^+(x,q)\ c^-(x,q) - s^+(x,q)\ s^-(x,q) \tag{13c}$$

is everywhere unique and limited, and therefore, has the finite limit

$$A(q) \equiv \lim_{x\to\infty} A(x,q) \quad . \tag{14}$$

Using these properties of the functions (13), the identity (12a) and the known asymptotics of the Coulomb functions as $x \to \infty$, one can easily be convinced in that the wave functions (10a) will have the required asymptotics (7c) if the scattering phase $\delta(q)$ and normalisation factors $N^\pm$ and $\alpha(q)$ are determined as the limits (14) of the relevant functions (13).

It is to be noted that each of the functions $A = c^\pm$, $s^\pm$ and $A = \delta$, $N^\pm$, α determined by the relations (11) and (13) has a remarkable property

$$A(x,q) \equiv A(b,q) \quad , \qquad x \ge b \quad , \tag{15}$$

if $V(x) \equiv 0$ at $x \geq b$, and therefore, has a clear physical meaning. Indeed, the values of the functions $c^{\pm}(x,q)$ and $s^{\pm}(x,q)$ at some point $x = b$ are the amplitudes with which the Coulomb functions F and G are contained at $x = b$ in the wave functions (10b) nonnormalised to unit density of the flux as $x \to \infty$, whereas the functions $\delta(x,q)$, $N^{\pm}(x,q)$ and $\alpha(x,q)$ at the point $x = b$, as it follows from formulae (13)-(15), are the phase $\delta(q)$ and the normalisation factors $N^{\pm}(q)$, $\alpha(q)$ in the case when the potential V is cut off at that point.

So for the construction of solutions $u^{\pm}$ of the initial problem (7) by formulae (10) one should solve the problems (11) and then find the limit (14) for each function (13).

However, this is not the final stage of the reformulation of the problem (7). A further reformulation is prompted by the following obvious facts:

1. the structure of the problems (11) is so simple that their numerical solution in some finite interval $[0,b] \equiv \{x,b : 0 \leq x \leq b < \infty\}$ does not cause any difficulties;

2. usually, in the inner region, i.e. in that interval, the potential V is a function more complicated for analytical study of the problem (11) than in the outer region, i.e. in the infinite half-interval $[b,\infty) \equiv \{x,b : 0 < b \leq x < \infty\}$;

3. from the condition (8), determining the class of potentials used, it follows that $V(b) \to 0$ as $b \to \infty$.

From the above-mentioned facts it seems quite reasonable to calculate the functions $c^{\pm}$ and $s^{\pm}$ in the interval $[0,b]$ numerically, to supplement eqs. (11a) by the limiting values $c^{\pm}(b,q)$ and $s^{\pm}(b,q)$ found, and than to construct the solutions of thus obtained problems in the half-interval $[b,\infty)$ analytically, namely as limits $c^{\pm(\infty)}$ and $s^{\pm(\infty)}$ of some sequences $\{c^{\pm(m)}\}_{m=0}^{\infty}$ and $\{s^{\pm(m)}\}_{m=0}^{\infty}$ uniformly converging in the C^0-metric if $x \in [b,\infty]$, $m \to \infty$ and b is large enough.

To construct those sequences it is proposed to introduce instead of the functions $c^{\pm}$ and $s^{\pm}$ new unknown functions $y_1^{\pm}$ and $y_2^{\pm}$ satisfying the uncoupled integral Volterra problems [12] that can easily be investigated by the iteration method. The derivation of these equations is simple enough and can be realised as follows.

It is assumed that the functions $c^{\pm}$ and $s^{\pm}$ are known at some point $x = b$ and connected with new unknown functions $y_1^{\pm}$ and $y_2^{\pm}$ by the following formulae:

$$\left\{ \begin{array}{c} c^{\pm}(x,q) \\ s^{\pm}(x,q) \end{array} \right\} = \exp\left(\left\{ \begin{array}{c} +1 \\ -1 \end{array} \right\} B_3(b,x,q)\right) \left\{ \begin{array}{c} y_1^{\pm}(x,q) \\ y_2^{\pm}(x,q) \end{array} \right\} \qquad (16a)$$

Here B_3 is one of the three integrals used below and determined by

$$B_{l,n}(b,x,q) \equiv q^{-1} \int_b^x V(t)\left(G_l^2(\rho,\eta)\,\delta_{n,1} - F_l^2(\rho,\eta)\,\delta_{n,2} + F_l(\rho,\eta)\,G_l(\rho,\eta)\,\delta_{n,3}\right) dt \qquad (16b)$$

where $n = 1,2,3$; $\rho = tq$ and $\delta_{n,m}$ is the Kronecker symbol [8]. Owing to the condition (8) the integrals $B_{l,2}$ and $B_{l,3}$ are always limited, and the integral $B_{l,1}$ can diverge at the lower limit only in the case $b = 0$, $l > 0$.

Equations (11a) with the boundary conditions shifted to the point $x = b$ are reduced, by the substitution (16), to differential equations for new unknown functions $y_1^{\pm}$ and $y_2^{\pm}$ given at that point by

$$y_1^{\pm}(b,q) = c^{\pm}(b,q) \quad , \qquad y_2^{\pm}(b,q) = s^{\pm}(b,q) \quad . \tag{17}$$

The problems thus obtained are written in an equivalent integral form

$$y_i^{\pm}(x,q) = y_i^{\pm(-1)}(x,q) + \langle\, x \,|\hat{P}_i(b,q)|\, y_j^{\pm}(t,q)\,\rangle \quad . \tag{18a}$$

Hereafter the indices i and $j = j(i)$ take the values $1,2$ and $1 + \delta_{i,1}$; by definition it is assumed that

$$y_i^{\pm(-1)}(x,q) \equiv y_i^{\pm}(b,q) \quad , \qquad x \geq b \quad , \tag{18b}$$

and the operators $\hat{P}_i$ map any function $z(x,q)$ into the integrals

$$\langle\, x \,|\hat{P}_i(b,q)|\, z(t,q)\,\rangle \equiv \int_b^x P_i(b,t,q)\, z(t,q)\, dt \tag{18c}$$

with the kernals

$$P_i(b,x,q) \equiv \partial_x B_i(b,x,q)\ \exp(\, (-1)^i\, 2B_3(b,x,q)\,) \tag{18d}$$

containing the functions (16b).

As early as the first iteration eqs. (18a) are diagonalised and take the form

$$y_i^{\pm}(x,q) = y_i^{\pm(0)}(x,q) + \langle\, x \,|\hat{T}_i(b,q)|\, y_i^{\pm}(t,q)\,\rangle \quad , \tag{19a}$$

where for brevity the following notation is used:

$$y_i^{\pm(0)}(x,q) \equiv y_i^{\pm(-1)}(x,q) + \langle\, x \,|\hat{P}_i(b,q)|\, y_j^{\pm(-1)}(t,q)\,\rangle \tag{19b}$$

and the operator products $\hat{T}_i \equiv \hat{P}_i\, \hat{P}_j$ are determined in a standard way: for any function z it is assumed that $\hat{T}_i\, z \equiv \hat{P}_i\,(\,\hat{P}_j\, z\,)$ and

$$\langle\, x \,|\hat{T}_i(b,q)|\, z(t',q)\,\rangle \equiv \int_b^x P_i(b,x,q)\, dt \int_b^t P_j(b,t',q)\, z(t',q)\, dt' \quad . \tag{19c}$$

According to (17), (18b) and (19b), eqs. (19a) determining the functions y_1^+ and y_2^+ or y_1^- and y_2^- are connected with each other only by the constants, known by assumption. These constants are the values of the functions c^+ and s^+ or c^- and s^- at the point $x = b$. Such a simple connection, achieved due to a properly chosen substitution, allows one to analyse the solutions y_1^+ and y_2^+ or y_1^- and y_2^- of the problems (18) independently from each other and to realise rather elegantly the remaining stages.

To a great extent, this is favoured by the simplicity and smoothness of the representation (1) of each sought function of the starting problem (7) and each auxiliary function (13). These representations are easily found by substituting (16) into formulae (10) and (13).

Stage 2. To investigate new problems (3), i.e. the problems (18) in the half-interval $[b,\infty)$, we introduce iteration sequences $\{y_i^{\pm(m)}\}_{m=-1}^{\infty}$ with the elements determined by formulae (2) in the following recurrent way: $y_i^{\pm(-1)}$ are the constants (18b), $y_i^{\pm(0)}$ are the functions (19b), and then as the order of the index m increases ($m = 1,2,\dots$) it is assumed that $y_i^{\pm(m)}$ is the right-hand side of the relevant eq. (18a) in which $y_i^{\pm}$ is replaced by $y_i^{\pm(m-1)}$. By virtue of this definition and the relations (18b) and (19c), two equivalent representations hold:

$$y_i^{\pm(m)}(x,q) = y_i^{\pm(-1)}(b,q) + \langle\, x\,|\hat{P}_i(b,q)|\, y_j^{\pm(m-1)}(t,q)\,\rangle \quad , \tag{20a}$$

$$y_i^{\pm(m)}(x,q) = y_i^{\pm(-1)}(b,q) \sum_{p=0}^{m} \langle\, x\,|\hat{T}_i^p(b,q)|\,\theta(t)\,\rangle$$

$$+ y_j^{\pm(-1)}(b,q) \sum_{p=0}^{m} \langle\, x\,|\hat{T}_i^p\, \hat{P}_i(b,q)|\,\theta(t)\,\rangle \,, \tag{20b}$$

where $m = 0, 1, \ldots$, θ is the theta function [8] and the integer degrees of the operators $\hat{T}_i$ are determined in a standard way: $\hat{T}_i^0\, z \equiv z$, and $\hat{T}_i^p\, z \equiv \hat{T}_i\,(\,\hat{T}_i^{p-1}\, z\,)$ for any function z and any $p = 1, 2, \ldots$.

The simplicity and equivalence of these representations essentially simplify the proof of the key statement of the proposed theory. This statement establishes the relation (4) and is formulated below as the theorem.

Stage 3.

Theorem

Let $x \in [b, \infty)$, $b > 0$ and the function (8) be limited so that

$$I_l(b,x) < (1/2)\ln 3 \quad , \qquad x \in [b, \infty) \quad . \tag{21}$$

Then, the sequences $\{y_{i,l}^{\pm(m)}\}_{m=-1}^{\infty}$ uniformly converge in the C^0-metric to the solutions $y_{i,l}^{\pm}$ of the problem (18) and the differences ${}^{(m)}y_{i,l}^{\pm} \equiv y_{i,l}^{\pm} - y_{i,l}^{\pm(m)}$ satisfy the following inequalities:

$$|\, {}^{(m)}y_{i,l}^{\pm}(x,q)\,| < D_{i,l,m}^{\pm}(b,x,q)\ \cosh v_l(b,x)\ v_l^{2m+2}(b,x)\,/\,\Gamma(2m+3) \quad , \tag{22a}$$

in which $i = 1, 2$; $j = 1 + \delta_{i,1}$; $m = -1, 0, \ldots$; Γ is the gamma function [8];

$$D_{i,l,m}^{\pm}(b,x,q) \equiv |\, y_{i,l}^{\pm(-1)}(b,q)\,|\ w_l^{i-1}(b,x,q)\ \big(\ \theta(m) + \theta(-m-1)\ v_l^2(b,x)/2\ \big)$$

$$+\,|\, y_{j,l}^{\pm(-1)}(b,q)\,|\ w_l^{2-i}(b,x,q)\ v_l(b,x)/(2m+3) \quad ; \tag{22b}$$

$$v_l(b,x) \equiv \Big(\ \exp\big(\,2I_l(b,x)\,\big) - 1\ \Big)/2 \quad ; \tag{22c}$$

$$w_l(b,x,q) \equiv \max_{b \le \rho/q \le x} \Big\{\ \big(\,(2l+1)/(2\pi\rho^2)\,\big)^{1/2}\ G_l^2(\rho,\eta)\ \Big\} \quad . \tag{22d}$$

Proof.

The Klarsfeld inequalities [13]

$$F_l^2(\rho,\eta)\,, \quad |\,F_l(\rho',\eta)\, G_l(\rho,\eta)\,| < q\big(\ 2\pi\, x'x\,/\,(2l+1)\ \big)^{1/2} \quad , \tag{23}$$

valid under the conditions $\rho' \equiv qx' \le \rho \equiv qx$. are the key ones for proving the theorem by the method of contracting mappings [6].

First, it is necessary to prove auxiliary majorant estimates for absolute values of the integrals B_2, B_3 of (16b), the kernals P_i of (18d), all the images $\hat{P}_i\,\theta$, $\hat{T}_i\,\theta$, $\hat{T}_i\,\hat{P}_i\,\theta$ of the theta function entering into the representations (20), and finally, for the differences $y_i^{\pm(n)} - y_i^{\pm(m)}$.

By virtue of the relations (8), (16b) and (23)

$$| B_n(b,x,q) | < I(b,x) \quad , \qquad n = 2,3 \quad . \tag{24}$$

If in the definitions (18d) one majorizes $q^{-1}F^2$ and B_2, B_3 by the right-hand sides of inequalities (23) and (24) and then uses the notation (8), (22c) and obvious identity $\partial_x v \equiv \partial_x I \, \exp(2I)$, one can get the following estimates:

$$| P_i(b,x,q) | < \Big(\delta_{i,1} \left((2l+1)/2\pi\rho^2 \right)^{1/2} G^2(\rho,\eta) + \delta_{i,2} \Big) \, \partial_x v(b,x) \quad . \tag{25}$$

Owing to them and the definitions (18c), (22c) and (22d),

$$| \langle x | \hat{P}_i(b,q) | \theta(t) \rangle | < v(b,x) \, w^{2-i}(b,x,q) \quad . \tag{26}$$

To prove the relations

$$| \langle x | \hat{T}_1^p(b,q) | \theta(t) \rangle | < \int_b^x \partial_{t_1} v(b,t_1) dt_1 \int_b^{t_1} \partial_{t_2} v(b,t_2) dt_2 \cdots \int_b^{t_{2p-1}} \partial_{t_{2p}} v(b,t_{2p}) dt_{2p} \quad (27a)$$

$$= v^{2p}(b,x) \,/\, \Gamma(2p+1) \quad (27b)$$

in the case of $p = 1$, one should assume in the integral (19c) $z = \theta$, majorise B_3 and $q^{-1}\, G(qt_1,\eta)\, F(qt_2,\eta)$ by the right-hand sides of inequalities (24) and (23) and then use the definitions (8), (22c) and the identity $\partial_x v \equiv \partial_x I \, \exp(2I)$. Further, taking into account the identities $\hat{T}_1^p \equiv \hat{T}_1^{p-1}\, \hat{T}_1$, one can easily prove by induction the validity of the relations (27) for any $p = 2,3,\ldots$.

Unfortunately, the functions $\langle x | \hat{T}_2^p(b,q) | \theta(t) \rangle$, $p = 1,2,\ldots$, cannot be estimated in an analogous way. The fact is that according to formulae (16b), (18c) and (19c) the arguments $\rho_1 = qt_1$ and $\rho_2 = qt_2$ of the Coulomb functions $F(\rho_1,\eta)$ and $G(\rho_2,\eta)$ which are comprised in the kernels of the operators $\hat{T}_2^p$, $p = 1,2,\ldots$, do not satisfy the condition $\rho_1 < \rho_2$ under which for $|q^{-1}\, F\, G|$ inequality (23) holds. However, by virtue of the definitions $\hat{T}_i \equiv \hat{P}_i\, \hat{P}_j$ and $\hat{T}_i^p \equiv \hat{T}_i^{p-1}\, \hat{T}_i$, $p = 1,2,\ldots$, the equalities $\hat{T}_2^p = \hat{P}_2\, \hat{T}_1^{p-1}\, \hat{P}_1$, $p = 1,2,\ldots$ are valid. Owing to them and the estimates (24-27) one has

$$| \langle x | \hat{T}_2^p(b,q) | \theta(t) \rangle | < w(b,x,q) \int_b^x \partial_t v(b,t) \, | \langle t | \hat{T}_1^{p-1}(b,q) | \partial_{t'} v(b,t') \rangle | \, dt \quad (28a)$$

$$< w(b,x,q) \, v^{2p}(b,x) \,/\, \Gamma(2p+1) \quad p = 1,2,\ldots . \quad (28b)$$

To prove the bounds

$$| \langle x | \hat{T}_i^p(b,q) \, \hat{P}_i(b,q) | \theta(t) \rangle | < w^{2-i}(b,x,q) \, v^{2p+1}(b,x) \,/\, \Gamma(2p+2) \tag{29}$$

in the case $i = 1$ one should first majorize the function $\langle t | \hat{P}_1(b,q) | \theta(t') \rangle$ in the identity $\hat{T}_1^p\, \hat{P}_1\, \theta \equiv \hat{T}_1^p (\; \hat{P}_1\, \theta \;)$ by inequality (26) and then apply the estimate (27a); in the case $i = 2$ one has to use the identity $\hat{T}_2^p\, \hat{P}_2 \equiv \hat{P}_2\, \hat{T}_1^p$ and the estimates (25) and (27b).

Using the representations (20), the definitions (22b), (22c) and the results (26)-(29) obtained one can easily show that

$$| y_i^{\pm(n)}(x,q) - y_i^{\pm(m)}(x,q) | < D_{i,m}^{\pm}(b,x,q) \sum_{p=0}^{n-m-1} v^{2(p+m+1)}(b,x) \,/\, \Gamma(2(p+m+1)+1) \quad (30)$$

for any $i = 1,2$; $j = 1 + \delta_{i,1}$; $n = 0,1,\ldots$ and $m = -1,\ldots,n-1$.

Now, having all necessary estimates, one can immediately prove both the statements of the theorem. Inequalities $0 \leq v(b,x) < 1$, (following from the condition (21) and the definition (22c)) and the estimates (27)-(30) imply that in the half-interval $[b,\infty)$ the operators $\hat{T}_i$ and $\hat{T}_i \hat{P}_i$ are contracting ones [6] and the sequences $\{y_i^{\pm(m)}\}_{m=-1}^{\infty}$ converge uniformly [6] to the functions $y_i^{\pm}$ satisfying eqs. (18a). Due to thise factes, in inequalities (30) one can put $n = \infty$ and $y_i^{\pm(\infty)} \equiv y_i^{\pm}$ in order to get the estimates (22), using the known power expansions [8] of the hyperbolic cosinuse, and thus to complete the proof.

By virtue of the theorem the condition (21) is sufficient for the fulfillment of the relations (4) in the C^0-metric in the half-interval $[b,\infty)$.

Stage 4. Let the problem (11) or (18) be solved in the interval $[0,b]$, where b is such that the inequality (21) is fulfilled, and the sequences $\{c^{\pm(m)}\}_{m=0}^{\infty}$ and $\{s^{\pm(m)}\}_{m=0}^{\infty}$, are defined as follows:

$$\left\{ \begin{array}{c} c^{\pm(m)}(x,q) \\ s^{\pm(m)}(x,q) \end{array} \right\} \equiv \left\{ \begin{array}{c} c^{\pm}(x,q) \\ s^{\pm}(x,q) \end{array} \right\} = \exp(\left\{ \begin{array}{c} +1 \\ -1 \end{array} \right\} B_3(b,x,q)) \left\{ \begin{array}{c} y_1^{\pm}(x,q) \\ y_2^{\pm}(x,q) \end{array} \right\} \quad , \quad (31a)$$

if $x \leq b$ and

$$\left\{ \begin{array}{c} c^{\pm(m)}(x,q) \\ s^{\pm(m)}(x,q) \end{array} \right\} \equiv \exp(\left\{ \begin{array}{c} +1 \\ -1 \end{array} \right\} B_3(b,x,q)\, \theta(m-1)) \left\{ \begin{array}{c} y_1^{\pm(m-1)}(x,q) \\ y_2^{\pm(m-1)}(x,q) \end{array} \right\} \quad , \quad (31b)$$

if $b \leq x \leq \infty$.

Here $m = 0,1,\ldots$, B_3 is the integral (16b), $y_i^{\pm(-1)}$ are the constants (18b) and $y_i^{\pm(m)}$ are the functions (20).

These sequences converge uniformly in the whole semiaxis $\mathcal{R}^+$ to the solutions of the problems (11). The functions $c^{\pm(0)}$ and $s^{\pm(0)}$, owing to equalities (18b) and (31), have the property (15) and are the exact solutions of these problems if the potential is cut off at the point $x = b$.

Due to the above-mentioned properties of the sequences $\{c^{\pm(m)}\}_{m=0}^{\infty}$ and $\{s^{\pm(m)}\}_{m=0}^{\infty}$ the following two assertions are valid.

First, to each function $f = \delta, N^{\pm}, \alpha, U^{\pm}, u^{\pm}$ there can be put into correspondence (5) the sequence $\{f^{(m)}\}_{m=0}^{\infty}$ uniformly converging on $\mathcal{R}^+$ to this function. For this purpose, one should determine the elements $f^{(m)}$ as the right-hand sides of the relevant representations (10) and (13) in which the functions $c^{\pm}$ and $s^{\pm}$ are substituted by the functions (31), i.e. to assume that at any $m = 0,1,\ldots$ and $x \in \mathcal{R}^+$

$$\delta^{(m)}(x,q) \equiv \arctan(s^{+(m)}(x,q) \,/\, c^{+(m)}(x,q)) \quad , \quad (32a)$$

$$N^{\pm(m)}(x,q) \equiv \Big(\big(c^{+(m)}(x,q)\big)^2 + \big(s^{+(m)}(x,q)\big)^2 \Big)^{\mp 1/2} \quad , \quad (32b)$$

$$\alpha^{(m)}(x,q) \equiv -c^{+(m)}(x,q)\; c^{-(m)}(x,q) - s^{+(m)}(x,q)\; s^{-(m)}(x,q) \quad , \tag{32c}$$

$$U^{\pm(m)}(x,q) \equiv c^{\pm(m)}(x,q)\; F(\rho,\eta) + s^{\pm(m)}(x,q)\; G(\rho,\eta) \quad , \tag{32d}$$

$$u^{\pm(m)}(x,q) \equiv N^{\pm(m)}(\infty,q)\; U^{\pm(m)}(x,q) + \left\{ \begin{array}{c} 0 \\ \alpha^{(m)}(\infty,q)\; u^{+(m)}(x,q) \end{array} \right\} \quad . \tag{32e}$$

Second, the functions δ^0, $N^{\pm(0)}$, α^0, $U^{\pm(0)}$ and $u^{\pm(0)}$ thus determined have an apparent physical meaning: they are the relevant functions (10) and (13) in the case when the potential V is cut at the point $x = b$.

Using formulae (10), (13), (22), (31), (32) and the identities $f \equiv f^{(\infty)}$ one can easily estimate from above the differences ${}^{(m)}f \equiv f - f^{(m)}$ for the functions $f = c^{\pm}, s^{\pm}$,

$$\left\{ \begin{array}{c} |\,{}^{(m)}c^{\pm}(x,q)\,| \\ |\,{}^{(m)}s^{\pm}(x,q)\,| \end{array} \right\} < \exp(\left\{ \begin{array}{c} +1 \\ -1 \end{array} \right\} B_3(b,x,q)\,\theta(m-1)\,) \left\{ \begin{array}{c} D^{\pm}_{1,m-1}(b,x,q) \\ D^{\pm}_{2,m-1}(b,x,q) \end{array} \right\}$$

$$\times \cosh v(b,x)\; v^{2m}(b,x)\,/\,\Gamma(2m+1) \;, \quad m = 0, 1, \ldots \;, \tag{33a}$$

and then for all the functions $f = \delta,\ N^{\pm},\ \alpha,\ U^{\pm},\ u^{\pm}$. After this one can easily verify that these estimates have the form of the following asymptotic inequalities

$$|\,{}^{(m)}f_l(x,q)\,| \le \theta(x-b)\; O(\; v^{2m+\theta(-m)}(b,x)\,/\,\Gamma(2m+1)\;) \quad , \qquad f \ne u^{\pm} \quad ,$$

$$|\,{}^{(m)}u^{\pm}_l(x,q)\,| < O(\; v^{2m+\theta(-m)}(b,\infty)\,/\,\Gamma(2m+1)\;) \quad , \tag{33b}$$

if b and l are fixed and $m \to \infty$, or if m is fixed and $v_l(b,x) \to 0$ for all $x \ge b$.

The validity of the estimates (33b) in the first case implies that relations (6) are proved under the condition (21). Consequently, the fourth stage is accomplished.

The validity of these estimates in the second case allows one to use perturbation theory for constructing asymptotics of the functions (10) and (13) in the region $x \ge b$ in two interesting, from the physical point of view, limits: $l \to \infty$ at fixed q and $q \to 0$ at fixed l. To show how to do that, one should first analyse the condition (21) and the estimates (33).

Stage 5. At $x \ge b$ the functions (8) and (22b) are monotonously vanishing if l is fixed and b increases ,

$$I_l(b,x) \quad , \quad v_l(b,x) \to 0 \quad , \qquad b \to \infty \quad , \tag{34}$$

or vice versa, if b is fixed and l increases ,

$$I_l(b,x) \quad , \quad v_l(b,x) = O(\, l^{-1/2}\,) \quad , \qquad l \to \infty \quad . \tag{35}$$

Therefore, inequality (21) is certainly valid in two cases: first, at any fixed l and any b exceeding the root $b_{min}(l)$ of the equation

$$I_l(b_{min}(l),\infty) \equiv \left(\, 2\pi/(2l+1)\,\right)^{1/2} \int_{b_{min}(l)}^{\infty} t\,|\,V(t)\,|\,dt = (\ln 3)/2 \quad , \tag{36}$$

and second, at any fixed b and any l exceeding the root

$$l_{min}(b) \equiv \pi\Big((2/\ln 3) \int_b^\infty t\,|\,V(t)\,|\,dt \Big)^2 - 1/2 \qquad (37)$$

of the equation

$$I_{l_{min}(b)}(b,\infty) = (\ln 3)/2 \quad .$$

Thus, perturbation theory constructed can certainly be applied at $x \geq b > 0$ in the two above-mentioned cases. Due to relations (34) and (35), the estimates (33) characterizing the efficiency of this theory, improve in the first case with increasing b and in the second case with increasing l.

The qualitative explanation of these conclusions is the following. According to inequality (8), in the region $x \geq b > 0$ the potential V is screened $(\,|\,V(x)\,| \leq l(l+1)x^{-2}\,)$ by the repulsive centrifugal barrier, thus being perturbation if l is fixed and b is rather large $\big(\,b > b_{min}(l)\,\big)$ or vice versa, if b is fixed and l is rather large $\big(\,l > l_{min}(b)\,\big)$. Obviously, the degree of screening improves in the first case with increasing b and in the second case with increasing l.

It is intuitively clear that at sufficiently large l the centrifugal barrier can screen the potential, satisfying the condition (8), everywhere, i.e. at all $x \in \mathcal{R}^+$. Therefore, it is interesting to generalize perturbation theory to the case $b = 0$. For this purpose, it is necessary to reconsider the proof of the theorem and all the subsequent constructions first for the functions with the sign " + " and then for the functions with the sign " − ".

Let $b = 0$ and the condition (21) be fulfilled. Then, owing to formulae (11b) and (17), $y_i^{+(-1)}(0,q) = \delta_{i,1}$, $i = 1,2$. Therefore, the representations (20b) for the functions $y_i^{+(m)}$ are simplified ,

$$y_i^{+(m)}(x,q) = \sum_{p=0}^{m} (\,x\,|\hat{T}_i^p(0,q)\,\hat{P}_2^{i-1}(0,q)|\,\theta(t)\,) \quad , \qquad m = 0,1,\ldots, \qquad (38)$$

and what is more important, contain only limited operators. Using formulae (38) and assuming $w \equiv 1$, one can easily be convinced in the following.

For the functions y_i^+, $y_i^{+(m)}$ and ${}^{(m)}y_i^+$ the theorem remains valid. Consequently, valid are also all the subsequent assertions concerning the functions c^+, s^+, δ, $N^\pm$, U^+ and u^+ whose representations (10), (13) and (16) do not contain the functions y_1^- and y_2^-.

Then, the relevant formulae (31) and (32) are essentially simplified. For instance, at $m = 0$ they reduce to the identities

$$c^{+(0)} = N^{\pm(0)} \equiv 1 \;, \quad s^{+(0)} = \delta^{(0)} \equiv 0 \;, \quad U^{+(0)} = u^{+(0)} \equiv F \;, \qquad (39)$$

and at $m = 1$ to the equalities

$$c^{+(1)}(x,q) = \exp(\,B_3(0,x,q)\,) \quad , \quad s^{+(1)}(x,q) = (\,x\,|\hat{P}_2(0,q)|\,\theta(t)\,)\,/\,c^{+(1)}(x,q) \quad , \; (40a)$$

$$\delta^{(1)}(x,q) = \arctan\Big(\,\exp(\,-2B_3(0,x,q)\,)\,(\,x\,|\hat{P}_2(0,q)|\,\theta(t)\,)\,\Big) \quad , \qquad (40b)$$

$$N^{\pm(1)}(x,q) = \Big(\,\cos\delta^{(1)}(x,q)\,\exp(\,-B_3(0,x,q)\,)\,\Big)^{\pm 1} \quad , \qquad (40c)$$

$$U^{+(1)} = \exp(\ B_3(0,x,q)\ )(\ F(\rho,\eta) + \tan\delta^{(1)}(x,q)\,G(\rho,\eta)\ )\quad , \qquad (40d)$$

$$u^{+(1)}(x,q) = \cos\delta^{(1)}(\infty,q)\ \exp(\ B_3(x,\infty,q)\ )\ (\ F(\rho,\eta) + \tan\delta^{(1)}(x,q)\,G(\rho,\eta)\ )\quad , \ (40e)$$

Finally, the estimates (33a) for the functions ${}^{(m)}c^+$ and ${}^{(m)}s^+$ are also simplified. For instance, at $m = 0, 1$

$$\begin{aligned} |\,{}^{(m)}c^+(x,q)\,| &< (1/2)\ \exp(\ B_3(0,x,q)\,\delta_{m,0}\ )\ v^2(0,x)\ \cosh v(0,x)\quad , \\ |\,{}^{(m)}s^+(x,q)\,| &< \exp(\ -B_3(0,x,q)\,\delta_{m,0}\ )\ v^{2m+1}(0,x)\ \cosh v(0,x)\,/\,(1+5\,\delta_{m,1})\quad . \end{aligned} \qquad (41)$$

Let now $b \to 0$ and the condition (21) be fulfilled at $b = 0$. In virtue of the relations (11b) and (17) the representations (20) for the functions $y_i^{-(m)}$ always (even at $b = 0$) contain the mappings $\hat{P}_1\,\theta$, $\hat{T}_2^p\,\theta$, $\hat{T}_1^p\,\hat{P}_1\,\theta$ of the theta function. The estimates (26), (28) and (29) of these mappings become meaningless at $b = 0$, as $w(b,x,q) \to \infty$, if $b \to 0$. Moreover, as it follows from the definitions (18c) and (18d),

$$|\,(\,x\,|\hat{P}_1(b,q)|\,\theta(t)\,)\,| \to \infty \quad , \quad b \to 0 \quad , \quad V\,G^2 \not\subset \mathcal{L}^1_{[0,x_0]} \quad .$$

From the afore-said the following construction seems to be reasonable. First, by the method described at stage 1. the functions c^- and s^- are found in the interval $[0, x_0]$. Then, perturbation theory is used in the half-interval $[b, \infty)$. Under a construction like that it is assumed in formulae (16)-(32) that $b = x_0$, the functions $c^{-(m)}$, $s^{-(m)}$, $\alpha^{(m)}$, $U^{-(m)}$, $u^{-(m)}$ have a correct asymptotics at zero, and the relevant estimates (33) are valid at all $x \geq 0$.

So if inequality (21) is valid at $b = 0$, then perturbation theory can be used to approximate the functions c^+, s^+, δ, $N^\pm$, U^+ and u^+ on the whole semiaxis $\mathcal{R}^+$ and to approximate the functions c^-, s^-, α, U^-, and u^- on the region $x \geq x_0$. According to equalities (36) and (37), the above condition is fulfilled if l is fixed and the potential V is such that $b_{min}(l) = 0$ or if V is an arbitrary (satisfying the condition (8)) potential and $l > l_{min}(0)$. In these cases formulae (38)-(41) hold.

Now, it is necessary to study the non-Coulomb limit $R \to \infty$. As $V(x) \equiv R^2\tilde{V}(x|R|)$, where $\tilde{V}$ is the potential in the r−representation, the integral (8), and consequently, the condition (21) are independent of R. This can be verified by writing them in the variable r. The key estimates (23) are also independent of R and remain valid [13,15] as $R \to \infty$, when [8] $F_l(\rho,\eta) \to j_l(\rho)$ and $G_l(\rho,\eta) \to -n_l(\rho)$.

Owing to the afore-mentioned facts, all said above (all conclusions, relations and formulae) remain also valid in the non-Coulomb limit ($V_c \equiv 0$, $R = \infty$) if everywhere beginning from eq. (7a) one assumes $\eta = 0$, $x \equiv \rho \equiv kr$, $q \equiv 1$, $F_l(\rho,\eta) \equiv j_l(x)$, $G_l(\rho,\eta) \equiv -n_l(x)$ and bears in mind that now $V(x) \equiv k^{-2}\tilde{V}(x/k)$.

The next interesting limit is $R \to 0+$. In this case, the repulsive Coulomb barrier increases ($V_c \to \infty$) and screens the potential V first at $x \geq b > 0$ and then at all $x \geq 0$. Unfortunately, we did not succeed in taking this effect into account in the framework of perturbation theory constructed. Indeed, the estimates (33), characterising its efficiency, do not improve at $R \to 0+$, as contain only the function v which by definition is independent of R.

Completing the analysis of the relations (21) and (33) it is useful to discuss the quality of the estimates (33) and to show the way of their improvement. According to the proof of the theorem, the condition (21) and then the definition (22c) of the function v and the structure of the relations (33) are generated by the key estimates (23). These estimates do not contain the Bohr radius R as a parameter and are rather rough especially as $x \to 0$ and $x \to \infty$ when [8] $F_l = O\big(x^{(l+1)}\, qC_l(q)\big)$ and $F_l,\ G_l = O(1)$. What is more important, the estimates (23) do not contain the Coulomb barrier factor

$$C_l(q) \equiv (2q)^l \mid \Gamma(l+1+i/2q) \mid \exp(\,-\pi/4kR\,)$$

and, therefore, they do not take into account the dependence $C_l(q) \to \infty$ as $R \to 0+$ reflecting the effect of Coulomb screening. It is evident that the estimates (33) also do not describe this dependence and are rather rough. Hence, for each function (10) and (13) the approximation $f \simeq f^{(m)}$ is indeed more accurate than the corresponding estimate (33) gives. Obviously, all these estimates can be essentially improved. For this purpose, instead of the relations (23), one should use less universal but more accurate estimates taking account of the structure of Coulomb functions in a proper way. For instance, as $q \to 0$ one can use the known [8,16] asymptotic ($|\eta| \to \infty$) representations (Bessel-Clifford series [8], WKB-asymptotics [14] and so on) and at $\eta = 0$ one can use uniform in x estimates [3]

$$j_l(x) = O\big(\,(1+x^{-1})^{-l-1}\,\big)\,, \quad n_l(x) = O\big(\,(1+x^{-1})^{l}\,\big)\,.$$

It is to be noted that perturbation theory can be generalised to the case when the potential V decreases more rapidly than centrifugal one but more slowly than the Coulomb potential and satisfies the condition that is more weak than the condition (8), namely:

$$x|\,V(x)\,| \subset \mathcal{L}^1_{[0,b]} \quad , \quad |\,V(x)\,| \subset \mathcal{L}^1_{[b,\infty]} \quad , \qquad 0 < b < \infty \ .$$

For a generalisation like that one should use at $\rho \gg 1$ the relations $F,\ G = O(1)$ instead of the inequalities (23).

It is customary to demonstrate the efficiency of the theory, using several examples, after its construction.

3. Examples of Application of Perturbation Theory

Example 1. Control and improvement of accuracy of the numerical solution of the problems (7) and (11).

In practice, the problems (11) are solved numerically not on the whole semiaxis $\mathcal{R}^+$ but on its certain finite interval $[0,b]$, i.e., the approximation $V(x) \equiv 0,\ x \geq b$, is used which is zeroth for the proposed perturbation theory. With its help one can: evaluate the accuracy of this approximation ${}^{(0)}f$; if necessary, to construct any function f of (10), (13) more exactly by formulae (31) and (32) with $m = 1$; to choose the point b so that the function $f^{(m)}$, $m = 0, 1$ found should approximate the sought one with the given absolute accuracy ε. Such a choice is made in a usual way: the function ${}^{(m)}Q(b,x,q)$, majorizing $|\,{}^{(m)}f\,|$, is calculated by formulae (33) and compared with ε at $x \geq b$; if ${}^{(m)}Q > \varepsilon$, then the value of b should be enlarged until the inverse equality is fulfilled.

In a special case, when the condition (21) is fulfilled at $b = 0$, the numerical solution of the problems (11) is not required, and therefore, perturbation theory becomes an effective method for analytical investigation of the initial problem (7). In this case, the construction of the functions $f^{(m)}$, $m = 0, 1, \ldots$, approximating the corresponding function (10) or (13) at all $x \geq 0$, reduces to the calculation of integrals of multiplicity not higher than $m + 1$, and the accuracy of approximation $f \simeq f^{(m)}$ is controlled by the estimates (33) in which $b = 0$ is assumed. Especially simple are formulae (39) and (40) determining the zeroth and first approximations of the functions c^+, s^+, δ, $N^\pm$, U^+ and u^+. These formulae and the estimates (41) are sufficient for deriving new qualitative results given below as examples 2 and 3.

Example 2. Qualitative study of the factor N^+

Let $b = 0$ and the condition (21) be fulfilled. Then, for the normalisation factor $N^+(q) \equiv N^+(\infty, q)$ one has the lower bound

$$N^+(q) \geq \Big(1+v^2(0,\infty) \cosh v(0,\infty) (1+\cosh v(0,\infty) (1+v^2(0,\infty)/4)) \Big)^{-1/2} \quad , \quad (42)$$

which is uniform in energy $E = q^2$ and can easily be proved by formulae (13b), (39)-(41) and equalities $c^+ = 1+{}^{(0)}c^+$ and $s^+ = {}^{(0)}s^+$. This bound allow one to estimate from below the function u^+ in the region of $qx \ll 1$, where, owing to the relations (10) and (11b), $u_l^+ \simeq N_l^+(q)\, x^{l+1}\, qC_l(q)$. Such a simple estimate may turn out to be rather useful for analysing many approximate formulae (for instance, Deser at. al formula [17]) containing asymptotics of the function u^+ at zero.

It is to be noted that the estimate (42) is rather rough: it depends neither on energy nor on the sign of the potential V. Within the first approximation, more accurate lower and upper estimates,

$$N^{+(1)}(q) > \exp(-B_3(0,\infty,q)) \Big(1 + \exp(-4B_3(0,\infty,q))\, v^2(0,\infty) \Big)^{-1/2} \quad , \quad (43a)$$

$$N^{+(1)}(q) < \exp(-B_3(0,\infty,q)) \quad , \quad (43b)$$

are valid. To prove inequalities (43a) and (43b) one should begin from the definition (32b), and correspondingly, from the representation (40c) and then to take into account formulae (40a) and (26).

The following asymptotic estimates

$$|\, N_l^+(q) - 1 \,| < O(l^{-1/2}) \quad , \qquad |\, N_l^{+(1)}(q) \,/\, N_l^+(q) \, - 1 \,| < O(l^{-1}) \quad (44)$$

determine the behaviour of the normalisation factor as $l \to \infty$ and are derived by formulae (13b), (39), (40c) and estimates (45) obtained below.

Example 3. The behaviour of the scattering phase and amplitude as $l \to \infty$

Let $l \to \infty$ and q is fixed. Then, as has been mentioned at stage 5, at any l exceeding $l_{min}(0)$ the function $f_l = c_l^+$, s_l^+, δ_l, $N_l^\pm$ can be approximated on the whole semiaxis $x \geq b = 0$ by the function $f_l^{(m)}$ given by the corresponding formula (39) or (40). By virtue of the relations (35) the accuracy of an approximation like that improves with increasing l. For instance, the estimates (41) take the form of asymptotic ($l \to \infty$) inequalities

$$|\,{}^{(m)}c_l^+(x,q)\,| < O(\,l^{-1}\,) \quad , \quad |\,{}^{(m)}s_l^+(x,q)\,| < O(\,l^{-m-1/2}\,) \quad , \qquad m = 0, 1. \tag{45}$$

The latter and equalities (13a), (39) and (40b) generate the following asymptotic estimates:

$$|\,\tan\delta_l(q)\,| < O(\,l^{-1/2}\,) \quad , \tag{46a}$$

$$|\,\tan\delta_l(q) - \tan\delta_l^{(1)}(q)\,| < O(\,l^{-3/2}\,) \quad , \qquad |\,\tan\delta_l^{(1)}(q)/\tan\delta_l(q) - 1\,| < O(\,l^{-1}\,) \quad ; \tag{46b}$$

specifying the behaviour of the scattering phase in the limit of a large l.

Using these estimates and usual definition of the scattering amplitude [1,3] ,

$$A_l(q) \equiv q^{-1}\,\sin\delta_l(q)\,\exp(\,i\delta_l(q)\,) \quad ,$$

and its first approximation ,

$$A_l^{(1)}(q) \equiv q^{-1}\,\sin\delta_l^{(1)}(q)\,\exp(\,i\delta_l^{(1)}(q)\,) \quad , \tag{47}$$

one can show that at fixed q

$$|\,A^{(1)}(q)\,/\,A_l(q)\,-1\,| < O(\,l^{-1}\,) \quad , \qquad l \to \infty \quad . \tag{48}$$

The estimates (46b) and (48) mean that with increasing l the phase and amplitude of scattering tend to zero as the functions $\delta_l^{(1)}$ and $A_l^{(1)}$, respectively.

The decrease of the scattering amplitude as $l \to \infty$ can be qualitatively explained by the effect of screening but its strict mathematical proof has first been given by Klarsfeld [13] . Comparing his result

$$|\,A_l^B(q)\,/\,A_l(q)\,-1\,| = O(\,l^{-1/2}\,) \quad , \qquad l \to \infty \quad ,$$

with the estimate (48) one can easily be convinced that at large l the functions $\delta_l^{(1)}$ and $A_l^{(1)}$ approximate the phase and amplitude of scattering more exactly than the functions δ_l^B and A_l^B given by the standard Born formulae [3]

$$\tan\delta_l^B(q) \equiv -q^{-1}\int_0^\infty V(t)\,F_l^2(\rho,\eta)\,dt \equiv q\,A_l^B(q) \quad . \tag{49}$$

Now pursueing the comparison of the Born approximations δ_l^B and A_l^B with the first approximations $\delta_l^{(1)}$ and $A_l^{(1)}$ of the theory proposed we should like to note that $\delta_l^{(1)} \to \delta_l^B$ and $A_l^{(1)} \to A_l^B$ as $B_{3,l}(0,x,q) \to 0$ for all $x \geq 0$. This can be verified by assuming $B_{3,l} \to 0$ in formulae (18c), (40b) and (47).

Example 4. Construction of low-energy representations

As is known [1,9], the low-energy scattering of two particles is mainly determined by the behaviour of the potential tail. Therefore, at $q \ll 1$ it is extremely necessary [18,19] to take into account of a long-range potential in the whole region of large distances though it is rather a difficult task. Its solution by numerical integration of the problem (7) or even (11) is rather an inefficient way in comparison with the construction of low-energy representations [9,20].

Representations of that type for the functions (10) and (13) can be obtained by using the known asymptotic forms of the Coulomb functions [8,16] as $|\eta| \to \infty$ and perturbation theory. This can be exemplified for the case $V_c > 0$.

The key idea of the construction proposed below is to choose the point b so that at $x \le b$ one could use the results of the previous paper [20]; and at $x > b$, the results of the present work.

Let $q \to 0$, l be fixed and by definition

$$b \equiv x_c^p \equiv (\eta/q)^p \left(1 + \left(1 + l(l+1)/\eta \right)^{1/2} \right)^p \quad , \tag{50}$$

where $2/3 < p < 1$, and x_c is the Coulomb turning point [1]. Then, $b \ll x_c$ and in the interval $[0, b]$ the conditions $q \to 0$, $x \ll x_c$ hold which allow one to change the functions F, G and c^+, s^+ by the corresponding finite sums of Bessel-Clifford series and expansions

$$\left\{ \begin{array}{c} c_l^{\pm}(x,q) \\ s_l^{\pm}(x,q) \end{array} \right\} = \left\{ \begin{array}{c} (qC_l^2(q))^{(-1\pm1)/2} \\ (qC_l^2(q))^{(+1\pm1)/2} \end{array} \right\} \sum_{n=0}^{\infty} q^{2n} \left\{ \begin{array}{c} c_{l,n}^{\pm}(x) \\ s_{l,n}^{\pm}(x) \end{array} \right\} \quad . \tag{51}$$

The way of constructing the latter has been proposed in Ref. [20]. Also, expansions of the functions (10b) and (13) as $q \to 0$ and $x \le b \ll x_c$ have been derived in that paper.

By the definition (50) $b \to \infty$ as $q \to 0$; therefore, for any potential satisfying inequality (8) the condition (21) is fulfilled at small enough q. At q like that and $x \ge b$ any of the functions (10) and (13) can be approximated by the function $f^{(m)}$, $m = 0, 1, \ldots$, given by the corresponding formula (32). To construct the asymptotic ($q \to 0$) estimates of accuracy ${}^{(m)}f$ of such an approximation, one should, first, consistently determine the behaviour of the functions I, v, w, $y_i^{\pm(-1)}$ and $D_{i,m}^{\pm}$ as $q \to 0$ and $x \ge b$, then by formulae (33a) obtain asymptotic estimates for the functions ${}^{(m)}c^+$ and ${}^{(m)}s^+$ and finally, using definitions (10), (13) and (32) construct asymptotic estimates for all other functions ${}^{(m)}f$.

As an example, it is useful to estimate a relative accuracy of the first approximation for the scattering phase generated by the long-range potential

$$V(x) \simeq ax^{-d} \quad , \quad d > 2 \quad , \quad x \gg 1 \quad , \tag{52}$$

and to reproduce from that estimate the known result [21]: $\delta_l(q) = O(\, \delta_l^B(q)\,)$ as $q \to 0$.

In what follows we assume that $x \ge b$, $q \to 0$ and l is fixed so that $2ql(l+1) \ll 1$.

By the definition (50) $b = O(\, q^{-2p}\,)$; therefore, for the potential (52) inequality (21) is valid at

$$q < q_{max}(l) \simeq \left(\left((2l+1) \,/\, 2\pi \right)^{1/2} (d-2)(\ln 3)/2|a| \right)^{1/2p(d-2)} \quad ,$$

and the functions (8) and (22c) are such that

$$I(b,x) \; ; \quad v(b,x) = O(\, q^{2p(d-2)}\,) \quad . \tag{53}$$

A rough estimate [8] $|\, G(\rho,\eta)\,| \le O(\, q^{-1/6}\,)$ is sufficient to derive from the definition (22d) the inequality

$$w(b,x,q) \le O(\, q^{2p-4/3}\,) \quad . \tag{54}$$

By virtue of the representations (51) and equalities (17) and (18b),

$$c^+(q,b)\ ,\quad y_1^{+(-1)}(q,x) = O(1)\quad ;\qquad s^+(q,b)\ ,\quad y_2^{+(-1)}(q,x) = O(\,qC^2(q)\,)\quad . \tag{55}$$

Relations (53)-(55) allow one to estimate the functions (22b) and then to obtain the asymptotic form of inequalities (33a):

$$\begin{aligned} |\,^{(m)}c^+(x,q)\,| \ &< \ O\big(\,q^{4(d-2)(m+\theta(-m))p}\,/\,\Gamma(\,2m+2\theta(-m)+1\,)\,\big)\quad , \\ |\,^{(m)}s^+(x,q)\,| \ &< \ O\big(\,q^{4(d-2)(m+1)p}\,/\,\Gamma(2m+2)\,\big)\quad ,\qquad m=0,1,\dots\ . \end{aligned} \tag{56}$$

Now, using the definitions (13a), (32a) and estimates (55) and (56) one can derive the sought relation

$$|\,\tan\delta^{(1)}(q)\,/\,\tan\delta(q)\ -1\,| < O\big(\,q^{4(d-2)p}\,\big)\quad . \tag{57}$$

and thus to prove for the first time the following statement: all terms of the asymptotic expansion of the function $\tan\delta^{(1)}(q)$ decreasing slower than $O\big(\,q^{4(d-2)p}\big)$ are the terms of the asymptotic expansion of the function $\tan\delta(q)$.

It remains to show that inequality (57) results in the relation

$$\tan\delta(q) = O(\,\tan\delta^B(q)\,) \tag{58}$$

that has first been established in Ref. [21] and implies that leading terms of low-energy asymptotics of the scattering phase and its Born approximation (49) depend on q in a similar way, namely as q^{2d-3}.

Owing to the estimates (26) and (53) the integral B_3 is such that $|\,B_3\,| < O(\,q^{2p(d-2)}\,)$; therefore, the definition (32a) results in the asymptotic equality $\delta^{(1)}(q) = O(\delta^B(q))$. The latter and inequality (57) generate the relation (58), which was to be proved.

4. Conclusion

The main results of the present paper are the following.

The complete construction and analysis of perturbation theory are given for the one-dimensional scattering problem (7) with the condition (8). For this theory we have established: a sufficient condition (21), the range of applicability ($b > b_{min}(l)$ or $l > l_{min}(b)$ independently of whether $V_c < 0$, $V_c > 0$ or $V_c \equiv 0$) and majorant estimates (33) and (41) of absolute accuracy $|\,^{(m)}f\,|$ of approximation $f \simeq f^{(m)}$ of each function f investigated. It is shown that these estimates can be improved if the structure of the Coulomb functions is taken into account in more detail.

It is explained how the constructed theory can be applied in order to take correctly into account the potential V at $x \ge b > 0$ (in some cases, at all $x \ge 0$), to get estimates for the normalization factor N^+ and to study the problem (7) in the low-energy and large angular momentum limit. It is the first time that estimates (42)-(44), (48) and (57) are obtained.

In conclusion, we would like to note the following.

In the present paper, the linear version of the variable phase approach [9,10] is supplemented by a method of constructing an irregular wave function.

Usually, a perturbation theory is constructed for studying only one of the unknown functions, for instance, a scattering phase or a regular wave function [1-4]. The proposed perturbation theory allows one not only to investigate in detail all the functions connected with the initial problem (7) but is an asymptotic method in two physically interesting limits.

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