Application of the *J*-matrix method to Faddeev-Merkuriev equations for $(e,2e)$ reactions: Beyond pseudostates

S. A. Zaytsev* and V. A. Knyr
Pacific National University, Khabarovsk, 680035, Russia

Yu. V. Popov
Nuclear Physics Institute, Moscow State University, 119992, Moscow, Russia

A. Lahmam-Bennani
Laboratoire des Collisions Atomiques et Moleculaires (UMR 8625) and Federation Lumiere Matiere(FR 2764), Bâtiment 351, Université de Paris-Sud XI, F91405 Orsay Cedex, France

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A version of the *J*-matrix method for solving numerically the three-body Faddeev-Merkuriev differential equations is proposed. This version allows one to take into account the full spectrum of the two-body Coulomb subsystem. As a result, a discrete analog of the Lippmann-Schwinger equation is obtained which allows one to interpret correctly the three-body wave function in two-body domains. The scheme is applied to calculations of the fully resolved absolute differential cross sections for the $\mathrm{He}(e,2e)\mathrm{He}^+$ reactions leaving the residual ion in an excited state, at small energy and momentum transfer. The results are in good agreement with the experiment both in shape and in absolute value.

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I. INTRODUCTION

The few-body Coulomb problem is one of the most fundamental problems in physics and being yet to be exactly solved. In recent years, it has attracted numerous theoretical studies which involve different approaches and/or approximations. Among these is the *J*-matrix method widely used in the quantum scattering theory. It was first proposed in atomic physics [1] and later on (independently) in nuclear physics [2–4]. Within this approach the full Hamiltonian of the atomic system is split into two parts: $H=H_c+V$. The operator H_c determines a discrete basis of square-integrable functions which are used for expansion of the many-body wave function. In atomic physics, a Laguerre basis is the most widely used because it provides a tridiagonal representation of the radial part of the operator H_c, and this infinite three-termed recurrence can be solved analytically. At the same time, the short-range interaction V is approached by its projection V^N on a subspace of N basic functions. Hence, the *J*-matrix method supplies the exact solution of the scattering problem for the model potential V^N. The *J*-matrix approach is proved to be an efficient and rather accurate numerical method. Formally and from the viewpoint of numerical realization, the *J*-matrix method is similar to the *R*-matrix scattering theory (for an overview, see, for example, [5]). It is also equivalent to the so-called Coulomb-Sturmian separable expansion method (see, for instance, Ref. [6] and references therein).

The most important problem in a few-body Coulomb scattering theory is the description of the continuum-state wave function in terms of square-integrable functions. The method of pseudostates and its recent avatar, the convergent close-coupling method (CCC) [7], replace the continuous energy spectrum of a selected two-body subsystem by a finite number of positive energy levels. In contrast, we present here a scheme which allows one to take into account both the summation and integration over, respectively, the bound and continuum states of the two-body subsystem.

An approach to the continuum-state wave function in the framework of the *J*-matrix method was formulated in [8] for a system of three nuclear particles interacting via short-range potentials using an oscillator basis. Later on, this approach was extended to the case of long-range Coulomb potentials [9]. In brief, we start with the Faddeev-Merkuriev differential equations for components ψ_α of the full wave function $\Psi=\Sigma_\alpha\psi_\alpha$. Any component ψ_α is presented as a series expansion over eigenfunctions of the two-body subsystem $(\beta\gamma)$ with the total charge Z_α. This choice allows one to factor out the long-range part of the interaction and, consequently, to describe correctly the asymptotic behavior of the function Ψ only in the two-body domain Ω_α, where the mutual distance $\mathbf{x}_\alpha$ between particles β and γ is much smaller than the distance $\mathbf{y}_\alpha$ between their center of mass and the particle α. In turn, the eigenfunctions are developed into the standard bispherical basis for the angular variables plus a Laguerre basis for radial variables. In this way, we obtain a discrete analog of the Lippmann-Schwinger equation for the component ψ_α in Ω_α. This is a general scheme of our approach, and the details are presented below. Note that our approach is an attempt to improve the method of pseudostates by correctly accounting for the whole two-body spectrum and is close to that proposed and developed by Papp *et al.* (see, for example, [10]).

The present paper is organized as follows. A detailed theoretical formulation of the general scheme is presented in Sec. II. In Sec. III, the convergence and stability of the numerical results depending on the number of basis functions and the choice of parameters of the "separation" function,

*Email address: zaytsev@fizika.khstu.ru

respectively, are inspected in the case of low-energy elastic electron scattering on a hydrogen atom. In Sec. IV, the efficiency of the presented numerical scheme is demonstrated in the light of comparison with experimental data. We calculate the triple differential cross section (TDCS) for ionization excitation of helium by fast electron impact. The convergence and stability of these results depending on the choice of parameters are also demonstrated.

II. THEORY

The Hamiltonian of a three-body system has the form

$$H = H_0 + \sum_{\alpha=1}^{3} V_\alpha^C(x_\alpha), \tag{1}$$

where H_0 is the kinetic energy operator

$$H_0 = -\Delta_{x_\alpha} - \Delta_{y_\alpha} \tag{2}$$

and

$$V_\alpha^C(x_\alpha) = \frac{Z_\alpha}{x_\alpha}. \tag{3}$$

The couple $(\mathbf{x}_\alpha, \mathbf{y}_\alpha)$ stands for the set of Jacobi coordinates [11]

$$\mathbf{x}_\alpha = \tau_\alpha(\mathbf{r}_\beta - \mathbf{r}_\gamma),$$

$$\mathbf{y}_\alpha = \mu_\alpha\left(\mathbf{r}_\alpha - \frac{m_\beta \mathbf{r}_\beta + m_\gamma \mathbf{r}_\gamma}{m_\beta + m_\gamma}\right), \tag{4}$$

where m_i are the particle masses and

$$\tau_\alpha = \sqrt{2\frac{m_\beta m_\gamma}{m_\beta + m_\gamma}}, \quad \mu_\alpha = \sqrt{2m_\alpha\left(1 - \frac{m_\alpha}{m_1 + m_2 + m_3}\right)}. \tag{5}$$

The corresponding conjugate momenta are

$$\mathbf{k}_\alpha = \frac{1}{\tau_\alpha}\frac{m_\gamma \mathbf{q}_\beta - m_\beta \mathbf{q}_\gamma}{m_\beta + m_\gamma},$$

$$\mathbf{p}_\alpha = \frac{1}{\mu_\alpha}\frac{(m_\beta + m_\gamma)\mathbf{q}_\alpha - m_\alpha(\mathbf{q}_\beta + \mathbf{q}_\gamma)}{m_1 + m_2 + m_3}, \tag{6}$$

where $\mathbf{q}_\alpha$ is the momentum of a particle with the radius vector $\mathbf{r}_\alpha$ $(\mathbf{q}_1 + \mathbf{q}_2 + \mathbf{q}_3 = 0)$.

The interaction V_α can be decomposed into the short- and long-range parts ($V_\alpha^{(s)}$ and $V_\alpha^{(l)}$, respectively) [11]

$$V_\alpha^{(s)}(x_\alpha, y_\alpha) = V_\alpha(x_\alpha)\zeta_\alpha(x_\alpha, y_\alpha),$$

$$V_\alpha^{(l)}(x_\alpha, y_\alpha) = V_\alpha(x_\alpha)[1 - \zeta_\alpha(x_\alpha, y_\alpha)], \tag{7}$$

with the "separation" function of the form [12]

$$\zeta(x_\alpha, y_\alpha) = 2/\{1 + \exp[(x_\alpha/x_0)^\nu/(1 + y_\alpha/y_0)]\}, \tag{8}$$

where $\nu > 2$. Thus, the function $V_\alpha^{(s)}$ decreases rather rapidly in the "true" three-body asymptotic domain Ω_0 and coincides with the initial potential in the two-body asymptotic domain Ω_α $(x_\alpha \ll y_\alpha)$. In the general case of different particles, the total wave function is represented as a sum of three components ψ_α satisfying the set of equations [11]

$$[H_0 + V_\alpha(x_\alpha) + V_\beta^{(l)}(x_\beta) + V_\gamma^{(l)}(x_\gamma) - E]\psi_\alpha = -V_\alpha^{(s)}(\psi_\beta + \psi_\gamma). \tag{9}$$

For the system (e, e, He^{++}) particles 1 and 2 (electrons) are identical, and the solution reduces to the sum of two components ψ_1 and ψ_2 (see, for instance, [12]). They are related to each other as follows: $\psi_2 = gP_{12}\psi_1$ ($g = +1$ and $g = -1$ for, respectively, singlet and triplet spin states, P_{12} is the permutation operator). Taking into account the spatial symmetry of the total wave function, Eq. (9) can be reduced to single equation [12]

$$[H_0 + V_1(x_1) + V_3(x_3) + V_2^{(l)}(x_2) - E]\psi_1(\mathbf{x}_1, \mathbf{y}_1) = -gV_1^{(s)}P_{12}\psi_1(\mathbf{x}_1, \mathbf{y}_1) \tag{10}$$

for the component ψ_1.

The angular decomposition of the function $\Psi^{(-)}_{n_0\ell_0 m}$ of the system (e, He^+) with two bound particles (2,3) and one free particle 1 with the momentum $\mathbf{p}_0$ is given by

$$\Psi^{(-)}_{n_0\ell_0 m} = \sqrt{\frac{2}{\pi}}\frac{1}{p_0}\frac{(1 + gP_{12})}{\sqrt{2}} \times \sum_{L\lambda_0\mu_0} (\ell_0 m \lambda_0 \mu_0 | LM) i^{\lambda_0} e^{-i\sigma_{\lambda_0}} Y^*_{\lambda_0\mu_0}(\hat{p}_0)\psi^{LM}_{\ell_0\lambda_0}, \tag{11}$$

where the quantum numbers $(n_0\ell_0 m)$ describe the state of the He^+ ion. The spatial part $\psi^{LM}_{\ell_0\lambda_0}$ of the component ψ_1 in Eq. (11) can be presented in the form of a bispherical expansion

$$\psi^{LM}_{\ell_0\lambda_0}(\mathbf{x}, \mathbf{y}) = \sum_{\ell\lambda} \frac{\psi^L_{\ell_0\lambda_0,\ell\lambda}(x, y)}{xy}\mathcal{Y}^{LM}_{\ell\lambda}(\hat{x}, \hat{y}), \quad \mathbf{x} \equiv \mathbf{x}_1, \ \mathbf{y} \equiv \mathbf{y}_1, \tag{12}$$

$$\mathcal{Y}^{LM}_{\ell\lambda}(\hat{x}, \hat{y}) = \sum_{m\mu} (\ell m \lambda \mu | LM) Y_{\ell m}(\hat{x}) Y_{\lambda\mu}(\hat{y}). \tag{13}$$

In turn, and in accord with [8], we look for the radial functions $\psi^L_{\ell_0\lambda_0,\ell\lambda}(x, y)$ in the form

$$\psi^L_{\ell_0\lambda_0,\ell\lambda}(x, y) = \sum_\nu \int dk a^{\ell\lambda}_\nu(k)\varphi_{k,\ell}(x)\phi^\lambda_\nu(y), \tag{14}$$

where $\varphi_{k,\ell}(x)$ are the eigenfunctions of the Hamiltonian

$$h_x = -\Delta_x + \frac{Z_1}{x} \tag{15}$$

describing the subsystem (2, 3). Note that here we put $Z_1 = -2\sqrt{2}$ in the limit $m_3 \to \infty$.

In Eq. (14) and hereafter $\int dk$ means the summation over the discrete states and integration over the continuous states of the subsystem (2, 3), i.e.,

$$\int dk a_\nu^{\ell\lambda}(k)\varphi_{k,\ell}(x) = \sum_j \varphi_\ell^{(j)}(x) a_\nu^{\ell\lambda}(i\kappa_j) + \frac{2}{\pi}\int_0^\infty dk \varphi_\ell(k,x) a_\nu^{\ell\lambda}(k), \quad (16)$$

with $\varphi_\ell^{(j)}$ and $\varphi_\ell(k,x)$ being the corresponding eigenfunctions of the Hamiltonian (15) [see Eqs. (A2) and (A3) of the Appendix]. The Laguerre basis functions ϕ_ν^λ are used in Eq. (14),

$$\phi_\nu^\lambda(r) = [(\nu+1)_{(2\lambda+1)}]^{-1/2}(2ur)^{\lambda+1}e^{-ur}L_\nu^{2\lambda+1}(2ur), \quad (17)$$

with u being the basis parameter whose suitable choice affects the convergence rate for the numerical results.

The functions $\varphi_\ell^{(j)}$ and $\varphi_\ell(k,x)$ can also be expanded over the basis functions ϕ_n^ℓ (17). We use analytical expressions for the coefficients $\mathcal{S}_{n\ell}^{(j)}$ and $\mathcal{S}_{n\ell}(k)$ of such expansion [see Eqs. (A5) and (A6) of the Appendix]. Thus, the function $\psi_{\ell_0\lambda_0}^{LM}$ reads

$$\psi_{\ell_0\lambda_0}^{LM} = \sum_{\ell,\lambda,n,\nu} C_{n\nu}^{L(\ell\lambda)}(E)|n\ \ell\ \nu\lambda;LM\rangle, \quad (18)$$

$$|n\ \ell\ \nu\lambda;LM\rangle = \frac{\phi_n^\ell(x)\phi_\nu^\lambda(y)}{xy}\mathcal{Y}_{\ell\lambda}^{LM}(\hat{x},\hat{y}). \quad (19)$$

The coefficients $C_{n\nu}^{L(\ell\lambda)}$ are of the form

$$C_{n\nu}^{L(\ell\lambda)}(E) = \int dk \mathcal{S}_{n\ell}(k) a_\nu^{\ell\lambda}(k). \quad (20)$$

Projection of Eq. (10) onto the functions $|n\ell\,\nu\lambda;LM\rangle$ yields an infinite set of equations,

$$\sum_{\substack{\ell',\lambda'\\ n',\nu'}} \langle n\ \ell\ \nu\lambda;LM|[h_x + h_y + V(\mathbf{x},\mathbf{y}) - E]C_{n'\nu'}^{L(\ell'\lambda')}(E) \times |n'\ell'\nu'\lambda';LM\rangle = 0. \quad (21)$$

Here $h_y = -\Delta_y + Z_{11}/y$. The potential Z_{11}/y describes the Coulomb interaction of the particle 1 with the center of mass of the subsystem (2,3) and

$$V(\mathbf{x},\mathbf{y}) = V_3(x_3) + V_2^{(l)}(x_2) - \frac{Z_{11}}{y} + gV_1^{(s)}P_{12}. \quad (22)$$

The system (21) can be rewritten as

$$\sum_{n',\nu'} [h_{nn'}^\ell Q_{\nu\nu'}^\lambda + h_{\nu\nu'}^\lambda Q_{nn'}^\ell - EQ_{nn'}^\ell Q_{\nu\nu'}^\lambda]C_{n'\nu'}^{L(\ell\lambda)}(E) = -\sum_{\substack{\ell',\lambda'\\ n',\nu'}} V_{n\nu,n'\nu'}^{L(\ell\lambda)(\ell'\lambda')} C_{n'\nu'}^{L(\ell'\lambda')}(E), \quad (23)$$

where $h_{nn'}^\ell$ and $h_{\nu\nu'}^\lambda$ are the matrix elements of the partial Hamiltonian h_x^ℓ and h_y^λ, respectively (see the Appendix). $V_{n\nu,n'\nu'}^{L(\ell\lambda)(\ell'\lambda')}$ denotes the matrix element of the operator (22)

$$V_{n\nu,n'\nu'}^{L(\ell\lambda)(\ell'\lambda')} = \langle n\ \ell\ \nu\lambda;LM|V(\mathbf{x},\mathbf{y})|n'\ell'\nu'\lambda';LM\rangle. \quad (24)$$

Let us multiply Eq. (23) by $\mathcal{S}_{n\ell}(k)$ and sum the result over n:

$$\sum_{n,n',\nu'} \mathcal{S}_{n\ell}(k)[h_{nn'}^\ell Q_{\nu\nu'}^\lambda + h_{\nu\nu'}^\lambda Q_{nn'}^\ell - EQ_{nn'}^\ell Q_{\nu\nu'}^\lambda] \times \int dk' \mathcal{S}_{n'\ell}(k') a_{\nu'}^{\ell\lambda}(k') = -\sum_{\substack{\ell',\lambda'\\ n,n',\nu'}} \mathcal{S}_{n\ell}(k) V_{n\nu,n'\nu'}^{L(\ell\lambda)(\ell'\lambda')} C_{n'\nu'}^{L(\ell'\lambda')}(E). \quad (25)$$

In the left-hand side of Eq. (25) we use Eq. (20) for the coefficients $C_{n\nu}^{L(\ell\lambda)}(E)$. We have to note that the function $\mathcal{S}_{n\ell}(k)$ is the eigenfunction of the matrix of the operator h_x^ℓ (see the Appendix):

$$\sum_{n'} h_{nn'}^\ell \mathcal{S}_{n'\ell}(k) = k^2 \sum_{n'} Q_{nn'}^\ell \mathcal{S}_{n'\ell}(k). \quad (26)$$

Thus, the first and third terms on the left-hand side of Eq. (25) can be reduced to the expression

$$-(E-k^2)\sum_{\nu'} Q_{\nu\nu'}^\lambda \sum_{nn'} \mathcal{S}_{n\ell}(k) Q_{nn'}^\ell \int dk' \mathcal{S}_{n'\ell}(k') a_{\nu'}^{\ell\lambda}(k') = -p^2 \sum_{\nu'} Q_{\nu\nu'}^\lambda a_{\nu'}^{\ell\lambda}(k), \quad (27)$$

with $p^2 = E - k^2$. The second term on the left-hand side of Eq. (25) can be transformed in the same manner. In the issue we obtain

$$\sum_{\nu'} \mathcal{J}_{\nu\nu'}^\lambda(p) a_{\nu'}^{\ell\lambda}(k) = -\sum_{\substack{n,n',\nu'\\ \ell',\lambda'}} \mathcal{S}_{n\ell}(k) V_{n\nu,n'\nu'}^{L(\ell\lambda)(\ell'\lambda')} C_{n'\nu'}^{L(\ell'\lambda')}(E), \quad (28)$$

$$k^2 + p^2 = E.$$

We take into account that $h_{\nu\nu'}^\lambda - p^2 Q_{\nu\nu'}^\lambda = \mathcal{J}_{\nu\nu'}^\lambda(p)$ are the elements of the J matrix [see the Appendix, Eqs. (A7)–(A9)]. The set of algebraic equations for the coefficients $a_\nu^{\ell\lambda}(k)$ was obtained in the papers of Refs. [8,9].

Within the two-body domain Ω_α where $x \ll y \to \infty$, the potential $V(\mathbf{x},\mathbf{y})$ is a short-ranged one. This circumstance allows one to take into account only a finite number of terms on the right-hand side of Eq. (28). This means that $V_{n\nu,n'\nu'}^{L(\ell\lambda)(\ell'\lambda')} = 0$ if at least one of the indices $\{n,\nu,n',\nu'\}$ exceeds some rather large number N. Thus, if $\nu \geq N$ then the right-hand side of Eq. (28) turns to zero, and the coefficients $a_\nu^{\ell\lambda}$ satisfy the "free" equation

$$\mathcal{J}_{\nu\nu-1}^\lambda(p) a_{\nu-1}^{\ell\lambda}(k) + \mathcal{J}_{\nu\nu}^\lambda(p) a_\nu^{\ell\lambda}(k) + \mathcal{J}_{\nu\nu+1}^\lambda(p) a_{\nu+1}^{\ell\lambda}(k) = 0. \quad (29)$$

Now we use the expression [14]

$$\mathcal{G}^{\lambda(\pm)}_{\nu\nu'}(p) = -\frac{1}{p}\mathcal{S}_{\nu_<\lambda}(p)\mathcal{C}^{(\pm)}_{\nu_>\lambda}(p),$$

$$\nu_< = \min\{\nu,\nu'\}, \quad \nu_> = \max\{\nu,\nu'\}, \tag{30}$$

for the matrix elements $[\mathcal{G}^{\lambda(\pm)}(p)]$ of the radial Green's function. The functions $\mathcal{C}^{(\pm)}_{\nu\lambda}(p)$ are determined by Eq. (A14) of the Appendix. Since formally the infinite matrix $[\mathcal{G}^{\lambda(\pm)}(p)]$ is the matrix inverse of the infinite J matrix $[\mathcal{J}^{\lambda}(p)]$ [14], i.e.,

$$-[\mathcal{G}^{\lambda(\pm)}(p)][\mathcal{J}^{\lambda}(p)] = 1, \tag{31}$$

the set of equations (28) can be rewritten as follows:

$$a^{\ell\lambda}_{\nu}(k) = \mathcal{S}_{\nu\lambda_0}(p_0)\delta_{(\ell\lambda)(\ell_0\lambda_0)}\delta_{j,n_0} + \sum_{n',\nu',n'',\nu''=0}^{N-1}\left(\sum_{\ell'',\lambda''}\mathcal{G}^{\lambda(-)}_{\nu\nu'}(p) \times \mathcal{S}_{n'\ell}(k)V^{L(\ell\lambda)(\ell''\lambda'')}_{n'\nu',n''\nu''}C^{L(\ell''\lambda'')}_{n''\nu''}(E)\right), \quad \nu = 0,1,\ldots. \tag{32}$$

Note that for $(e,2e)$ reactions $k_0^2 = E - p_0^2 < 0$, i.e., $k_0 = i\kappa_{n_0}$ [see the Eq. (A6)]. This fact explains the appearance of the δ symbol δ_{j,n_0} in the free term in Eq. (32). The case $k_0 > 0$ is beyond the scope of the present paper.

Inserting Eq. (32) into Eq. (20) and taking into account the boundary conditions for the function $\Psi^{(-)}_{n_0\ell_0 m}$ (11), we obtain a set of equations for the expansion coefficients $C^{L(\ell\lambda)}_{n\nu}$ in Eq. (18). In the case of two asymptotically bound particles the set of equations takes the form

$$C^{L(\ell\lambda)}_{n\nu}(E) = \delta_{(\ell\lambda)(\ell_0\lambda_0)}\mathcal{S}^{(n_0)}_{n\ell_0}\mathcal{S}_{\nu\lambda_0}(p_0) + \sum_{n',\nu',n''\nu''=0}^{N-1}\left(\sum_{\ell'',\lambda''}\left[\int dk\mathcal{S}_{n\ell}(k)\mathcal{S}_{n'\ell}(k)\mathcal{G}^{\lambda(-)}_{\nu\nu'}(p)\right] \times V^{L(\ell\lambda)(\ell''\lambda'')}_{n'\nu',n''\nu''}C^{L(\ell''\lambda'')}_{n''\nu''}(E)\right). \tag{33}$$

To simplify the solution of the algebraic system of equations, the authors of the CCC scheme suppose that $C_{n\nu} = A_n B_\nu$, where A_n is a result of the diagonalization of the two-body Hamiltonian $h_x = -\Delta_x + \frac{Z_1}{x}$ describing the subsystem of particles (2,3). This operation replaces the two-body continuum by a discrete number of pseudostates with positive energies.

In contrast to this method, we do not make such *a priori* assumptions regarding the structure of the coefficients $C_{n\nu}$ [see Eq. (20)], and applying the J-matrix approach we eventually obtain a discrete analog of the integral equation of the Lipmann-Schwinger-type which already includes the boundary conditions (see also [10]). Solving it numerically we keep the information on the full spectrum of the two-body Hamiltonian. In this respect, we have to note that the expression in the square brackets on the right-hand side of Eq. (33)

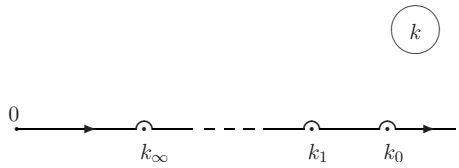

FIG. 1. The integration contour of the integral in parentheses in Eq. (33). The poles of the integrand are shown by full circles.

$$\int dk\mathcal{S}_{n\ell}(k)\mathcal{S}_{n'\ell}(k)\mathcal{G}^{\lambda(-)}_{\nu\nu'}(p) \equiv \sum_{j=0}^{\infty}\mathcal{S}^{(j)}_{n\ell}\mathcal{S}^{(j)}_{n'\ell}\mathcal{G}^{\lambda(-)}_{\nu\nu'}(\sqrt{E+\kappa_j^2}) + \frac{2}{\pi}\int_0^{\infty} dk\mathcal{S}_{n\ell}(k)\mathcal{S}_{n'\ell}(k)\mathcal{G}^{\lambda(-)}_{\nu\nu'}(p) \quad (E = p^2 + k^2), \tag{34}$$

plays a role of the matrix elements $G^{\ell\lambda(-)}_{nn';\nu\nu'}(E)$ of the asymptotic three-body Green's function $\widetilde{G}^{(-)}(E)$ in the two-body domain.

The integrals (34) can be calculated directly. Note that the integrand has the following poles at the points $k_j = \sqrt{E+\eta_j^2}$ ($\eta_j = -Z_{11}/[2(\lambda+j+1)]$) which correspond to the discrete spectrum of the Hamiltonian h_y and have an accumulation point at $k_\infty = \sqrt{E}$. The presence of the matrix element of the radial Green's function $\mathcal{G}^{\lambda(-)}_{\nu\nu'}(p)$ in the integrand means that the poles have to be rounded in a clockwise direction (Fig. 1).

Let us note that the poles can be allocated more uniformly along the integration contour if one carries out a transformation of variable. For example, if one puts $q = -Z_{11}/(2\sqrt{k^2 - E})$ then the poles are disposed at the points $q_j = \lambda + 1 + j$. Thus, the integral under consideration can be performed as an infinite sum of integrals I_j along segments L_j, in which the poles are localized, and an integral I_c with a smooth integrand, which is calculated along the segment L_c. Using the well-known Sokhotsky formula we obtain

$$I_j = \frac{2}{\pi}\int_{L_j} dk\mathcal{S}_{n\ell}(k)\mathcal{S}_{n'\ell}(k)\mathcal{G}^{\lambda(-)}_{\nu\nu'}(p) - 2i\mathcal{S}_{n\ell}(k_j)\mathcal{S}_{n'\ell}(k_j)\underset{k=k_j}{Res}\mathcal{G}^{\lambda(-)}_{\nu\nu'}(p) = \frac{2}{\pi}\int_{L_j} dk\mathcal{S}_{n\ell}(k)\mathcal{S}_{n'\ell}(k)\mathcal{G}^{\lambda(-)}_{\nu\nu'}(p) + \frac{i}{k_j}\mathcal{S}_{n\ell}(k_j)\mathcal{S}_{n'\ell}(k_j)\mathcal{S}^{(j)}_{\nu\lambda}\mathcal{S}^{(j)}_{\nu'\lambda}. \tag{35}$$

For $E < 0$ the matrix elements $G^{\ell\lambda(-)}_{nn';\nu\nu'}(E)$ can be calculated without difficulties because the number of poles is finite and (usually) not numerous. For $E > 0$ we must calculate an infinite number of integrals in Eq. (35). To avoid this time-consuming operation we use another representation for

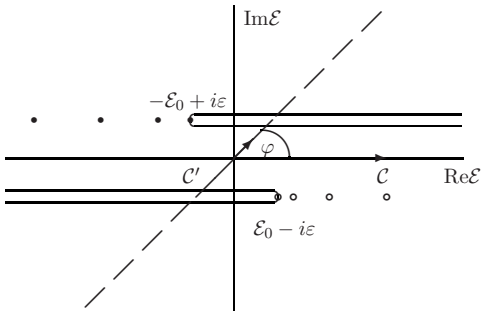

FIG. 2. The path of integration of the convolution integral (37). The poles which are associated with the discrete spectrum of the Hamiltonian h_x are depicted as full circles. $-\mathcal{E}_0+i\varepsilon$ denotes the initial point of the corresponding unitary branch cut. Open circles and $\mathcal{E}_0-i\varepsilon$ are the same for the Hamiltonian h_y.

the expression (34). As was mentioned above, the expression (34) coincides with the matrix element $G^{\ell\lambda(-)}_{nn';\nu\nu'}(E)$ of a convolution integral of the two-body Green's functions $G^{(-)}_x$ and $G^{(-)}_y$ [11]

$$\widetilde{G}^{(-)}(E)=\frac{1}{2\pi i}\oint_{\mathcal{C}} d\mathcal{E}G^{(-)}_x(\mathcal{E})G^{(-)}_y(E-\mathcal{E}). \tag{36}$$

Here the contour $\mathcal{C}$ surrounds the spectrum of the operator h_x in a counterclockwise direction. We should note that Eq. (34) coincides with the matrix element of the channel-distorted Coulomb Green's operator $\widetilde{G}$, which is used by Papp *et al.* [10] in their Lippman-Schwinger-type integral equation.

To calculate the convolution integral (36) being written now for the matrix elements

$$G^{\ell\lambda(-)}_{nn';\nu\nu'}(E)=\frac{1}{2\pi i}\int_{\mathcal{C}} d\mathcal{E}\mathcal{G}^{\ell(-)}_{nn'}(\sqrt{\mathcal{E}_0+\mathcal{E}})\mathcal{G}^{\lambda(-)}_{\nu\nu'}(\sqrt{\mathcal{E}_0-\mathcal{E}}), \tag{37}$$

with $\mathcal{E}_0=\frac{1}{2}E$, we use the method of Shakeshaft [15]. The poles and cuts of the integrand in Eq. (37) are shown in Fig. 2 (here ε is not infinitesimal for visualization). To simplify calculations we rotate the contour $\mathcal{C}$ by a positive angle φ, and the contour $\mathcal{C}'=\mathcal{E}_0e^{i\varphi}t$ is depicted by the dotted line.

TABLE I. The convergence rate of the singlet *s* phase (in rad) of the elastic $e+H$ scattering with the $s+p+d+f$ contributions calculated (a) without and (b) with smoothing factors (45). *N* is the number of basis functions (17) used in the expansion.

		k_1 (a.u.)							
	N	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8
(a)	10	2.5800	2.0662	1.7009	1.4177	1.2001	1.0408	0.9316	0.8811
	11	2.5728	2.0726	1.6941	1.4209	1.1989	1.0428	0.9259	0.8913
	12	2.5657	2.0763	1.6956	1.4144	1.2049	1.0376	0.9333	0.8806
	13	2.5602	2.0745	1.7011	1.4130	1.2000	1.0441	0.9267	0.8900
	14	2.5555	2.0707	1.7010	1.4187	1.1986	1.0394	0.9336	0.8827
	15	2.5530	2.0665	1.6969	1.4173	1.2039	1.0396	0.9282	0.8899
	16	2.5525	2.0650	1.6949	1.4131	1.2001	1.0424	0.9312	0.8843
	17	2.5533	2.0670	1.6968	1.4154	1.1993	1.0386	0.9293	0.8894
	18	2.5552	2.0698	1.6996	1.4177	1.2028	1.0422	0.9299	0.8838
	19	2.5576	2.0712	1.6985	1.4150	1.1997	1.03998	0.9313	0.8889
	20	2.5596	2.0704	1.6957	1.4136	1.1999	1.0396	0.9286	0.8846
	21	2.5611	2.0679	1.6952	1.4163	1.2022	1.0419	0.9318	0.8884
(b)	10	2.5484	2.0645	1.6944	1.4142	1.1975	1.0374	0.9270	0.8871
	11	2.5517	2.0641	1.6943	1.4136	1.1999	1.0373	0.9274	0.8850
	12	2.5518	2.0649	1.6946	1.4134	1.1994	1.0394	0.9273	0.8846
	13	2.5519	2.0652	1.6948	1.4134	1.1994	1.0394	0.9288	0.8842
	14	2.5524	2.0651	1.6952	1.4136	1.1991	1.0397	0.9290	0.8852
	15	2.5525	2.0652	1.6951	1.4140	1.1991	1.0393	0.9295	0.8854
	16	2.5525	2.0654	1.6951	1.4140	1.1994	1.0393	0.9294	0.8860
	17	2.5526	2.0654	1.6952	1.4139	1.1996	1.0393	0.9294	0.8862
	18	2.5526	2.0655	1.6953	1.4140	1.1996	1.0396	0.9292	0.8862
	19	2.5526	2.0655	1.6953	1.4140	1.1996	1.0397	0.9293	0.8862
	20	2.5526	2.0655	1.6953	1.4141	1.1996	1.0397	0.9294	0.8861
	21	2.5527	2.0656	1.6954	1.4141	1.1997	1.0397	0.9295	0.8861

TABLE II. Singlet ($g=+1$) and triplet ($g=-1$) phases (in rad) of the elastic e^-+H scattering using the s, $s+p$, $s+p+d$, and $s+p+d+f$ contributions.

k_1 (a.u.)	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8
				$g=+1$				
s[a]	2.4176	1.8974	1.5364	1.2697	1.0658	0.9106	0.7975	0.7261
$s-p$[a]	2.5452	2.0553	1.6849	1.4040	1.1899	1.0300	0.9199	0.8769
$s-p-d$[a]	2.5514	2.0637	1.6935	1.4124	1.1979	1.0380	0.9278	0.8845
$s-p-d-f$[a]	2.5527	2.0656	1.6954	1.4141	1.1997	1.0397	0.9295	0.8861
$s-p-d-f$[b]	2.5526	2.0656	1.6954	1.4141	1.1997	1.0397	0.9295	0.8863
$s-p-d-f$[c]	2.5526	2.0656	1.6954	1.4141	1.1997	1.0397	0.9294	0.8863
Ref. [18]	2.553	2.0673	1.6964	1.4146	1.202	1.041	0.930	0.886
				$g=-1$				
s[a]	2.9077	2.6794	2.4616	2.2579	2.0710	1.9019	1.7507	1.6165
$s-p$[a]	2.9374	2.7160	2.4982	2.2926	2.1031	1.9316	1.7784	1.6427
$s-p-d$[a]	2.9383	2.7172	2.4996	2.2940	2.1045	1.9329	1.7796	1.6439
$s-p-d-f$[a]	2.9384	2.7174	2.4998	2.2941	2.1046	1.9331	1.7798	1.6441
$s-p-d-f$[b]	2.9384	2.7174	2.4998	2.2941	2.1046	1.9331	1.7797	1.6443
$s-p-d-f$[c]	2.9384	2.7174	2.4998	2.2941	2.1046	1.9331	1.7797	1.6442
Ref. [18]	2.9388	2.7171	2.4996	2.2938	2.1046	1.9329	1.7797	1.643

[a] $x_0=3$.
[b] $x_0=2$.
[c] $x_0=4$.

The integral (37) is calculated numerically along the contour $\mathcal{C}'$. To explain details of integration we subdivide the integration path conventionally into two parts: $\mathcal{C}'_1$ $(t<0)$ and $\mathcal{C}'_2(t>0)$. We also introduce for brevity two variables: $p=\sqrt{\mathcal{E}_0-\mathcal{E}}$ and $k=\sqrt{\mathcal{E}_0+\mathcal{E}}$.

Note that $\arg(p)>0$ for $t<0$, whereas $\mathcal{C}^{(-)}_{\nu\lambda}(p)$ and $\mathcal{G}^{\lambda(-)}_{\nu\nu'}(p)$ are defined at $-\pi<\arg(p)<0$. To define $\mathcal{G}^{\lambda(-)}_{\nu\nu'}(p)$ in $\mathcal{C}'_1$ we use the analytic continuation [13] $\mathcal{C}^{(-)}_{\nu\lambda}(p)=\mathcal{C}^{(+)}_{\nu\lambda}(p)-2i\mathcal{S}_{\nu\lambda}(p)$, or

$$\mathcal{G}^{\lambda(-)}_{\nu\nu'}(p)=\mathcal{G}^{\lambda(+)}_{\nu\nu'}(p)+\frac{2i}{p}\mathcal{S}_{\nu\lambda}(p)\mathcal{S}_{\nu'\lambda}(p). \tag{38}$$

At the same time, the contour $\mathcal{C}'_1$ passes in the domain of definition of the function $\mathcal{G}^{\ell(-)}_{nn'}(k)$.

Reasoning by analogy allows us to integrate along the contour $\mathcal{C}'_2$. Finally, we obtain in the limit $\varepsilon\to 0$,

$$G^{\ell\lambda(-)}_{nn';\nu\nu'}(E)=\frac{\mathcal{E}_0 e^{i\varphi}}{2\pi i}\left\{\int_{-\infty}^{0}dt\mathcal{G}^{\ell(-)}_{nn'}(k)\left[\mathcal{G}^{\lambda(+)}_{\nu\nu'}(p)+\frac{2i}{p}\mathcal{S}_{\nu\lambda}(p)\mathcal{S}_{\nu'\lambda}(p)\right]+\int_{0}^{\infty}dt\left[\mathcal{G}^{\ell(+)}_{n,n'}(k)+\frac{2i}{k}\mathcal{S}_{n\ell}(k)\mathcal{S}_{n'\ell}(k)\right]\mathcal{G}^{\lambda(-)}_{\nu\nu'}(p)\right\}. \tag{39}$$

Calculating the second term in Eq. (38), we accept in accordance with [13] that

$$|\Gamma(\ell+1+it)|^2\to\Gamma(\ell+1+it)\Gamma(\ell+1-it), \tag{40}$$

as well as calculating ξ^{-2it} we choose a minimal value of the argument ξ in the range $-\pi<\arg(\xi)\le\pi$.

III. EXAMPLE: ELASTIC ELECTRON-HYDROGEN SCATTERING

The low-energy elastic scattering of an electron on a hydrogen atom is considered. Thus, we inspect the stability and the convergence of the S matrix (phase shifts) with respect to the number of basis functions.

In our case, taking into account the asymptotic behavior of the coefficients $a^{\ell\lambda}_{\nu}$ at $\nu\ge N-1$ [see also the remark after Eq. (32)] we have

$$a^{\ell\lambda}_{\nu}(k)=\frac{i}{2}\left\{\mathcal{C}^{(-)}_{\nu\lambda}(p_0)\delta_{(\ell_0\lambda_0)(\ell\lambda)}\delta_{j,n_0}-\sqrt{\frac{p_0}{p}}\mathrm{S}^{(\ell\lambda)(\ell_0\lambda_0)}_{jn_0}\mathcal{C}^{(+)}_{\nu\lambda}(p)\right\}, \tag{41}$$

and the S-matrix element can be obtained in the following form

$$S^{(\ell\lambda)(\ell_0\lambda_0)}_{jn_0}=\delta_{(\ell_0\lambda_0)(\ell\lambda)}\delta_{j,n_0}-\frac{2i}{\sqrt{pp_0}}\sum_{\ell',\lambda'}\sum_{n,\nu,n',\nu'=0}^{N-1}\mathcal{S}_{n\ell}(k)\mathcal{S}_{\nu\lambda}(p)\times V^{L(\ell\lambda)(\ell'\lambda')}_{n\nu,n'\nu'}C^{L(\ell'\lambda')}_{n'\nu'}(E). \tag{42}$$

Consequently, the s phase follows from the expression

TABLE III. Convergence of the singlet *s* phase (in rad) of the elastic e^-+H scattering in the case of $s+p+d+f$ contributions calculated for parameters $x_0=2$ and $x_0=4$.

		k_1 (a.u.)							
	N	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8
$x_0=2$	10	2.5528	2.0641	1.6917	1.4150	1.2005	1.0377	0.9249	0.8908
	11	2.5508	2.0656	1.6945	1.4121	1.2003	1.0398	0.9275	0.8836
	12	2.5513	2.0650	1.6954	1.4130	1.1986	1.0403	0.9291	0.8826
	13	2.5525	2.0646	1.6952	1.4139	1.1987	1.0392	0.9300	0.8842
	14	2.5524	2.0653	1.6948	1.4141	1.1991	1.0390	0.9294	0.8862
	15	2.5523	2.0654	1.6950	1.4139	1.1997	1.0390	0.9291	0.8866
	16	2.5526	2.0653	1.6953	1.4137	1.1996	1.0396	0.9288	0.8864
	17	2.5526	2.0654	1.6953	1.4140	1.1994	1.0397	0.9292	0.8859
	18	2.5526	2.0655	1.6952	1.4141	1.1995	1.0397	0.9294	0.8858
	19	2.5526	2.0655	1.6953	1.4141	1.1996	1.0396	0.9296	0.8860
	20	2.5526	2.0655	1.6954	1.4141	1.1997	1.0396	0.9295	0.8862
	21	2.5526	2.0656	1.6954	1.4141	1.1997	1.0397	0.9295	0.8863
$x_0=4$	10	2.5487	2.0650	1.6939	1.4130	1.1967	1.0388	0.9287	0.8861
	11	2.5500	2.0646	1.6952	1.4125	1.1987	1.0375	0.9290	0.8855
	12	2.5520	2.0641	1.6949	1.4140	1.1982	1.0386	0.9280	0.8861
	13	2.5522	2.0650	1.6945	1.4139	1.1995	1.0382	0.9285	0.8853
	14	2.5522	2.0653	1.6949	1.4135	1.1995	1.0392	0.9280	0.8856
	15	2.5524	2.0652	1.6952	1.4137	1.1994	1.0395	0.9287	0.8850
	16	2.5525	2.0653	1.6952	1.4139	1.1993	1.0397	0.9291	0.8853
	17	2.5526	2.0654	1.6952	1.4140	1.1994	1.0395	0.9295	0.8856
	18	2.5526	2.0655	1.6953	1.4141	1.1996	1.0395	0.9295	0.8860
	19	2.5526	2.0655	1.6953	1.4140	1.1996	1.0395	0.9295	0.8862
	20	2.5526	2.0655	1.6954	1.4141	1.1997	1.0396	0.9294	0.8862
	21	2.5526	2.0656	1.6954	1.4141	1.1997	1.0397	0.9294	0.8863

$$e^{2i\delta_0} = 1 - \frac{2i}{p_0}\sum_{\ell}\sum_{n,\nu,n',\nu'=0}^{N-1} \mathcal{S}_{n0}^{(j=0)}\mathcal{S}_{\nu 0}(p_0)V_{n\nu,n'\nu'}^{L=0(00)(\ell\ell)}C_{n'\nu'}^{L=0(\ell\ell)}(E). \tag{43}$$

Note that now $Z_{11}=0$ and the integrand on the right-hand side of Eq. (34) has no singularities and decreases as $k^{-(2\ell+4)}$ if $k\to\infty$. Such integrals can be calculated with the help of a standard code. The sum converges rapidly as well.

We choose the following values of parameters:

$$x_0 = 3, \quad y_0 = 20, \quad \nu = 2.1, \tag{44}$$

for the "separation" function $\zeta(x_\alpha, y_\alpha)$ (8), and $u=0.6$ for the basis function (17) [16]. The convergence of the singlet *s*-phase depending on the number of the basis functions is displayed in Table I(a). Here $k_1=\mu_1 p_0$ denotes the momentum of the scattering electron, and $k_1=\sqrt{2}p_0$ if $m_3\to\infty$.

The use of the so-called smoothing factors [17]

$$\sigma_n^N = \frac{1-\exp\{-[\alpha(n-N)N]^2\}}{1-\exp(-\alpha^2)}, \quad \alpha = 5, \tag{45}$$

allows to improve the convergence considerably. Here we do the replacement in Eqs. (33) and (43)

$$V_{n\nu,n'\nu'}^{L(\ell\lambda)(\ell'\lambda')} \to \sigma_n^N\sigma_\nu^N V_{n\nu,n'\nu'}^{L(\ell\lambda)(\ell'\lambda')}\sigma_{n'}^N\sigma_{\nu'}^N. \tag{46}$$

The convergence in this case is shown in Table I(b).

We also demonstrate the convergence of the phase with respect to the number of partial waves taken into account (Table II).

Note that the choice of x_0 in the "separation" function ζ (8) does not influence noticeably neither the convergence, nor the resulting value of the phase in this example (Table III and Table II). It is a positive sign, because the wave function should not depend on the way of "separation" in the limit of an infinite number of partial waves [19].

IV. RESULTS AND DISCUSSION

To illustrate the efficiency of the presented numerical scheme, calculations of the triple differential cross section (TDCS) for the $(e,2e)$ reaction on the helium atom in a singlet state were performed. If a fast projectile electron of energy about several kiloelectronvolts transfers to the atom relatively small amounts of energy and momentum, the respective four-body problem can be considerably simplified by examining only the first Born approximation for the in-

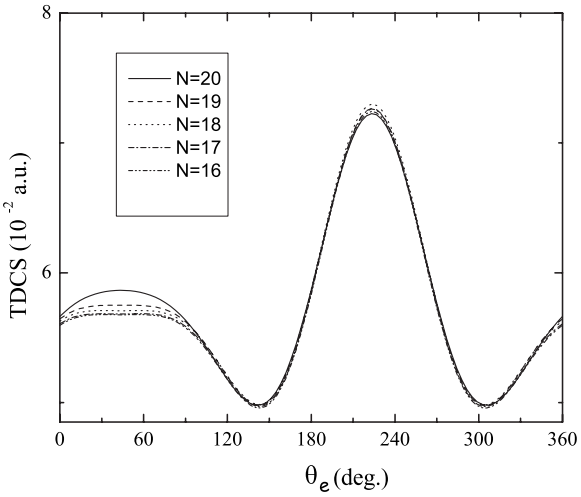

FIG. 3. Dependence of the absolute TDCS (47) for single ionization of helium on the number N of the radial basis functions. E_s=5500 eV, E_e=5 eV, θ_s=0.35°. The parameters of the "separation" functions are x_0=3, y_0=20, ν=2.1.

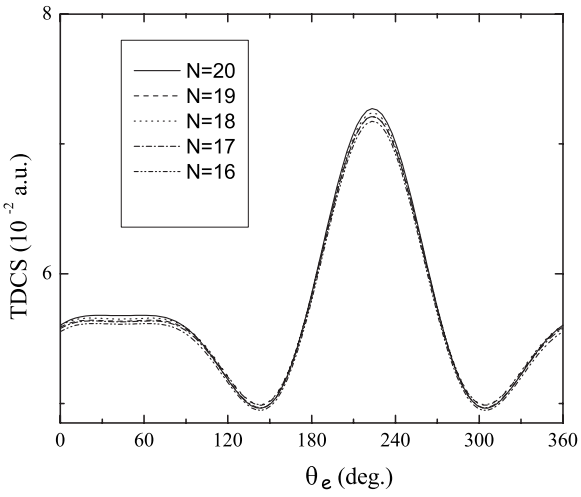

FIG. 4. As in Fig. 3, but x_0=5, y_0=50, ν=2.1.

teraction of the projectile electron with the atom.

The calculations were performed in the limit $m_3 \to \infty$; that is, $\mathbf{x}_1=\sqrt{2}\mathbf{r}_2$ and $\mathbf{y}_1=\sqrt{2}\mathbf{r}_1$ (atomic units are used $m_e=e=\hbar=1$). The triple differential cross section (TDCS) of $\mathrm{He}(e,2e)\mathrm{He}^+$ reaction when the residual He^+ ion remains in an exited state is expressed as [20]

$$\sigma_{n_0}^{(3)} \equiv \frac{d^3\sigma_{n_0}}{d\Omega_s dE_e d\Omega_e} = \frac{p_s k_e}{p_i}\frac{4}{Q^4}\sum_{\ell_0 m}|\langle\Psi_{n_0\ell_0 m}^{(-)}|\exp(i\mathbf{Q}\cdot\mathbf{r}_1) + \exp(i\mathbf{Q}\cdot\mathbf{r}_2) - 2|\Psi_0\rangle|^2. \quad (47)$$

In Eq. (47) $(E_i,\mathbf{p}_i)$, $(E_s,\mathbf{p}_s)$, and $(E_e,\mathbf{k}_e)$ are the energy and momentum of, respectively, the incident (fast), scattered (fast), and ejected (slow) electron; $\mathbf{Q}=\mathbf{p}_i-\mathbf{p}_s$ is the transferred momentum.

The angular distributions of the slow electron in the case of the $(e,2e)$ ionization-excitation reaction are calculated for two sets of experiments [21]. In these experiments the residual ion remains in the n_0=2 state, the energy of the scattered electron is E_s=5500 eV, and the ejected electron is characterized by the following kinematical conditions: (a) E_e=5 eV and θ_s=0.35°; (b) E_e=75 eV and θ_s=1°, where θ_s is the angle of the scattered electron and θ_e is the in-plane emission angle with respect to the vector $\mathbf{p}_i$.

The helium ground-state wave function Ψ_0 is obtained as a result of diagonalization of the matrix (1) which was calculated in the basis (19). Here we put ℓ_{max}=3 and $n_{max}=\nu_{max}$=15. Choosing the basis parameter u_0=1.193 yields the value E_0=−2.903 256 for the ground-state energy.

The final-state wave function $\Psi_{n_0\ell_0 m}^{(-)}$ (11) is obtained using the method described in Sec. II. We have restricted ourselves to the maximum value of the total orbital angular momentum L_{max}=2 and $\ell,\lambda \le 3$ and we have used "smoothing," Eqs. (45) and (46).

Here we would like to say a few words about the role of the parameters x_0 and y_0 in the "separation" function (8). The parameter x_0 determines the effective radius of the short-range potential $V_1^{(s)}P_{12}$ (10), whose matrix is nondiagonal with respect to the indices $(\ell\lambda)$. Besides that, the term $V_3(x_3)$ also couples partial waves with different $(\ell\lambda)$ in Eq. (10). In this respect, the value x_0 governs the nondiagonal part of the interaction which gives the dominant contribution into the TDCS. Consequently, a stability of our calculations with respect to the choice of x_0 might indicate a good convergence of the partial wave decomposition.

For the case (a) the total energy $E<0$, that allows one to use Eq. (34) for calculations of the Green's functions. The integrand on the right-hand side of Eq. (34) has the only pole at the point $k_0=\sqrt{E+Z_{11}^2/4}$ (for $\lambda=0$) and decreases rapidly enough $(k^{-(2\ell+4)})$ if $k\to\infty$. The basis parameter u=0.6 (17) is used in this calculation. We found that the convergence rate for the results is practically independent of the values of the parameters x_0 and y_0. The convergence of the angular distribution of the slow electron versus its emission angle θ_e is presented in Fig. 3 (x_0=3, y_0=20, ν=2.1) and Fig. 4 (x_0=5, y_0=50, ν=2.1). N denotes the number of Laguerre basis functions.

In Fig. 5, our results are presented in comparison with the experiment [21] and with two models: CCC [22] and the 5-channel R-matrix calculation (5MC) [21]. All theories need multiplicative factors to fit the experiment (~1.45 for our model and ~1.6 for 5MC). Note that the TDCS shape of our model is better than both the other ones.

In case (b) $E>0$, and we resort to the integrals in Eq. (39). For the energy E_e=75 eV, the TDCS $\sigma_{n_0}^{(3)}$ is approximately 40 times less than in case (a), and all the numerical inaccuracies are more noticeable here. The convergence of the angular distribution of the slow electron versus its emission angle θ_e is shown in Fig. 6 (x_0=3, y_0=20, ν=2.1, u=0.3). In Fig. 7, our results are presented in comparison with the experiment [21], CCC calculations, and 5MC. Our model reproduces the experiment better, at least the binary peak is

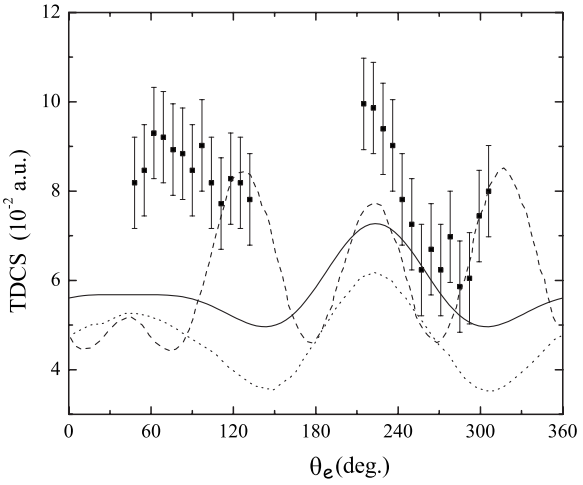

FIG. 5. Absolute TDCS (47) for the ionization excitation of helium. E_s=5500 eV, E_e=5 eV, θ_s=0.35°. Full curve, this model; broken curve, CCC; dotted curve, 5MC (all without multiplicative factors). The parameters of the "separation" functions as in Fig. 4.

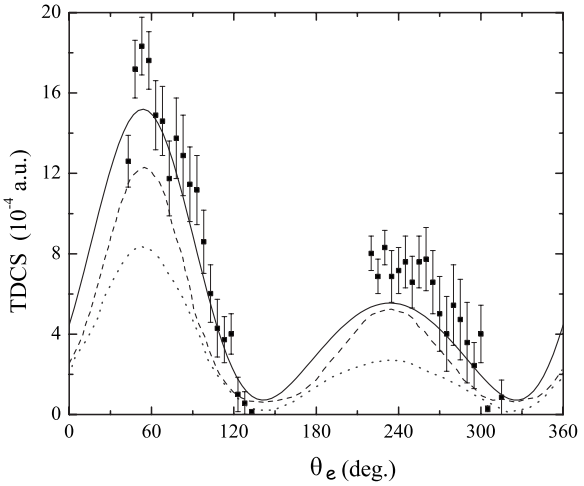

FIG. 7. Absolute TDCS (47) for single ionization excitation of helium. E_s=5500 eV, E_e=75 eV, θ_s=1°. Full curve, this model; broken curve, CCC; dotted curve, 5MC (all without multiplicative factors). The parameters of the "separation" functions as in Fig. 6.

reproduced without resorting to any fitting factors.

Let us discuss the problem of the multiplicative, fitting factors. The exact final state wave function $|\Psi_n^{(-)}(\mathbf{k}_e)\rangle$ must be normalized as follows:

$$\langle \Psi_{n'}^{(-)}(\mathbf{k}'_e)|\Psi_n^{(-)}(\mathbf{k}_e)\rangle = \delta(\mathbf{k}_e - \mathbf{k}'_e)\,\delta_{nn'}.$$

It is obvious that the function $\Psi_n^{(-)}$ being decomposed into a finite sum of square-integrable functions can never be normalized to a δ function. Possibly this is the nature of the necessity of using the fitting factors.

As a summary, we formulate the following three statements:

(i) The numerical method is suggested for solving the Faddeev-Merkuriev equations, which allows to obtain many-body wave functions including single continuum states. Its convergence rate depending on the amount of the basis functions has been studied.

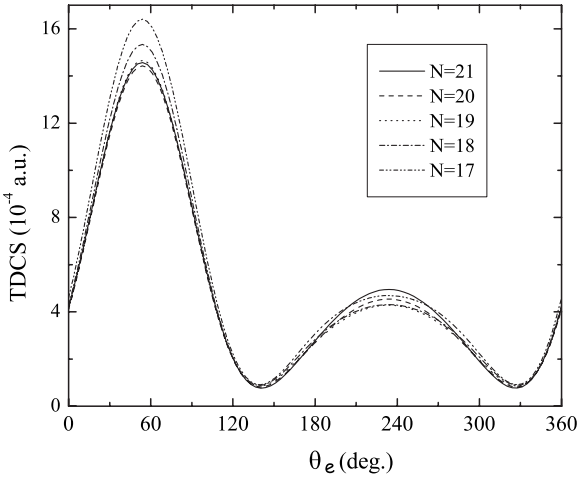

FIG. 6. As in Fig. 3, except E_e=75 eV and θ_s=1°.

(ii) The performed calculations demonstrate the importance of accounting for the whole two-body continuum spectrum. The present method gives better results than that of pseudostates which replaces the continuum by a finite number of states with positive energies.

(iii) The present method based on the *J*-matrix approach leads to the numerical scheme which can be effective for various applications in atomic physics.

The efficiency of the *J*-matrix approach to $(e,3e)$ reactions will be presented in another paper.

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APPENDIX

The Hamiltonian

$$h^\ell = -\frac{d^2}{dr^2} + \ell(\ell+1)/r^2 + 2Z/r \tag{A1}$$

has the following wave functions of the bound spectrum ($Z<0$)

$$\varphi_\ell^{(j)}(r) = (2\kappa_j r)^{\ell+1} e^{-\kappa_j r} \frac{\sqrt{-Z(j+1)_{2\ell+1}}}{(j+\ell+1)(2\ell+1)!}\,{}_1F_1(-j;2\ell+2;2\kappa_j r), \tag{A2}$$

and continuous spectrum

$$\varphi_\ell(k,r) = \frac{1}{2}(2kr)^{\ell+1}e^{-\pi t/2}e^{ikr}\frac{|\Gamma(\ell+1+it)|}{(2\ell+1)!}{}_1F_1(\ell+1+it;2\ell+2;-2ikr). \quad \text{(A3)}$$

They can be expanded over a set of the Laguerre basis functions [1]

$$\phi_n^\ell(r) = [(n+1)_{(2\ell+1)}]^{-1/2}(2ur)^{\ell+1}e^{-ur}L_n^{2\ell+1}(2ur). \quad \text{(A4)}$$

The expansion coefficients $\mathcal{S}_{n\ell}^{(j)}$ and $\mathcal{S}_{n\ell}(k)$ are given by [1,13]

$$\mathcal{S}_{n\ell}^{(j)} = (-1)^n\left(\frac{4u\kappa_j}{(u+\kappa_j)^2}\right)^{\ell+1}\left(\frac{u-\kappa_j}{u+\kappa_j}\right)^{n+j}\frac{\sqrt{-Z(j+1)_{2\ell+1}(n+1)_{2\ell+1}}}{(j+\ell+1)(2\ell+1)!}{}_2F_1\left[-n,-j;2\ell+2;1-\left(\frac{u+\kappa_j}{u-\kappa_j}\right)^2\right], \quad \text{(A5)}$$

$$\mathcal{S}_{n\ell}(k) = \frac{1}{2}\sqrt{(n+1)_{2\ell+1}}(2\sin\zeta)^{\ell+1}e^{-\pi t/2}\xi^{-it}\frac{|\Gamma(\ell+1+it)|}{(2\ell+1)!}(-\xi)^n{}_2F_1(-n,\ell+1+it;2\ell+2;1-\xi^{-2}). \quad \text{(A6)}$$

Here $\kappa_j=-Z/(j+\ell+1)$, $t=Z/k$, and $\xi=e^{i\zeta}=(iu-k)/(iu+k)$.

It is proved [1] that the functions $\mathcal{S}_{n\ell}^{(j)}$, $\mathcal{S}_{n\ell}$ are the regular solutions of the infinite trinomial recurrence which is a discrete analog of the Schrödinger equation

$$\mathcal{J}_{n,n-1}^\ell(k)d_{n-1} + \mathcal{J}_{n,n}^\ell(k)d_n + \mathcal{J}_{n,n+1}^\ell(k)d_{n+1} = 0 \quad (n=1,2,\ldots) \quad \text{(A7)}$$

with the initial condition

$$\mathcal{J}_{0,0}^\ell(k)d_0 + \mathcal{J}_{0,1}^\ell(k)d_1 = 0. \quad \text{(A8)}$$

In Eq. (A7) $\mathcal{J}_{n,n'}^\ell(k)$ are the elements of a three-diagonal matrix of the operator $(h^\ell-k^2)$ (i.e., J matrix) calculated using the basis functions ϕ_n^ℓ

$$\mathcal{J}_{nn}^\ell(k) = \frac{u^2-k^2}{u}(n+\ell+1)+2Z,$$

$$\mathcal{J}_{nn-1}^\ell(k) = \frac{u^2+k^2}{2u}\sqrt{n(n+2\ell+1)},$$

$$\mathcal{J}_{nn+1}^\ell(k) = \frac{u^2+k^2}{2u}\sqrt{(n+1)(n+2\ell+2)}. \quad \text{(A9)}$$

The coefficients $\mathcal{S}_{n\ell}^{(j)}$, $\mathcal{S}_{n\ell}$ satisfy the normalization conditions

$$\sum_{n,n'=0}^{\infty}\mathcal{S}_{n\ell}^{(j)}Q_{n,n'}^\ell\mathcal{S}_{n'\ell}^{(j')} = \delta_{j,j'},$$

$$\frac{2}{\pi}\sum_{n,n'=0}^{\infty}\mathcal{S}_{n\ell}(k)Q_{n,n'}^\ell\mathcal{S}_{n'\ell}(k') = \delta(k-k'), \quad \text{(A10)}$$

where $Q_{nn'}^\ell$ are the elements of the three-diagonal matrix and are given by the overlapping integrals

$$Q_{nn'}^\ell = \int_0^\infty \phi_n^\ell(r)\phi_{n'}^\ell(r)dr, \quad \text{(A11)}$$

$$Q_{nn-1}^\ell = -\frac{1}{2u}\sqrt{n(n+2\ell+1)},$$

$$Q_{nn+1}^\ell = -\frac{1}{2u}\sqrt{(n+1)(n+2\ell+2)},$$

$$Q_{nn}^\ell = \frac{1}{u}(n+\ell+1). \quad \text{(A12)}$$

The corresponding completeness condition takes the form

$$\frac{2}{\pi}\int_0^\infty dkQ_{n,n''}^\ell\mathcal{S}_{n''\ell}(k)\mathcal{S}_{n'\ell}(k) + \sum_{j=0}^{\infty}Q_{n,n''}^\ell\mathcal{S}_{n''\ell}^{(j)}\mathcal{S}_{n'\ell}^{(j)} = \delta_{nn'}. \quad \text{(A13)}$$

The second solution of Eq. (A7) can be presented in the form [1,13]

$$\mathcal{C}_{n\ell}^{(\pm)}(k) = -\sqrt{n!\,(n+2\ell+1)!}\frac{e^{\pi t/2}\xi^{it}}{(2\sin\zeta)^\ell}\frac{\Gamma(\ell+1\pm it)}{|\Gamma(\ell+1\pm it)|}\frac{(-\xi)^{\pm(n+1)}}{\Gamma(n+\ell+2\pm it)}{}_2F_1(-\ell\pm it,n+1;n+\ell+2\pm it;\xi^{\pm 2}). \quad \text{(A14)}$$

The function $\mathcal{C}_{n\ell}^{(+)}(k)$ ($\mathcal{C}_{n\ell}^{(-)}(k)$) is determined at $\mathrm{Im}(k)>0$ [$\mathrm{Im}(k)<0$] of the complex plane k. The analytical continuation can be done with the help of the following relation [13]:

$$\mathcal{C}_{n\ell}^{(+)}(k) = \mathcal{C}_{n\ell}^{(-)}(k) + 2i\mathcal{S}_{n\ell}(k). \tag{A15}$$

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