Relativistic *J*-matrix method

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The relativistic version of the *J*-matrix method for a scattering problem on the potential vanishing faster than the Coulomb one is formulated. As in the nonrelativistic case it leads to a finite algebraic eigenvalue problem. The derived expression for the tangent of phase shift is simply related to the nonrelativistic case formula and gives the latter as a limit case. It is due to the fact that the used basis set satisfies the ''kinetic balance condition.''

I. INTRODUCTION

The *J*-matrix method, introduced by Heller and Yamani [1,2] and developed by Yamani and Fishman [3], is an example of an algebraic method in quantum scattering theory. Comparing with the algebraic variational theories the method has been shown to be free of the false resonances problem [4]. It has been used in construction of the Gauss quadrature of the continuum [5] (see also Ref. [6]), in the definition and analysis of a reproducing kernel in the context of Harris eigenvalues [7]. Quite recently, it has been used in formulation of complex-scaling method [8] and in development of the multichannel Green's functions [9] by means of a complete L^2 basis.

The crux of the method is representation of the Hamiltonian in a suitable nonorthogonal basis changing the differential scattering problem into the purely algebraic one. Thus far only the nonrelativistic version of the method has been formulated. The aim of this paper is to develop the simple relativistic formulation of the method in its theoretical framework for potentials sufficiently regular at the origin and vanishing at infinity faster than the Coulomb one.

II. NONRELATIVISTIC *J*-MATRIX: RADIAL KINETIC ENERGY CASE

First we briefly review the non-relativistic Jacobi matrix approach introduced in Refs. [1,2] and extended in Ref. [3]. We recall only the case when the potential vanishing faster than the Coulomb one is involved, as we shall formulate the relativistic formalism for this kind of potential. The Coulomb case is much more complicated and it will be considered elsewhere. Let $\{\phi_n^l\}_{n=0}^{\infty}$ be either Laguerre or Gaussian (Hermite) basis set. The explicit forms of both bases as well as some other formulas concerning non-relativistic problem (see Ref. [3]) are collected in Table I. Only the second basis, i.e., the Gaussian one, forms an orthogonal set, hence, in general, the notion of biorthonormality is needed. The set $\{\bar{\phi}_n^l\}_{n=0}^{\infty}$ is biorthonormal to $\{\phi_n^l\}_{n=0}^{\infty}$ with respect to the unitary scalar product if $\langle \bar{\phi}_m^l|\phi_n^l\rangle \equiv \int_0^{\infty}\bar{\phi}_m^l(\lambda r)\phi_n^l(\lambda r)dr = \delta_{mn}$. Biorthonormal basis functions $\{\bar{\phi}_n^l\}$ are also given in Table I. The important feature of the sets $\{\phi_n^l\}$ is that the radial kinetic energy operator

$$H_0 - \frac{k^2}{2} \equiv -\frac{1}{2}\frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} - \frac{k^2}{2} \qquad (1)$$

if expanded in any of them, takes the tridiagonal or Jacobi form

$$J_{mn} \equiv \langle \phi_m^l|(H_0 - k^2/2)\phi_n^l\rangle,$$

$$J_{mn} \neq 0 \quad \text{only for} \quad m = n, n \pm 1. \qquad (2)$$

In the above k is a wave number related to the energy $\mathcal{E}$ and mass m of the projectile

$$k^2 = \frac{2m\mathcal{E}}{\hbar^2}. \qquad (3)$$

It must be stressed here that the matrix elements J_{mn} are functions of k, i.e., $J_{mn} = J_{mn}(k)$. The regular solution $S(k,r)$ of the equation

$$(H_0 - k^2/2)S(k,r) = 0 \qquad (4)$$

is simply proportional to the Riccati-Bessel function, satisfying $S(k,r) \sim r^{l+1}$ as $r \to 0$ and $S(k,r) \underset{r\to\infty}{\sim} \sin(kr - (\pi l/2))$. Using an expansion of $S(k,r)$ in the basis $\{\phi_n^l\}$, i.e., $S(k,r) = \Sigma_{n=0}^{\infty} s_m^l \phi_n^l(\lambda r)$, one can write Eq. (4) in the form

$$\sum_{n=0}^{\infty} J_{mn}s_n^l = 0. \qquad (5)$$

As shown in Ref. [3], using the explicit form of the matrix elements J_{mn} one can find the expansion coefficients s_n^l in terms of Gegenbauer polynomials (see Table I). Again we have $s_n^l = s_n^l(k)$. In the *J*-matrix method to solve a scattering problem one introduces the second, cosinelike function $C(k,r)$, which is required to satisfy $C(k,r) \sim r^{l+1}$ as $r \to 0$ and $C(k,r) \underset{r\to\infty}{\sim} \cos(kr - (\pi l/2))$. It cannot be the second solution of the original, homogeneous problem as this solution, proportional to the Riccati-Neumann function, is singular at the origin.

The required $C(k,r)$ function has been found [1–3], in another way, namely, by solving an inhomogeneous equation

$$(H_0 - k^2/2)C(k,r) = \beta\bar{\phi}_0^l(\lambda r), \quad \beta = -\frac{k}{2s_0^l} \qquad (6)$$

with s_0^l being the first expansion coefficient of sine solution. Then the expansion coefficients of $C(k,r)$ satisfy the equation

TABLE I. Elements of expansion of sine- and cosine-like solutions in the Laguerre and the Gaussian basis set [3]. The $L_n^{(\alpha)}$ and $C_n^{(\alpha)}$ are the Laguerre and the Gegenbauer polynomials, respectively while $_2F_1$ and $_1F_1$ are the Gauss and the Kummer (confluent) hypergeometric functions (see Ref. [11]), respectively; $\lambda > 0$ is a scaling parameter.

Quantity	Laguerre set	Gaussian set
ϕ_n^l	$(\lambda r)^{l+1}\exp(-\lambda r/2)L_n^{(2l+1)}(\lambda r)$	$(\lambda r)^{l+1}\exp(-\lambda^2 r^2/2)L_n^{(2l+1)}(\lambda^2 r^2)$
$\bar{\phi}_n^l$	$\dfrac{n!}{\lambda n+2l+1}(\lambda r)^{-1}\phi_n^l$	$\dfrac{2n!}{\lambda^2\Gamma(n+2l+3/2)}\phi_n^l$
s_n^l	$\dfrac{2^l l! n!(\sin\theta)^{l+1}}{n+2l+1}C_n^{(l+1)}(\cos\theta)$	$\dfrac{\sqrt{2\pi}n!(-1)^n}{\Gamma(n+l+3/2)}\exp(-\eta^2/2)L_n^{(l+1/2)}(\eta^2)$
c_n^l	$\dfrac{-2^l\Gamma(l+1/2)n!}{\sqrt{\pi}\Gamma(n+2l+2)(\sin\theta)^l}$ $\times {}_2F_1\left(-n-2l-1,n+1;\dfrac{1}{2}-l;\sin^2(\theta/2)\right),$ $\sin\theta\equiv\dfrac{k\lambda^{-1}}{k^2\lambda^{-2}+1/4}$	$\dfrac{\sqrt{2/\pi}\Gamma(n+1/2)(-1)^n n!}{\Gamma(n+l+3/2)}\exp(-\eta^2/2)\eta^{-l}$ $\times {}_1F_1\left(-n-l-\dfrac{1}{2},\dfrac{1}{2}-l,\eta^2\right),$ $\eta\equiv\dfrac{k}{\lambda}$

$$\sum_{n=0}^{\infty} J_{mn}c_n^l = \beta\bar{\phi}_0^l. \qquad (7)$$

The corresponding coefficients $c_n^l = c_n^l(k)$ (see Table I) have also been found [3] by some differential technique. The calculated expansions $S(k,r) = \sum_{n=0}^{\infty} s_n^l \phi_n^l(\lambda r)$ and $C(k,r) = \sum_{n=0}^{\infty} c_n^l \phi_n^l(\lambda r)$ have been used in an approximate solution of the original scattering problem on the radial potential $V = V(r)$ vanishing faster than the Coulomb potential

$$\left(H_0 + V - \frac{k^2}{2}\right)\psi_E = 0. \qquad (8)$$

Namely, the potential V has been replaced by a truncated potential operator

$$V^N = P_N^\dagger V P_N, \qquad (9)$$

where P_N is the generalized projection operation

$$P_N = \sum_{n=0}^{N-1} |\phi_n^l\rangle\langle\bar{\phi}_n^l|. \qquad (10)$$

The new potential operator can be written in the basis $\{\phi_n^l\}$ as an $N\times N$ matrix with the matrix elements $V_{mn}^N = \langle\bar{\phi}_n^l|V\phi_n^l\rangle$. Then the exact solution ψ_E^N of the new problem

$$\left(H_0 + V^N - \frac{k^2}{2}\right)\psi_E^N = 0. \qquad (11)$$

has been expanded in the basis $\{\phi_n^l\}$ as

$$\psi_E^N(r) = \sum_{n=0}^{N-1} a_n^l\phi_n^l + \sum_{n=N}^{\infty}(s_n^l + \tan\delta_N c_n^l)\phi_n^l \qquad (12)$$

to satisfy the boundary requirement $\psi_E^N(r)\underset{r\to\infty}{\sim}\sin(kr - (\pi l/2)) + \tan\delta_N\cos(kr - (\pi l/2))$. The $\tan\delta_N$ is an approximation of the tangent of the sought phase shift δ of the exact solution ψ_E of the problem (8). The left-hand side projection of Eq. (11) onto the basis $\{\phi_n^l\}$ gives then infinitely many equations depending on n. However all equations for $n \geq N + 1$ are satisfied automatically as coefficients s_n^l, c_n^l satisfy the same recursion relation (5) for any $m > 0$. The remaining finite set on equations involve $N+1$ unknowns $\tan\delta_N, \{a_{nl}\}_{n=0}^{N-1}$. Those equations can be easily solved [1,2]. In particular, using the recursion relation for matrix elements J_{nm} the tangent can be calculated giving

$$\tan\delta_N = -\frac{s_{N-1}^l + g_{N-1,N-1}(\mathcal{E})J_{N,N-1}s_N^l}{c_{N-1}^l + g_{N-1,N-1}(\mathcal{E})J_{N,N-1}c_N^l}, \qquad (13)$$

where $g_{N-1,N-1}(\mathcal{E}) = \sum_{n=0}^{N-1}\Gamma_{N-1,m}^2/(\mathcal{E}_m - \mathcal{E})$ with the matrix Γ diagonalizing the finite-dimensional problem $[\Gamma^\dagger P^\dagger(H_0 + V - k^2/2)P\Gamma]_{mn} = (\mathcal{E}_n - \mathcal{E})\delta_{mn}$. Here the energy dependent quantity $g_{N-1,N-1}(\mathcal{E})$ can be viewed as the matrix element of the inverse of the truncated operator $P^\dagger(H_0 + V^N - (k^2/2))P$ if restricted to the N-dimensional space where it does not vanish. The quantities $\mathcal{E}_n$ [10] are called Harris eigenvalues (see also Ref. [7], and references therein).

III. RELATIVISTIC JACOBI-MATRIX PROBLEM

Now we shall turn to the relativistic problem. Before the formulation of the method we shall find the relativistic counterparts of $S(k,r)$ and $C(k,r)$ in some suitable basis. We shall also calculate the relativistic Jacobi matrix elements in this basis. For this purpose consider the free Dirac equation

$$(\mathcal{H}_0 - E/c\hbar)\Psi$$

$$\equiv\begin{pmatrix}(mc^2 - E)/c\hbar & -d/dr + \kappa/r \\ d/dr + \kappa/r & (-mc^2 - E)/c\hbar\end{pmatrix}\begin{pmatrix}F(r) \\ G(r)\end{pmatrix} = \begin{pmatrix}0 \\ 0\end{pmatrix}. \qquad (14)$$

In the above the total energy E is related to the rest energy $\mathcal{E}$ as $E = \mathcal{E} + mc^2$. Let $l(\kappa)$ be the non-negative solution of the equation $l(l+1) = \kappa(\kappa+1)$, i.e., $l(\kappa) = \kappa$ and $l(\kappa) = -\kappa$

-1 for positive and negative κ, respectively. We shall usually omit the symbol κ in the notation throughout the text and write l only, remembering that the latter depends on κ. Then Eq. (14) has two independent solutions. The first one, regular at the origin

$$\Psi_{\mathrm{reg}}(r) = \begin{pmatrix} F_{\mathrm{reg}}(r) \\ G_{\mathrm{reg}}(r) \end{pmatrix} \sim \begin{pmatrix} \hat{j}_l(\tilde{k}r) \\ \pm \epsilon \hat{j}_{l\mp 1}(\tilde{k}r) \end{pmatrix} \quad (15)$$

is constituted by the Riccati-Bessel functions with boundary behavior

$$\hat{j}_l(x) \underset{x \to 0}{\sim} \frac{x^{l+1}}{(2l+1)!!} \quad \text{and} \quad \hat{j}_l(x) \underset{x \to \infty}{\sim} \sin\left(x - \frac{\pi l}{2}\right). \quad (16)$$

The numbers ϵ and $\tilde{k}$ in Eq. (15) are standard abbreviations

$$\epsilon \equiv \sqrt{\frac{E - mc^2}{E + mc^2}}, \quad \tilde{k} \equiv \frac{\sqrt{(E - mc^2)(E + mc^2)}}{c\hbar}. \quad (17)$$

The quantity $\tilde{k}$ converges in the nonrelativistic limit $c \to \infty$ to the number $k = \sqrt{2m\mathcal{E}/\hbar^2}$. The second solution of Eq. (14), irregular at zero is given by

$$\Psi_{\mathrm{irr}}(r) = \begin{pmatrix} F_{\mathrm{irr}}(r) \\ G_{\mathrm{irr}}(r) \end{pmatrix} \sim \begin{pmatrix} -\hat{n}_l(\tilde{k}r) \\ \pm \epsilon \hat{n}_{l\mp 1}(\tilde{k}r) \end{pmatrix}. \quad (18)$$

Here we have the Ricatti-Neumann functions with properties

$$\hat{n}_l(x) \underset{x \to 0}{\sim} -\frac{(2l-1)!!}{x^l} \quad \text{and} \quad \hat{n}_l(x) \underset{x \to \infty}{\sim} -\cos\left(x - \frac{\pi l}{2}\right). \quad (19)$$

In both solutions (15) and (18) the upper and lower signs in the small components correspond to negative and positive κ, respectively. From the above it can be immediately seen that the regular solution Ψ_{reg} is the relativistic counterpart of nonrelativistic function $S(k,r)$. For the sake of consistency with the nonrelativistic case, hereafter we shall denote the relativistic sinelike solution Ψ_{reg} by Ψ_S. To develop the Jacobi matrix analysis we have to introduce a suitable basis set.

A. The basis set

In the Hilbert space $L^2(0,\infty) \otimes C^2$ on which the Dirac operator from Eq. (14) is defined. Let again $\{\phi_n^l(x)\}$ be either the Laguerre or the Gaussian basis set and let $\psi_n^l(\lambda r) = (\kappa/r + d/dr)\phi_n^l(\lambda r)$.[1] Then the basis set defined for our purposes is

$$\Phi_{n\kappa}^+(r) \equiv \begin{pmatrix} \phi_n^l(\lambda r) \\ 0 \end{pmatrix}, \quad \Phi_{n\kappa}^-(r) \equiv \begin{pmatrix} 0 \\ \psi_n^l(\lambda r) \end{pmatrix}. \quad (20)$$

The above set depends on the positive reals number λ which can be treated as a nonlinear variational parameter (see, for instance, Ref. [12]). Note that the set (20) satisfies the "ki-

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[1]One should keep in mind that here dependence on κ is not only present via l coefficient, but via operator $(\kappa/r + d/dr)$.

netic balance condition." The latter condition is generally defined as a requirement that, if the functions $\{\gamma_i\}$ are used to expand the large component of the solution of the Dirac equation, then the basis $\{\omega_i\}$ used for expansion of the small component should consist of linear combinations of functions $\{(\kappa/r + d/dr)\gamma_i\}$. Use of such a basis is the simplest way [13,14] to omit the problem of the so called "finite basis set disease" (see Refs. [16–18]) in estimation of bound states of the atomic system. It seems that it would also be interesting in the future to consider the relativistic *J*-matrix problem in the context of the relativistic Sturmian basis (see Ref. [19], and references therein) as it is known that the relativistic free particle Green function takes a particularly simple form in this basis.

The biorthonormal elements to the functions (20) obviously are $\bar{\Phi}_{n\kappa}^+(r) = (\bar{\phi}_n^l(\lambda r),0)^T$, $\bar{\Phi}_{n\kappa}^-(r) = (0,\bar{\psi}_n^l(\lambda r))^T$. As usual, we denote by $\bar{f}_n$ the element biorthonormal to f_n. The elements $\bar{\phi}_n^{l(\kappa)}$ [3] are recalled in Table I. Here we shall calculate the biorthonormal elements $\bar{\psi}_n^{l(\kappa)}$.

It is easy to show (integrating by parts) that biorthonormal elements $\{\bar{\psi}_n^l(x)\}_{n=0}^\infty$ should satisfy the equation

$$\int_0^\infty \left[\left(\frac{\kappa}{r} - \frac{d}{dr}\right)\bar{\psi}_m^l(\lambda r)\right]\phi_n^l(\lambda r)dr = \delta_{mn}. \quad (21)$$

Hence it suffices only to solve the following inhomogeneous differential equation

$$\left(\frac{\kappa}{x} - \frac{d}{dx}\right)\bar{\psi}_n^l(x) = \bar{\phi}_n^l(x), \quad x = \lambda r. \quad (22)$$

The resulting functions are given in Table II. They all belong to the space $L^2(0,\infty)$. This fact is obvious apart from the case of negative κ for the Gaussian set. This case needs more careful analysis as here it is not possible to give the functions by explicit formula. For all $\kappa < 0$ the functions $\{\bar{\psi}_n^l\}$ due to Gaussian set behave as r^{l+2} at the origin, and vanish at infinity not slower than $r^{-(l+1)}$ as the limit of the occurring integral is finite. Then $(\psi_n^l)^2$ behaves for $r \to \infty$ as $r^{-2(l+1)}$ and, as l is nonnegative, $\|\psi_n^l\|$ exists. Thus in both cases, when $\{\phi_n^l\}$ is either the Laguerre or the Gaussian basis set, all elements $\{\bar{\psi}_n^l\}$ biorthonormal to new functions $\psi_n^l = (\kappa/r + d/dr)\phi_n^l$ belong to $L^2(0,\infty)$. Then obviously biorthonormal elements $\bar{\Phi}_{n\kappa}$ due to the relativistic case belong to the Hilbert space $L^2(0,\infty) \otimes C^2$. Note that we do not need the explicit forms of biorthonormal functions in our considerations.

B. Expansions of relativistic sine and cosine solutions

Now we are in the position to find the expansions of sinelike $\Psi_S = \Psi_{\mathrm{reg}}$ and cosinelike Ψ_C solutions. The latter are to satisfy three requirements: (1) Ψ_C should have Ψ_{irr} type asymptotic form, (2) Ψ_C should exhibit regular behavior at the origin, (3) coefficients of the Ψ_C expansion should satisfy (apart from at most the few first ones) the same recurrence equations as the ones of $\Psi_{\mathrm{reg}} = \Psi_S$.

Consider first the solution

TABLE II. Biorthonormal elements $\bar{\psi}_n^l$ due to the small component.

Quantity	Laguerre set	Gaussian set
$\bar{\psi}_n^l$ for $\kappa > 0$	$-\dfrac{n!}{n+2l+1}(\lambda r)^l \exp(-\lambda r/2)$	$-\dfrac{n!}{\lambda^2\Gamma(n+2l+3/2)}\exp(-\lambda^2 r^2/2)(\lambda r)^l$
	$\times \sum\limits_{k=0}^{n}(-2)^{k+1}L_{n-k}^{(2l+k+1)}(\lambda r)$	$\times \sum\limits_{k=0}^{n}(-2)^{k+1}L_{n-k}^{(2l+k+1)}(\lambda^2 r^2)$
$\bar{\psi}_n^l$ for $\kappa < 0$	$-\dfrac{n!}{n+2l+1}\exp(-\lambda r/2)\sum\limits_{k=0}^{n}(-2)^{k+1}$	$-\dfrac{n!}{\lambda^2\Gamma(n+2l+3/2)}(\lambda r)^{-(l+1)}$
	$\times \sum\limits_{i=0}^{k}\dfrac{(2l+1)!}{(2l+1-i)!}(\lambda r)^{2l+1-i}(-1)^i L_{n-i}^{(2l+1+i)}(\lambda r)$	$\times \int_0^{(\lambda r)^2} t^{l+1/2}\exp(-t^2/2)L_n^{(l+1/2)}(t)\,dt$

$$\Psi_U(\tilde{k},r) = (F_U(\tilde{k},r), G_U(\tilde{k},r))^T$$

of the inhomogeneous equation of type (14):

$$\left(\mathcal{H}_0 - \frac{E}{c\hbar}\right)\Psi_U \equiv \Phi_{\text{inh}}. \qquad (23)$$

In the above the index $U = S, C$ corresponds to sinelike and cosinelike solution. The inhomogeneity is chosen as $\Phi_{\text{inh}} = \Phi_{0\kappa}^+ = (\Omega_U \bar{\phi}_0^l, 0)^T$ and the coefficients Ω_U are $\Omega_S = 0$, $\Omega_C = -\epsilon/s_0^l$.

Equation (23) can be also written as

$$(\kappa/r - d/dr)G_U - \tilde{k}\epsilon F_U = \Omega_U \bar{\psi}_0^l,$$

$$(\kappa/r + d/dr)F_U - \frac{\tilde{k}}{\epsilon}G_U = 0. \qquad (24)$$

We can introduce the relativistic counterpart of the Jacobi matrix

$$\mathcal{J}_{mn}^{ss'} \equiv \langle \Phi_{m\kappa}^s | (\mathcal{H}_0 - E/c\hbar)\Phi_{n\kappa}^s \rangle,$$

$$s, s' = \pm, \quad m, n = 0, 1, 2, \ldots. \qquad (25)$$

The matrix elements of $\mathcal{J}$ can be expressed in an extremely simple form. To see this, let us define the 2×2 matrices $\mathcal{J}_{mn}$ defined by their matrix elements as $\{\mathcal{J}_{mn}\}_{ss'} \equiv \mathcal{J}_{mn}^{ss'}$. Then it can be easily seen that in the spinor basis the new matrix takes the particularly simple form

$$\mathcal{J}_{mn} = \begin{pmatrix} -\tilde{k}\epsilon\langle \phi_m^l | \phi_n^l \rangle & \langle \psi_m^l | \psi_n^l \rangle \\ \langle \psi_m^l | \psi_n^l \rangle & -\dfrac{\tilde{k}}{\epsilon}\langle \psi_m^l | \psi_n^l \rangle \end{pmatrix}. \qquad (26)$$

The explicit forms of the integrals constituting elements of the above matrix are given in Table III. They are simply related to the nonrelativistic J-matrix elements (2) (see Ref. [3]):

$$J_{mn} = \frac{1}{2}\langle \psi_m^l | \psi_n^l \rangle - \frac{k^2}{2}\langle \phi_m^l | \phi_n^l \rangle. \qquad (27)$$

Now we shall predict the expansions of the two solutions in basis (20) in the following form:

$$\Psi_U = \sum_{s=\pm}\sum_{n=0}^{\infty} u_{n\kappa}^s \Phi_{n\kappa}^s \equiv \sum_{n=0}^{\infty} u_n^l(\tilde{k})\begin{pmatrix} \phi_n^l \\ (\epsilon/\tilde{k})\psi_n^l \end{pmatrix},$$

$$U = S, C; \quad u = s, c, \qquad (28)$$

i.e., we predict that large components of sine-like and cosine-like solutions are given by the same expansion coefficients s_n^l, c_n^l as in the non-relativistic case, only taken in the modified point $\tilde{k}$ and that the small components coefficients are only rescaled by $\epsilon/\tilde{k}$.

It can be easily verified that Eq. (28) really solves Eq. (14). Namely putting the above expansion into the equation and using the definition of matrix elements (25) we get the infinite set of equations

$$\sum_{s'=\pm}\sum_{n=0}^{\infty} \mathcal{J}_{mn}^{ss'} u_{n\kappa}^{s'} = \Omega_U \bar{\phi}_0^l \delta_{m0}\delta_{s,+},$$

$$s = \pm, m = 0, 1, 2, \ldots \qquad (29)$$

as for any pair m, n fixed the second element in the lower row of the matrix (26) is rescaled by $-\tilde{k}/\epsilon$ we obtain immediately that all equations (29) with a negative "index" $s =$ "$-$" are

TABLE III. The overlap integrals proportional to the elements of $\mathcal{J}$ matrix.

Integral	Laguerre set	Gaussian set
$\langle \phi_m^l | \phi_n^l \rangle$	$\dfrac{\Gamma(n+2l+2)}{\lambda n!}[2(n+2l+2)\delta_{mn}-n\delta_{m,n-1}$	$\dfrac{\Gamma(n+l+3/2)}{2n!}\delta_{mn}$
	$-(n+2n+3)\delta_{m,n+1}]$	
$\langle \psi_m^l | \psi_n^l \rangle$	$\dfrac{\Gamma(n+2l+2)}{4n!}[2(n+2l+2)(2\lambda-1)\delta_{mn}$	$\dfrac{\lambda^2\Gamma(n+l+3/2)}{2n!}[(2n+l+3/2)\delta_{mn}$
	$+n\delta_{m,n-1}+(n+2n+3)\delta_{m,n+1}]$	$+n\delta_{m,n-1}+(n+l+3/2)\delta_{m,n+1}]$

satisfied trivially. Recalling the definition of $l=l(\kappa)$ [see cf. the remark following Eq. (14)] after integration by parts one gets

$$\langle \psi_m^l | \psi_n^l \rangle = \left\langle \left(\frac{\kappa}{r} + \frac{d}{dr} \right) \phi_m^l \middle| \left(\frac{\kappa}{r} + \frac{d}{dr} \right) \phi_n^l \right\rangle$$
$$= \left\langle \phi_m^l \middle| \left(-\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} \right) \phi_n^l \right\rangle.$$

Taking into account the form of the upper row of the matrix (26) and the identity (27) we obtain immediately that equations (29) with the ''index'' $s=$''$+$'' have the identical form with the sets of equations (5), (7) if the latter are evaluated at $\tilde{k}$ instead of k. Thus we have shown that the expansions (28) are in fact solutions of Eq. (24). From the nonrelativistic case we see that their large components have the desired behavior at the origin and at infinity. Moreover, as the equations of the type (14) are coupled and the behavior of the one component determines the behavior of the other one. Hence both the components of the solutions Ψ_S, Ψ_C have the asymptotic behavior we need for purposes of our method, i.e., Ψ_S is simply the regular solution, Ψ_C behaves as Ψ_{irr} at infinity and as Ψ_{reg} at the origin. As the inhomogeneity involves only one biorthonormal element $\Psi_{0\kappa}^+$ both functions satisfy the same set of equations apart from the first one [see formula (26)].

IV. POTENTIAL SCATTERING

Now we shall consider the central problem of our paper which is the approximate solution within the $\mathcal{J}$-matrix formalism. Consider again the radial part of the scattering problem of a projectile on a target described by a sufficiently regular potential $V=V(r)$ vanishing at infinity faster than the Coulomb potential. To solve the problem one has to find the solution of the following equation:

$$\left(\mathcal{H}_0 + \frac{V}{c\hbar} - \frac{E}{c\hbar} \right) \Psi_E = 0. \tag{30}$$

A solution Ψ_E of the above equation is required to satisfy the boundary condition $\Psi_E(\tilde{k},r) \underset{r\to\infty}{\sim} \Psi_S(\tilde{k},r) + \tilde{t}\Psi_C(\tilde{k},r)$ where the tangent of the phase shift, $\tilde{t}=\tan\tilde{\delta}$, is to be found.

To develop the formalism of the relativistic J-matrix (we shall denote it by $\mathcal{J}$ matrix to distinguish from the nonrelativistic case) we use the generalized projection operators

$$\mathcal{P}_N = \sum_{s=\pm} \sum_{n=0}^{N-1} |\Phi_{n\kappa}^s \rangle \langle \Phi_{n\kappa}^s|, \tag{31}$$

and introduce the truncated potential

$$\mathcal{V}^N = \mathcal{P}_N^\dagger \frac{V}{c\hbar} \mathcal{P}_N, \tag{32}$$

where $\mathcal{P}_N^\dagger$ corresponds to Hermitian conjugate of $\mathcal{P}_N$.

Now one can seek the exact solution of the equation with truncated potential

$$\left(\mathcal{H}_0 + \mathcal{V}^N - \frac{E}{c\hbar} \right) \Psi_E^N(r) = 0. \tag{33}$$

Note that for any $\psi \in L^2(0,\infty) \otimes C^2$ the function $\mathcal{V}^N \psi$ vanishes at infinity faster than $1/r$. Recall that we assumed that our original potentials vanish at infinity faster than $1/r^2$. Thus although Eq. (33) has not a standard Dirac equation form with the same scalar potential in its large and small part, still its solution asymptotically satisfies the free Dirac equation. Hence the solution Ψ_E^N satisfies the boundary condition

$$\Psi_E^N(\tilde{k},r) \sim \Psi_S(\tilde{k},r) + \tilde{t}_N \Psi_C(\tilde{k},r), \tag{34}$$

where $\tilde{t}_N$ is an approximated tangent of phase shift. As the potential operator $\mathcal{V}^N \xrightarrow[N\to\infty]{} V/c\hbar$. We expect that for $N \to\infty$, $\tilde{t}_N$ converges to correct value $\tilde{t}=\tan\tilde{\delta}$.

Now we shall find more details about the form of the solution Ψ_E^N. The most general formula is

$$\Psi_E^N = \sum_{s=\pm} \sum_{m=0}^{\infty} d_{m\kappa}^s |\Phi_{m\kappa}^s \rangle. \tag{35}$$

Consider the matrix representation of Eq. (33). Putting the expansion of the function Ψ_E^N in the basis $\{\Psi_{n\kappa}^\pm\}$ we get the infinite set of equations

$$\sum_{s'=\pm} \sum_{n=0}^{\infty} (\mathcal{J}+\mathcal{V}^N)_{mn}^{ss'} d_{n\kappa}^{s'} = 0, \quad s=\pm, m=0,1,2,\dots. \tag{36}$$

It can be easily seen by the right-hand side projection of Eq. (24) onto the basis $\{\Psi_{n\kappa}^\pm\}$.

According to analysis following the formula (29) the expansion coefficients $\{d_{n\kappa}^\pm\}$ of Ψ_E^N must satisfy (a) for the large component $\sum_{n=0}^{\infty} J_{mn}(\tilde{k}) d_{n\kappa}^+ = 0$, $m>N$ with elements $J_{mn}(\cdot)$ given by the nonrelativistic formula, (b) for the small component $d_{n\kappa}^- = (\epsilon/k) d_{n\kappa}^+$. Moreover we impose the additional condition (c) $F_E^N \sim S(\tilde{k},r) + \tilde{t}_N C(\tilde{k},r)$ [see condition (34)]. This gives us, together with the condition (b), the following required form of the sought solution Ψ_E^N of Eq. (33) (see Ref. [3]):

$$\Psi_E^N = \sum_{m=0}^{N-1} \begin{pmatrix} d_{m\kappa}^+ \phi_m^l \\ d_{m\kappa}^- \frac{\epsilon}{\tilde{k}} \psi_m^l \end{pmatrix} + \sum_{m=N}^{\infty} \begin{pmatrix} (s_{\kappa m}^+ + \tilde{t}_N c_{\kappa m}^+) \phi_n^l \\ (s_{\kappa m}^- + \tilde{t}_N c_{\kappa m}^-) \psi_n^l \end{pmatrix}, \tag{37}$$

where the abbreviations $s_{\kappa m}^\pm, c_{\kappa m}^\pm$ has been used according to Eq. (28). After adding and subtracting the term $\sum_{m=0}^{N-1}((s_{\kappa m}^+ + \tilde{t}_N c_{\kappa m}^+) \phi_n^l, (s_{\kappa m}^- + \tilde{t}_N c_{\kappa m}^-) \psi_n^l)^T$ to the left hand side of the above equation it is straightforward to see that the above function satisfies the asymptotic condition (34).

Let us turn back to equations (36). In general, in analogy to the nonrelativistic case, they can be schematically represented as follows:

$$
\begin{pmatrix}
\ddots & \cdots & & & & & & & & & & & & \cdots \\
& X & X & X & & & & 0 & & & & X & X & X \\
& & X & X & X & & & & & X & X & X \\
& & X & X & X & X & X & X & & & X & X & X \\
& & & X & X & X & X & X & & X & X & X \\
& & & X & X & X & X & X & & X & X & X \\
& & & X & X & X & X & X & X & X & X \\
& & & X & X & X & X & X & X & X & & 0 \\
& 0 & & & X & X & X & X & X & X & X & X \\
& & & X & X & X & X & X & X & X & X \\
& & X & X & X & & X & X & X & X & X \\
& & X & X & X & & X & X & X & X & X \\
& X & X & X & & & X & X & X & X & X & X \\
& X & X & X & & & & & & X & X & X \\
& X & X & X & & & 0 & & & & X & X & X \\
\ddots & \cdots & & & & & & & & & & & & \cdots
\end{pmatrix}
\begin{pmatrix}
\vdots \\ s^+_{N+1,l} \\ s^+_{N,l} \\ d^+_{N-1,l} \\ \vdots \\ d^+_{1,l} \\ d^+_{0,l} \\ d^-_{0,l} \\ d^-_{1,l} \\ \vdots \\ d^-_{N-1,l} \\ s^-_{N,l} \\ s^-_{N+1,l} \\ \vdots
\end{pmatrix}
=
\begin{pmatrix}
\vdots \\ 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \\ 0 \\ \vdots
\end{pmatrix}.
$$

From the construction of the required form (37) we see that all the equations for $m>N$ are satisfied automatically. Thus one has to solve the remaining $2N+2$ equations with the unknowns $\tilde{t}_N, d^+_{0\kappa}, d^+_{1\kappa}, \ldots, d^+_{N-1,\kappa}; d^-_{0\kappa}, d^-_{1\kappa}, \ldots, d^-_{N-1,\kappa}$. Note that here the number of equations is greater than the number of sought quantities $(2N+1)$, so in general the set of equations of such a form can have no solution. But in our particular case the solution certainly exists as the general theory of differential equations assures the existence of Ψ^N_E and, according to the previous analysis, Eq. (37) represents the most general required form of Ψ^N_E.

Using Eqs. (36) one obtains the following form of the remaining equations:

$$
\begin{pmatrix}
-\mathcal{J}^{++}_{N,N-1}c^+_{N-1} & \mathcal{J}^{++}_{N,N-1} & 0 & \cdots & 0 & \mathcal{J}^{+-}_{N,N-1} & -\mathcal{J}^{+-}_{N,N-1}c^-_{N-1} \\
\mathcal{J}^{++}_{N-1,N}c^+_N & (\mathcal{J}+\mathcal{V}^N)^{++}_{N-1,N-1} & (\mathcal{J}+\mathcal{V}^N)^{++}_{N-1,N-2} & \cdots & \mathcal{J}^{+-}_{N-1,N-2} & \mathcal{J}^{+-}_{N-1,N-1} & \mathcal{J}^{+-}_{N-1,N}c^-_N \\
0 & (\mathcal{J}+\mathcal{V}^N)^{++}_{N-2,N-1} & (\mathcal{J}+\mathcal{V}^N)^{++}_{N-2,N-2} & \cdots & \mathcal{J}^{+-}_{N-2,N-2} & \mathcal{J}^{+-}_{N-2,N-1} & 0 \\
\vdots & \vdots & \vdots & \cdots & \vdots & \vdots & \vdots \\
0 & (\mathcal{J}+\mathcal{V}^N)^{++}_{0,N-1} & (\mathcal{J}+\mathcal{V}^N)^{++}_{0,N-2} & \cdots & (\mathcal{J}+\mathcal{V}^N)^{+-}_{0,N-2} & (\mathcal{J}+\mathcal{V}^N)^{+-}_{0,N-1} & 0 \\
0 & (\mathcal{J}+\mathcal{V}^N)^{-+}_{0,N-1} & (\mathcal{J}+\mathcal{V}^N)^{-+}_{0,N-2} & \cdots & (\mathcal{J}+\mathcal{V}^N)^{--}_{0,N-2} & (\mathcal{J}+\mathcal{V}^N)^{+-}_{0,N-1} & 0 \\
\vdots & \vdots & \vdots & \cdots & \vdots & \vdots & \vdots \\
0 & \mathcal{J}^{-+}_{N-2,N-1} & \mathcal{J}^{-+}_{N-2,N-2} & \cdots & (\mathcal{J}+\mathcal{V}^N)^{--}_{N-2,N-2} & (\mathcal{J}+\mathcal{V}^N)^{--}_{N-2,N-1} & 0 \\
\mathcal{J}^{-+}_{N-1,N}c^+_N & \mathcal{J}^{-+}_{N-1,N-1} & \mathcal{J}^{-+}_{N-1,N-2} & \cdots & (\mathcal{J}+\mathcal{V}^N)^{--}_{N-1,N-2} & (\mathcal{J}+\mathcal{V}^N)^{--}_{N-1,N-1} & \mathcal{J}^{--}_{N-1,N}c^-_N \\
-\mathcal{J}^{-+}_{N,N-1}c^+_{N-1} & \mathcal{J}^{-+}_{N,N-1} & 0 & \cdots & 0 & \mathcal{J}^{--}_{N,N-1} & -\mathcal{J}^{--}_{N,N-1}c^-_{N-1}
\end{pmatrix}
$$

$$
\times
\begin{pmatrix}
\tilde{t}_N \\ d^+_{N-1} \\ d^+_{N-2} \\ \vdots \\ d^+_0 \\ d^-_0 \\ \vdots \\ d^-_{N-2} \\ d^-_{N-1} \\ \tilde{t}_N
\end{pmatrix}
=
\begin{pmatrix}
\mathcal{J}^{++}_{N,N-1}s^+_{N-1} + \mathcal{J}^{+-}_{N,N-1}s^-_{N-1} \\
-\mathcal{J}^{++}_{N-1,N}s^+_N - \mathcal{J}^{+-}_{N-1,N}s^-_N \\
0 \\ \vdots \\ 0 \\ 0 \\ \vdots \\ 0 \\
-\mathcal{J}^{-+}_{N-1,N}s^+_N - \mathcal{J}^{--}_{N-1,N}s^-_N \\
\mathcal{J}^{-+}_{N,N-1}s^+_{N-1} + \mathcal{J}^{--}_{N,N-1}s^-_{N-1}
\end{pmatrix}.
$$

Keeping in mind that the inner $2N \times 2N$ matrix $(\mathcal{J} + \mathcal{V}^N)_{nm}^{ss'}, s = \pm, m, n = 0, 1, ..., N-1$ is Hermitian and real, hence symmetric, and recalling the definition of $\mathcal{V}^N$ we can solve the above equations by some orthogonal matrix Γ (see the nonrelativistic case):

$$\left[\Gamma^{\dagger} \mathcal{P}_n^{\dagger} \left(\mathcal{H}_0 + \frac{V}{c\hbar} - \frac{E}{c\hbar} \right) \mathcal{P}_N \Gamma \right]_{mn}^{ss'} = \frac{1}{c\hbar} (E_n^s - E) \delta_{nm} \delta_{ss'}. \tag{38}$$

$2N \times 2N$ matrix $\mathcal{G}(E)$ with elements defined as

$$\mathcal{G}_{mn}^{ss'}(E) = \sum_{p=\pm} \sum_{i=0}^{N-1} c\hbar \frac{\Gamma_{m,i}^{sp} \Gamma_{n,i}^{s'p}}{E_i^p - E} \tag{39}$$

is an inverse of the $2N \times 2N$ matrix representation of the truncated operator $\mathcal{P}_N^{\dagger}(\mathcal{H}_0 + V/c\hbar - E/c\hbar)\mathcal{P}_N$. It can be viewed as the approximation of the relativistic Green function in the basis (20). The numbers E_n^p are the relativistic counterparts of the Harris eigenvalues [10]. They represent a finite approximation of the spectrum of the relativistic Hamiltonian $\mathcal{H}_0 + V/c\hbar$. In particular, they include positive approximations of the first N energy levels due to the potential V and the N negative pseudoenergies due to the continuous spectrum. As our basis (20) satisfies the kinetic balance condition [13,14] there is a hope that E_i^p satisfy the generalized form of the Hylleraas-Undheim theorem (see, for instance, Refs. [15,20], and references therein). It means, in particular, that (i) N positive values among set $\{E_i^p\}$ approximate the exact eigenenergies $\mathcal{H}_0 + V/c\hbar$ from the above and that (ii) the remaining N eigenvalues have values below $-mc^2$.

We can introduce now the $(2N+2) \times (2N+2)$ block-diagonal matrix

$$\tilde{\Gamma}_{(2N+2)\times(2N+2)} = \text{diag}(1, \Gamma_{2N\times2N}, 1) \tag{40}$$

and act with it on the left-hand side of the above set of $2N + 2$ equations. Using the fact that the matrix $\mathcal{J}_{N,N-1}$ given by Eq. (26) is nonsingular the set of $(2N+2) \times (2N+2)$ the equations can be solved with respect to the approximate tangent of phase shift. Using the properties of the coefficients of the matrix $\mathcal{J}$ one can derive the tangent of the approximated phase shift in the form similar to the nonrelativistic formula

$$\tilde{t}_N = -\frac{s_{N-1}^l(\tilde{k}) + (2\epsilon/\tilde{k})\mathcal{G}_{N-1,N-1}^{++}(E)J_{N,N-1}(\tilde{k})s_N^l(\tilde{k})}{c_{N-1}^l(\tilde{k}) + (2\epsilon/\tilde{k})\mathcal{G}_{N-1,N-1}^{++}(E)J_{N,N-1}(\tilde{k})c_N^l(\tilde{k})}. \tag{41}$$

Note that in the above the $J_{N,N-1}$ stands for the nonrelativistic *J*-matrix element [see Eq. (27)]. The fact that we have $2N+2$ equations and $2N+1$ unknows results in second, very similar formula for $\tilde{t}_N$ with $(\tilde{k}/\epsilon)\mathcal{G}_{N-1,N-1}^{-+}(E)$ instead of $\mathcal{G}_{N-1,N-1}^{++}(E)$. From the previous analysis we know that both equations must give *the same* $\tilde{t}_N$ which means that one has $\mathcal{G}_{N-1,N-1}^{-+}(E) = (\epsilon/\tilde{k})\mathcal{G}_{N-1,N-1}^{++}(E)$.

V. DISCUSSION

Comparing Eq. (41) with the nonrelativistic formula (13) one can see that apart from the quantity $(2\epsilon/\tilde{k})\mathcal{G}_{N-1,N-1}^{++}(E)$, all elements of the expression for tangent of the phase shift have the same form as in Eq. (13), they are only evaluated in relativistic wave number $\tilde{k}$.

Now let us note that for any N the above formula for tangent shift converges to the nonrelativistic limit as the speed of light c approaches infinity. Indeed, the basis (20) used ensures (see Refs. [14,15]) that in the limit of infinite c the large component satisfies the correct Schrödinger equation (11) with the wave number $k = \lim_{c\to\infty} \tilde{k}$. This means that the related tangent of the phase shift must also satisfy a correct limit, i.e.,

$$\lim_{c\to\infty} \tilde{t}_N = t_N. \tag{42}$$

From the above we get immediately

$$\lim_{c\to\infty} (2\epsilon/\tilde{k})\mathcal{G}_{N-1,N-1}^{++}(E) = g_{N-1,N-1}(\mathcal{E}).$$

Moreover $(2\epsilon/\tilde{k})\mathcal{G}_{N-1,N-1}^{++}(E)$ plays the analogous role as $g_{N-1,N-1}(\mathcal{E})$. In fact, the matrices $\mathcal{G}(E)$ and $g(\mathcal{E})$ can be viewed as the finite approximations of the Green functions of the relativistic and nonrelativistic Hamiltonians with the potential V, respectively. The form of the factor $2\epsilon/\tilde{k}$ is simply connected with the normalizations of the Green functions in both cases. It can be seen from the simple analysis of the set of second order equations derived in a standard way from the Dirac equation.

From the practical point of view, the convergence can be improved with the help of additional parameter λ. As we mentioned before, the latter can be treated as an additional variational parameter. In particular its optimal value will depend on the range of the potential. It can be seen simply that potentials of long range should be treated with small λ while potentials with support located close to the origin will require large values of the parameter.

In conclusion, we have provided the relativistic version of Jacobi matrix method for well defined class of potentials. The usage of the basis satisfying the ''kinetic balance condition'' allowed for a simple formulation of the method. In particular, the derived expression for the tangent of the phase shift is similar to its nonrelativistic counterpart and reproduces the latter as a correct nonrelativistic limit.

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