Relativistic *J*-matrix theory of scattering

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A systematic development of the relativistic *J*-matrix theory of scattering is presented. The reference Hamiltonian includes the Coulomb interaction, and the short-range perturbing potential may include spin-dependent coupling. The nonrelativistic limit is obtained and shown to be identical to the familiar nonrelativistic *J* matrix.

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I. INTRODUCTION

The *J*-matrix theory of quantum scattering is an algebraic method [1–4] which exploits the fact that the unperturbed (reference) Hamiltonian can be tridiagonalized in a certain complete set of L^2 basis functions. The resulting symmetric three-term recursion relation for the expansion coefficients of the unperturbed wave function is solved in terms of appropriate orthogonal polynomials. The method yields exact scattering information over a continuous range of energy for a model potential obtained by truncating the given short-range potential in a finite subset of this basis. This method has been applied successfully to a large number of nonrelativistic problems. It is shown to be free from the fictitious resonances that plague some algebraic variational scattering methods [5]. The group-theoretical foundation of the theory has been exploited to account for the class of analytic potentials that are compatible with the formalism [6,7].

Recently, Horodecki introduced a relativistic extension of the theory in which the unperturbed reference Hamiltonian included only the kinetic-energy term [8]. The recursion relation obtained is identical to the nonrelativistic one except for a rescaling of the energy variable. He derived an expression for the scattering phase shift that has the correct nonrelativistic limit. In this article, we make a systematic derivation of the relativistic theory starting from the basic principles of the *J*-matrix formalism together with manifest relativistic invariance. As an extension to Horodecki's work, we include the Coulomb interaction in the reference Hamiltonian and consider short-range perturbing potentials that may have spin-dependent coupling. The two-component relativistic L^2 basis, which is compatible with the requirements of the *J*-matrix formalism, is obtained. It turned out to be of the generalized Laguerre-type basis, which has been demonstrated to be numerically more accurate and stable in variational calculations as compared to other bases like the Slater type [9]. The recursion relation is derived. It differs from the nonrelativistic relation even for a vanishing Coulomb interaction, which is a point of departure from Horodecki's results. The orthogonal polynomials associated with this symmetric recursion relation are not calculated analytically; however, a numerical solution is obtained. The nonrelativistic limit of the theory is obtained and shown to coincide with the familiar nonrelativistic *J* matrix. The small component of the spinor wave function is related to the larger component by a parametrized first-order differential equation. The ''kinetic-balance condition'' [8,10] used by Horodecki for the small component is a special case of this differential equation; however, they coincide in the nonrelativistic limit.

The plan of the paper is as follows. In Sec. II, the two-component relativistic L^2 basis is obtained and the symmetric three-term recursion relation is derived. In Sec. III, the nonrelativistic limit of the theory is obtained and shown to coincide with the familiar nonrelativistic *J* matrix. This is also verified in the scattering examples of Sec. IV where we also calculate the relativistic effects in the phase shift. The matrix elements for a given short-range perturbing potential are obtained in Appendix A using the Gauss quadrature approximation [11]. Due to the fact that the basis is nonorthogonal, care must be taken in the calculation of the singular Green's functions. This is done in Appendix B. In Appendix C, we calculate the tridiagonal matrix elements of the reference Hamiltonian and the basis-overlap matrix, which are used in obtaining the recursion relation.

II. THE RELATIVISTIC COULOMB-DIRAC *J* MATRIX

In this section we make a systematic derivation of the relativistic theory starting with the basic principles of the *J*-matrix formalism applied to the Dirac equation. In atomic units, the two-component radial Dirac equation for a charged spinor in the Coulomb field $-Z/r$ is [12]

$$\begin{pmatrix} 1-\alpha^2\dfrac{Z}{r} & \alpha\left(\dfrac{\kappa}{r}-\dfrac{d}{dr}\right) \\ \alpha\left(\dfrac{\kappa}{r}+\dfrac{d}{dr}\right) & -1-\alpha^2\dfrac{Z}{r} \end{pmatrix} \begin{pmatrix} g(r) \\ f(r) \end{pmatrix} = \varepsilon \begin{pmatrix} g(r) \\ f(r) \end{pmatrix}, \tag{2.1}$$

where α is the fine-structure constant, ε is the relativistic energy, and κ is the spin-orbit coupling parameter defined by

$$\kappa = \pm\left(j+\tfrac{1}{2}\right) \quad \text{for } l = j \pm \tfrac{1}{2}, \tag{2.2}$$

where j is the total angular momentum quantum number. By eliminating the upper component in the coupled equation (2.1) we obtain a second-order differential equation for the lower component. This differential equation is not Schrödinger-like, i.e., it contains first-order derivatives. Therefore, we seek a general local unitary transformation that eliminates the first-order derivative:

$$r=q(r') \quad \text{and} \quad \begin{pmatrix} g(r) \\ f(r) \end{pmatrix} = \begin{pmatrix} \cos(\rho) & \sin(\rho) \\ -\sin(\rho) & \cos(\rho) \end{pmatrix} \begin{pmatrix} \phi(r') \\ \theta(r') \end{pmatrix}, \tag{2.3}$$

where ρ is a function of r'. The stated requirement gives the constraint

$$\frac{dq}{dr'}\left[\cos(2\rho)+\frac{\alpha\kappa}{q}\sin(2\rho)-\alpha^2\frac{Z}{q}-\alpha\frac{d\rho/dr'}{dq/dr'}\right]=\text{const.} \tag{2.4}$$

For a global fixed-coordinate transformation (i.e., $r=r'$ and $d\rho/dr'=0$), we obtain

$$\sin(2\rho)=\alpha Z/\kappa, \tag{2.5}$$

$$\cos(2\rho)=\pm\sqrt{1-(\alpha Z/\kappa)^2}, \tag{2.6}$$

giving two solutions, one for each sign. A change of sign in Eq. (2.6) is equivalent to a change of sign of κ in Eq. (2.2). For the upper sign, this transformation takes Eq. (2.1) into the form

$$\begin{pmatrix} -\frac{\gamma}{\kappa} & -\alpha\left(\frac{Z}{\kappa}+\frac{\gamma}{r}+\frac{d}{dr}\right) \\ -\alpha\left(\frac{Z}{\kappa}+\frac{\gamma}{r}-\frac{d}{dr}\right) & \frac{\gamma}{\kappa}-2\frac{\alpha^2 Z}{r} \end{pmatrix} \begin{pmatrix} \phi(r) \\ \theta(r) \end{pmatrix} = \varepsilon \begin{pmatrix} \phi(r) \\ \theta(r) \end{pmatrix}, \tag{2.7}$$

where

$$\gamma=\sqrt{\kappa^2-(\alpha Z)^2}. \tag{2.8}$$

Equation (2.7) gives

$$\phi(r)=\frac{-\alpha}{\varepsilon+\gamma/\kappa}\left(\frac{Z}{\kappa}+\frac{\gamma}{r}+\frac{d}{dr}\right)\theta(r) \tag{2.9}$$

for $\varepsilon\neq-\gamma/\kappa$. Substituting this back into the coupled equations in Eq. (2.7) gives the following Schrödinger-like equation for $\theta(r)$ [13,14]:

$$\left[-\frac{d^2}{dr^2}+\frac{\gamma(\gamma+1)}{r^2}-2\frac{Z\varepsilon}{r}-\frac{\varepsilon^2-1}{\alpha^2}\right]\theta(r)=0. \tag{2.10}$$

This is analogous to the Schrödinger-Coulomb equation

$$\left[-\frac{d^2}{dr^2}+\frac{l(l+1)}{r^2}-2\frac{\hat{Z}}{r}-2\hat{E}\right]\hat{\theta}(r)=0 \tag{2.11}$$

with the substitutions

$$\hat{Z}=Z\varepsilon, \quad \hat{E}=(\varepsilon^2-1)/2\alpha^2, \quad \text{and} \quad l=\gamma. \tag{2.12}$$

The well-known nonrelativistic bound-state spectrum of Eq. (2.11) is

$$\hat{E}_n=-\frac{\hat{Z}^2}{2(l+n)^2}, \quad n=1,2,\ldots. \tag{2.13}$$

Therefore, the substitution (2.12) gives the relativistic spectrum

$$\varepsilon_n=\left[1+\left(\frac{\alpha Z}{\gamma+n}\right)^2\right]^{-1/2}, \quad n=1,2,\ldots. \tag{2.14}$$

For building the relativistic J-matrix scattering formalism, we need to construct an L^2 discrete representation in which the reference Hamiltonian

$$H_0=\begin{pmatrix} -\frac{\gamma}{\kappa} & -\alpha\left(\frac{Z}{\kappa}+\frac{\gamma}{r}+\frac{d}{dr}\right) \\ -\alpha\left(\frac{Z}{\kappa}+\frac{\gamma}{r}-\frac{d}{dr}\right) & \frac{\gamma}{\kappa}-2\frac{\alpha^2 Z}{r} \end{pmatrix} \tag{2.15}$$

is tridiagonal so that the operator $J=H_0-\varepsilon$ gives a symmetric three-term recursion relation for the expansion coefficients of the wave function. The analytic solution of the recursion relation gives the two ''regularized'' solutions $\{c_n(\varepsilon),s_n(\varepsilon)\}_{n=0}^{\infty}$ of the relativistic wave equation (2.7) that behave asymptotically as $\cos(kr)$ and $\sin(kr)$, respectively. Therefore, the J-matrix formalism can be applied to give the relativistic S matrix after the addition of the perturbing short-range potential $\tilde{V}(r)$. The L^2 space is spanned by the two-component radial functions $\{\psi_n(r)\}_{n=0}^{\infty}$ whose upper component is $\phi_n(r)$ and lower component $\theta_n(r)$. The conjugate space is spanned by $\{\overline{\psi}_n(r)\}_{n=0}^{\infty}$ such that

$$\langle\overline{\psi}_n|\psi_m\rangle=\int_0^{\infty}\overline{\phi}_n(r)\phi_m(r)dr+\int_0^{\infty}\overline{\theta}_n(r)\theta_m(r)dr=\delta_{nm}. \tag{2.16}$$

Now, the analogy of the second-order Dirac-Coulomb equation (2.10) to the Schrödinger-Coulomb equation (2.11) suggests that the lower component is precisely the nonrelativistic J-matrix Laguerre basis function for the Coulomb problem with $\gamma=l$ [1–3]. That is,

$$\theta_n(r)=a_n(\lambda r)^{\gamma+1}e^{-\lambda r/2}L_n^{2\gamma+1}(\lambda r), \tag{2.17}$$

where λ is the basis scale parameter and $L_n^{\nu}(x)$ is the generalized Laguerre polynomial. The normalization constant a_n will be determined from the normalization condition (2.16). $\theta_n(r)$ satisfies the differential equation

$$\left[-\frac{d^2}{dr^2}+\frac{\gamma(\gamma+1)}{r^2}-\frac{\lambda(\gamma+n+1)}{r}+\frac{\lambda^2}{4}\right]\theta_n(r)=0. \tag{2.18}$$

The requirement that the basis-overlap matrix $\langle\psi_n|\psi_m\rangle$ and the reference Hamiltonian matrix be at most tridiagonal is satisfied by the following expression for the upper component:

$$\phi_n(r)=C\left(\frac{\xi}{2}+\frac{\gamma}{r}+\frac{d}{dr}\right)\theta_n(r), \tag{2.19}$$

where the small-component strength parameter C and scale parameter ξ are independent of n; and C is nonzero. This expression is also motivated by the solution of the wave equation in Eq. (2.9). The case $\xi=0$ is identical to the kinetic-balance condition used in Horodecki's work [8]. However, it will be shown below that this choice is necessary only in the nonrelativistic limit where $\alpha\to 0$. Using the differential and recursion properties of the Laguerre polynomials, we can write Eq. (2.19) as

$$\phi_n(r)=C\left(\frac{\xi-\lambda}{2}+\frac{2\gamma+n+1}{r}\right)\theta_n(r) - C\frac{a_n}{a_{n-1}}\frac{2\gamma+n+1}{r}\theta_{n-1}(r). \tag{2.20}$$

Explicitly, this reads

$$\phi_n(r)=\frac{\lambda C}{2}(1+\xi/\lambda)a_n(\lambda r)^{\gamma}e^{-\lambda r/2}\left[(2\gamma+n+1)L_n^{2\gamma}(\lambda r) + \frac{1-\xi/\lambda}{1+\xi/\lambda}(n+1)L_{n+1}^{2\gamma}(\lambda r)\right]. \tag{2.21}$$

The orthogonal conjugate representation defined in Eq. (2.16) requires that

$$\overline{\theta}_n(r)=\frac{[(2-\zeta)/4][1-(\xi/\lambda)^2]}{(\gamma+n+1)+\gamma\xi/\lambda}\theta_n(r)+\frac{\zeta}{\lambda r}\theta_n(r),$$

$$\overline{\phi}_n(r)=\frac{(2-\zeta)/\lambda^2C^2}{(\gamma+n+1)+\gamma\xi/\lambda}\phi_n(r), \tag{2.22}$$

where ζ is an arbitrary constant parameter. Simplicity is achieved by choosing $\xi=\lambda$. However, we stay with the general case for now and leave the parameters arbitrary. The normalization constant obtained is

$$a_n=\sqrt{\lambda\Gamma(n+1)/2\Gamma(2\gamma+n+2)}. \tag{2.23}$$

The matrix elements of the tridiagonal reference Hamiltonian in this basis are shown in Appendix C. The tridiagonal basis-overlap matrix is also given there.

The expansion coefficients of the wave function that solves the wave equation (2.7) satisfy the symmetric three-term recursion relation

$$J_{n,n-1}h_{n-1}+J_{n,n}h_n+J_{n,n+1}h_{n+1}=0, \quad n\geqslant 1, \tag{2.24}$$

where h_n stands for either s_n or c_n. The initial conditions are [3]

$$J_{00}s_0+J_{01}s_1=0,$$

$$J_{00}c_0+J_{01}c_1=-W/2s_0 \tag{2.25}$$

where $W(\varepsilon)$ is the Wronskian of the regular and irregular solutions of the free Dirac problem:

$$W(\varepsilon)=W(\psi_{\rm reg},\psi_{\rm irreg})=\psi_{\rm reg}\frac{d\psi_{\rm irreg}}{dr}-\psi_{\rm irreg}\frac{d\psi_{\rm reg}}{dr}= -2\alpha\sqrt{(\varepsilon-1)/(\varepsilon+1)}. \tag{2.26}$$

These coefficients also satisfy the Wronskian-like relation

$$J_{n,n-1}(c_ns_{n-1}-c_{n-1}s_n)=-W/2, \quad n\geqslant 1. \tag{2.27}$$

Using the matrix elements J_{nm} given in Appendix C we can write the homogeneous recursion relation (2.24) as

$$\left[\hat{a}_n+\frac{x(\lambda\xi\gamma C^2/2)+w}{xv+u}\right]h_n(x)+\hat{b}_{n-1}h_{n-1}(x)+\hat{b}_nh_{n+1}(x)=0, \quad n\geqslant 1, \tag{2.28}$$

where $x=\varepsilon-\gamma/\kappa$ and the recursion coefficients are

$$\hat{a}_n=(\gamma+n+1)\frac{x(v+\lambda^2C^2/2)+[u+\lambda^2C^2(\gamma/\kappa+\alpha/C)]}{xv+u} =(\gamma+n+1)\left[1+(\lambda^2C^2/2)\frac{x+2(\gamma/\kappa+\alpha/C)}{xv+u}\right],$$

$$\hat{b}_n=-\tfrac{1}{2}\sqrt{(n+1)(2\gamma+n+2)}, \quad n\geqslant 0 \tag{2.29}$$

with the constant parameters u, v, and w defined as

$$u=\alpha C\left(-\frac{\lambda^2}{2}+\frac{Z\xi}{\gamma}\right)+\frac{\gamma\lambda^2C^2}{2\kappa}\left(-1+\frac{\xi^2}{\lambda^2}\right),$$

$$v=1+(\lambda C/2)^2(-1+\xi^2/\lambda^2),$$

$$w=\alpha^2\lambda Z+\frac{\lambda\xi\gamma^2C^2}{\kappa}+\alpha\lambda\gamma C\left(\frac{\xi}{2}+\frac{Z}{\kappa}\right). \tag{2.30}$$

The symmetric recursion (2.28) can be rewritten as a three-parameter relation in terms of a new rescaled variable. Solving this recursion relation analytically gives orthogonal polynomials in terms of which the coefficients $\{s_n,c_n\}$ are obtained. Here, we are content with a numerical solution, which is more than sufficient for demonstrating the utility and implications of the theory.

The solution of Eq. (2.28) subject to the initial conditions in Eq. (2.25) gives the J-matrix kinematic coefficients $\{R_n^{\pm}\}_{n=1}^{\infty}$ and $\{T_n\}_{n=0}^{\infty}$, defined at the energy $\varepsilon-\gamma/\kappa$ as

$$T_n=\frac{c_n-is_n}{c_n+is_n}, \quad R_{n+1}^{\pm}=\frac{c_{n+1}\pm is_{n+1}}{c_n\pm is_n}. \tag{2.31}$$

Alternatively, starting with the initial coefficients $R_1^{\pm}$ and T_0, the rest can be calculated recursively using Eq. (2.24) as

$$R_{n+1}^{\pm}=-\frac{1}{J_{n,n+1}}\left(J_{n,n}+\frac{J_{n,n-1}}{R_n^{\pm}}\right) \quad \text{and}$$

$$T_n=T_{n-1}\frac{R_n^-}{R_n^+}, \quad n\geqslant 1. \tag{2.32}$$

These will be the coefficients that enter in the calculation of the Nth-order relativistic S matrix,

$$S^{(N)}(\varepsilon)=T_{N-1}(\varepsilon)\frac{1+g_{N-1,N-1}(\varepsilon)J_{N-1,N}(\varepsilon)R_N^-(\varepsilon)}{1+g_{N-1,N-1}(\varepsilon)J_{N-1,N}(\varepsilon)R_N^+(\varepsilon)}, \tag{2.33}$$

where $g_{N-1,N-1}(\varepsilon)$ is the finite Green's function in the conjugate space representation $\{\overline{\psi}_n(r)\}_{n=0}^{N-1}$, which carries the dynamical effects of the short-range potential $\widetilde{V}$:

$$g_{N-1,N-1}(\varepsilon)=\langle\overline{\psi}_{N-1}|(H_0+\widetilde{V}-\varepsilon)^{-1}|\overline{\psi}_{N-1}\rangle. \tag{2.34}$$

Due to the fact that the basis of the L^2 space $\{\psi_n(r)\}_{n=0}^{\infty}$ is nonorthogonal, the finite Green's function should be calculated as shown in Appendix B. Given the matrix elements $\widetilde{V}_{nm}$ of the potential, we may use any one of several alternative expressions for $g_{N-1,N-1}(\varepsilon)$ given in Appendix B.

Now, for the perturbing short-range *scalar* potential $\widetilde{V}(r)$, we replace $-Z/r$ by the expression $-Z/r+\widetilde{V}(r)$ when going from Eq. (2.1) to Eq. (2.7). The unitary transformation defined in Eqs. (2.3)–(2.6) results in the following wave equation, which replaces Eq. (2.7):

$$\begin{pmatrix} -\frac{\gamma}{\kappa}+\alpha^2\widetilde{V}(r) & -\alpha\left(\frac{Z}{\kappa}+\frac{\gamma}{r}+\frac{d}{dr}\right) \\ -\alpha\left(\frac{Z}{\kappa}+\frac{\gamma}{r}-\frac{d}{dr}\right) & \frac{\gamma}{\kappa}-2\frac{\alpha^2 Z}{r}+\alpha^2\widetilde{V}(r) \end{pmatrix}\begin{pmatrix}\phi(r)\\ \theta(r)\end{pmatrix} =\varepsilon\begin{pmatrix}\phi(r)\\ \theta(r)\end{pmatrix}. \tag{2.35}$$

Therefore, the matrix representation of $\widetilde{V}$ is

$$\widetilde{V}_{nm}=\alpha^2\int_0^{\infty}\theta_n(r)\widetilde{V}(r)\theta_m(r)dr +\alpha^2\int_0^{\infty}\phi_n(r)\widetilde{V}(r)\phi_m(r)dr. \tag{2.36}$$

With the help of Eqs. (2.17) and (2.21), this can be written as

$$\begin{aligned}\widetilde{V}_{nm}=&\frac{\alpha^2}{\lambda}a_n a_m\int_0^{\infty}e^{-y}y^{2\gamma+2}L_n^{2\gamma+1}(y)L_m^{2\gamma+1}(y)\widetilde{V}(y/\lambda)dy+\lambda\alpha^2C^2\left(\frac{1+\xi/\lambda}{2}\right)^2 a_n a_m\\ &\times\Bigg[(2\gamma+n+1)(2\gamma+m+1)\int_0^{\infty}e^{-y}y^{2\gamma}L_n^{2\gamma}(y)L_m^{2\gamma}(y)\widetilde{V}(y/\lambda)dy+\left(\frac{1-\xi/\lambda}{1+\xi/\lambda}\right)^2(n+1)(m+1)\\ &\times\int_0^{\infty}e^{-y}y^{2\gamma}L_{n+1}^{2\gamma}(y)L_{m+1}^{2\gamma}(y)\widetilde{V}(y/\lambda)dy+\left(\frac{1-\xi/\lambda}{1+\xi/\lambda}\right)(2\gamma+n+1)(m+1)\\ &\times\int_0^{\infty}e^{-y}y^{2\gamma}L_n^{2\gamma}(y)L_{m+1}^{2\gamma}(y)\widetilde{V}(y/\lambda)dy+\left(\frac{1-\xi/\lambda}{1+\xi/\lambda}\right)(2\gamma+m+1)(n+1)\int_0^{\infty}e^{-y}y^{2\gamma}L_{n+1}^{2\gamma}(y)L_m^{2\gamma}(y)\widetilde{V}(y/\lambda)dy\Bigg],\end{aligned} \tag{2.37}$$

where $y=\lambda r$. To evaluate these integrals we utilize a scheme based on Gauss quadrature as summarized in Appendix A. The result of this computation is

$$\begin{aligned}\widetilde{V}_{nm}\cong&\frac{\alpha^2}{2}[\sqrt{(2\gamma+n+2)(2\gamma+m+2)}F_{n,m}^{2\gamma+2}+\sqrt{nm}F_{n-1,m-1}^{2\gamma+2}-\sqrt{m(2\gamma+n+2)}F_{n,m-1}^{2\gamma+2}-\sqrt{n(2\gamma+m+2)}F_{n-1,m}^{2\gamma+2}]\\ &+\frac{(\alpha\lambda C)^2}{2}\left(\frac{1+\xi/\lambda}{2}\right)^2\Bigg\{\sqrt{(2\gamma+n+1)(2\gamma+m+1)}F_{n,m}^{2\gamma}+\left(\frac{1-\xi/\lambda}{1+\xi/\lambda}\right)^2\sqrt{(n+1)(m+1)}F_{n+1,m+1}^{2\gamma}+\left(\frac{1-\xi/\lambda}{1+\xi/\lambda}\right)\\ &\times[\sqrt{(m+1)(2\gamma+n+1)}F_{n,m+1}^{2\gamma}+\sqrt{(n+1)(2\gamma+m+1)}F_{n+1,m}^{2\gamma}]\Bigg\},\end{aligned} \tag{2.38}$$

where F_{nm}^{ν} is the integral defined in Appendix A and evaluated in Eq. (A12) as

$$F_{nm}^{\nu}\equiv\sum_{k=0}^{M-1}\Lambda_{nk}^{\nu}\Lambda_{mk}^{\nu}\widetilde{V}(\varepsilon_k^{\nu}/\lambda)=F_{mn}^{\nu}\quad\text{for } M>N. \tag{2.39}$$

In Appendix A, we also include details for the general case of a spin-dependent short-range potential matrix

$$\widetilde{V}(r)=\begin{pmatrix}\widetilde{V}_{\uparrow\uparrow}(r) & \widetilde{V}_{\uparrow\downarrow}(r)\\ \widetilde{V}_{\downarrow\uparrow}(r) & \widetilde{V}_{\downarrow\downarrow}(r)\end{pmatrix} \tag{2.40}$$

where $\widetilde{V}_{\downarrow\uparrow}(r)=\widetilde{V}_{\uparrow\downarrow}(r)$.

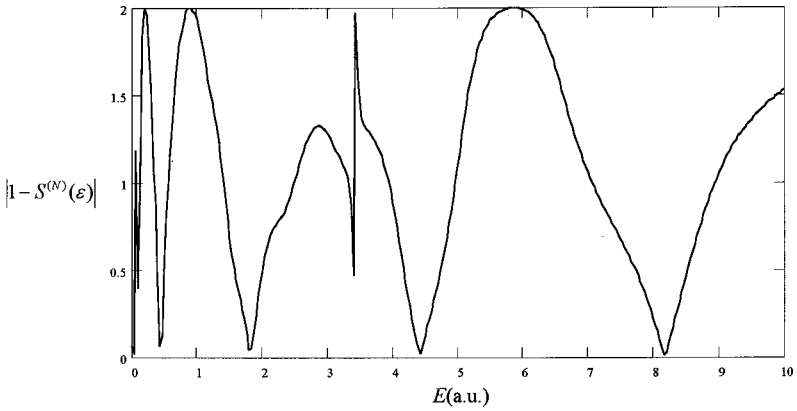

FIG. 1. Result of the numerical scheme as a plot of the nonrelativistic limit of $|1-S^{(N)}(\varepsilon)|$ vs E for the first scattering example in the presence of the short-range potential $\tilde{V}(r)=7.5r^2e^{-r}$. The energy variables are related by $E\cong(\varepsilon-\gamma/\kappa)/\alpha^2$ and we took the parameter values $Z=0$, $\kappa=l=0$, $\alpha=10^{-3}$, $\lambda=2$, $\xi=0$, $C=-\alpha/2$, $N=30$.

III. THE NONRELATIVISTIC *J*-MATRIX LIMIT

It is instructive at this point to compare the nonrelativistic limit of Eq. (2.28) with the nonrelativistic *J*-matrix recursion relation, which reads [3]

$$\left[(l+n+1)\frac{E-\tilde{\lambda}^2/8}{E+\tilde{\lambda}^2/8}+\frac{\tilde{\lambda}Z/2}{E+\tilde{\lambda}^2/8}\right]h_n(E)+\hat{b}_{n-1}h_{n-1}(E)$$
$$+\hat{b}_n h_{n+1}(E)=0, \quad n\geqslant 1, \tag{3.1}$$

where $\tilde{\lambda}$ is the nonrelativistic basis scale parameter and $\hat{b}_n$ is the same as that given in Eq. (2.29) with γ replaced by l. It is obvious that without some limiting process neither a choice of parameters nor a redefinition would put the recursion (2.28) into the form given by (3.1). The nonrelativistic limit of the development in the previous section is achieved by taking the limit $\alpha\to 0$ (i.e., $c\to\infty$), which gives

$$\gamma\cong|\kappa|=l,$$
$$\varepsilon-\gamma/\kappa\cong\varepsilon-1\cong\alpha^2E. \tag{3.2}$$

Moreover, in the same limit, the small spinor component $\phi_n(r)$ will be negligible compared to the larger component $\theta_n(r)$. That is, the small-component strength parameter C in Eq. (2.19) will be of the order of α. Taking this limit in the relativistic recursion relation defined in Eqs. (2.28)–(2.30) and using Eq. (3.2) above, we obtain

$$\left[(l+n+1)\frac{E-\tilde{\rho}}{E+\tilde{u}}+\frac{\tilde{w}}{E+\tilde{u}}\right]h_n(E)+\hat{b}_{n-1}h_{n-1}(E)$$
$$+\hat{b}_n h_{n+1}(E)=0, \tag{3.3}$$

where

$$\tilde{u}=\frac{C}{\alpha}\left(-\frac{\lambda^2}{2}+\frac{Z\xi}{\kappa}\right)+\frac{\lambda^2}{2}\left(\frac{C}{\alpha}\right)^2\left(-1+\frac{\xi^2}{\lambda^2}\right),$$
$$\tilde{p}=-\frac{C}{\alpha}\left(\frac{\lambda^2}{2}+\frac{Z\xi}{\kappa}\right)-\frac{\lambda^2}{2}\left(\frac{C}{\alpha}\right)^2\left(1+\frac{\xi^2}{\lambda^2}\right),$$
$$\tilde{w}=\lambda Z\left(1+\frac{C}{\alpha}\right)+l\lambda\xi\frac{C}{\alpha}\left(\frac{1}{2}+\frac{C}{\alpha}\right). \tag{3.4}$$

This nonrelativistic limit of the recursion relation can be identified with Eq. (3.1) if we require $\tilde{p}=\tilde{u}$ and the l dependence in $\tilde{w}$ vanishes. All of these requirements give $\xi=0$, which results in the recursion relation

$$\left[(l+n+1)\frac{E+(\lambda^2C/2\alpha)(1+C/\alpha)}{E-(\lambda^2C/2\alpha)(1+C/\alpha)}\right.$$
$$\left.+\frac{\lambda Z(1+C/\alpha)}{E-(\lambda^2C/2\alpha)(1+C/\alpha)}\right]h_n(E)+\hat{b}_{n-1}h_{n-1}(E)$$
$$+\hat{b}_n h_{n+1}(E)=0. \tag{3.5}$$

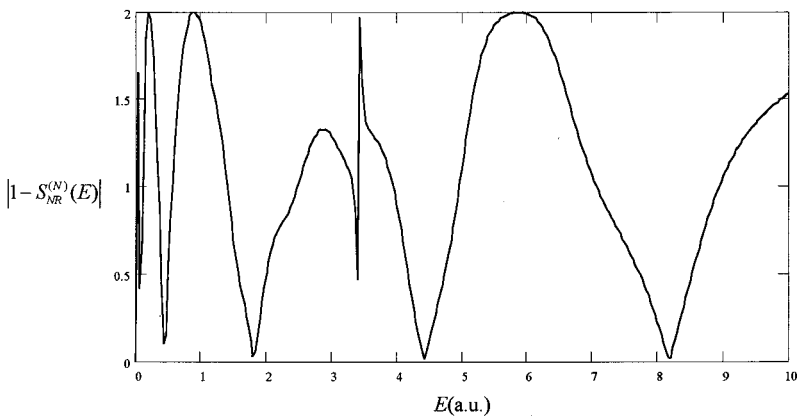

FIG. 2. Plot of the nonrelativistic $|1-S_{\mathrm{NR}}^{(N)}(E)|$ vs E resulting from the standard nonrelativistic *J*-matrix calculation for the same problem as in Fig. 1 with the same parameters $Z=0$, $l=0$, $\lambda=2$, $N=30$.

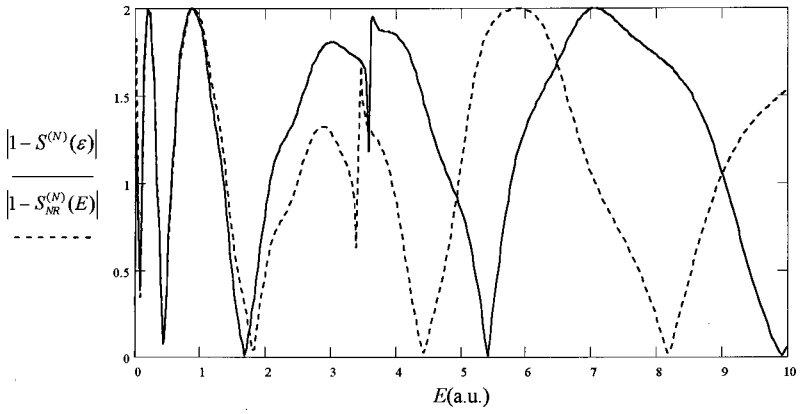

FIG. 3. Superposition of the two plots in Figs. 1 and 2, with the exception that the fine-structure parameter α is chosen to be large enough ($\alpha = 0.2$) so that relativistic effects become relevant.

Therefore, this equation will be identical to the nonrelativistic recursion (3.1) if we make the following choice of parameters:

$$C = -\alpha/2,$$

$$\lambda = \tilde{\lambda}. \tag{3.6}$$

In summary, the nonrelativistic *J*-matrix limit is achieved by making the following choice of parameters in the relativistic *J*-matrix formalism developed in the previous section:

$$\alpha \to 0,$$

$$|\kappa| = l,$$

$$\xi = 0,$$

$$C = -\alpha/2, \tag{3.7}$$

with the nonrelativistic energy $E \cong (\varepsilon - \gamma/\kappa)\alpha^2$. Note that when taking the limit $\alpha \to 0$ one should keep relativistic energy terms (including potential terms) up to order α^2 because at the end the α^2 factor will be divided out. The kinetic-balance condition used by Horodecki is therefore required only when taking the nonrelativistic limit.

IV. ILLUSTRATIVE EXAMPLES

We consider two examples. The first is a scattering by a short-range scalar potential $\tilde{V}(r) = 7.5r^2e^{-r}$ [15,16]. The aim of this exercise is to demonstrate the accuracy of the nonrelativistic limit of the theory and give first-order relativistic effects in the scattering phase shift. We take the physical parameters $Z = 0$ and $|\kappa| = l = 0$. The other parameters are chosen in the nonrelativistic limit as

$$\alpha = 10^{-3}, \quad \lambda = 2, \quad \xi = 0, \quad C = -\alpha/2, \quad N = 30. \tag{4.1}$$

The numerical *J*-matrix scheme developed in Ref. [17] is used to calculate the relativistic *S* matrix. The input to the scheme comes from the matrix elements of the reference Hamiltonian [Eq. (C7)], the basis-overlap matrix [Eqs. (C1) and (C4)], and the matrix elements of the short-range potential [Eq. (2.38)].

Figure 1 shows the results of the numerical scheme as a plot of $|1-S^{(N)}(\varepsilon)|$ vs E. Figure 2 is a plot of $|1-S^{(N)}_{\rm NR}(E)|$ vs E that is obtained by the standard nonrelativistic *J*-matrix calculation for the same problem with the same parameters ($Z = 0$, $l = 0$, $\lambda = 2$, and $N = 30$). The energy variables are related by $E \cong (\varepsilon - \gamma/\kappa)/\alpha^2$. Figure 3 is a superposition of the same two plots, with the only exception that the fine-structure parameter α is chosen to be large enough ($\alpha = 0.2$) so that relativistic effects become relevant. Aside from variations in the overall structure of the phase shift, it should be noted that resonance shifts are prominent in the relativistic *S* matrix. Sharp resonances, like the one seen on the graph at $E = 3.42$ a.u., are shifted only slightly. The direction of the shift is also to be noted. It is not only in one direction.

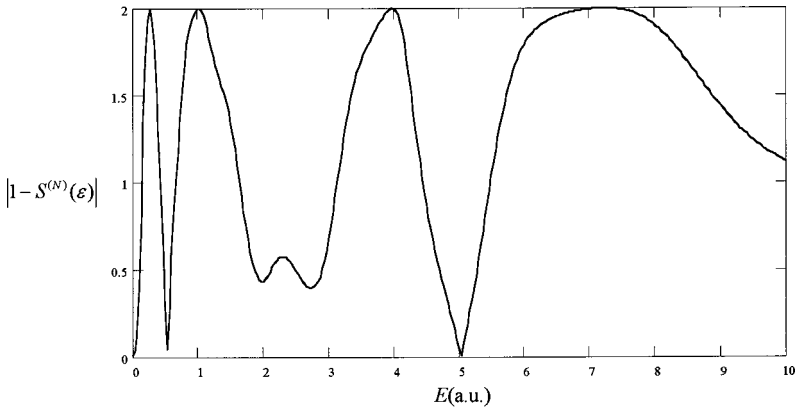

FIG. 4. Plot of the nonrelativistic limit of $|1 - S^{(N)}(\varepsilon)|$ vs E for the second example of Coulomb scattering in the presence of the short-range potential with spin-dependent coupling as given in Eq. (4.2). The parameter values are $Z = -1$, $\kappa = l = 1$, $\alpha = 10^{-4}$, $\lambda = 1$, $\xi = 0$, $C = -\alpha/2$, $N = 30$.

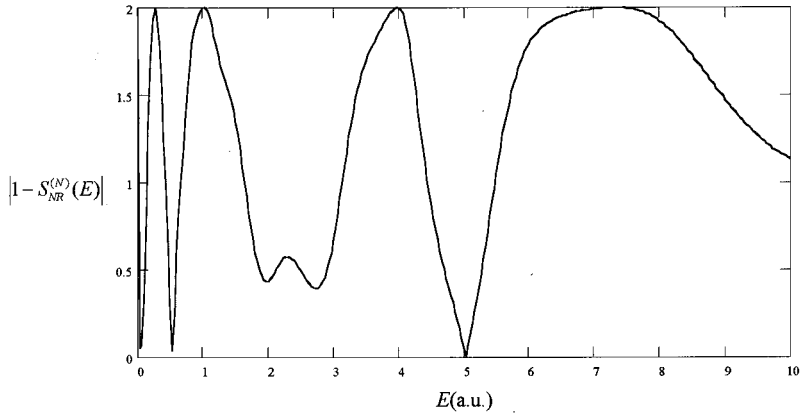

FIG. 5. Plot of the nonrelativistic $|1-S_{\mathrm{NR}}^{(N)}(E)|$ vs E for the same problem as in Fig. 4 with the parameters $Z=-1$, $l=1$, $\lambda=1$, $N=30$.

The second example is that of an electron scattering off a point charge in the presence of a perturbing short-range potential that includes spin-dependent couplings. The potential considered is

$$\tilde{V}(r)=\begin{pmatrix} 5 & -2 \\ -2 & 3 \end{pmatrix} r^2 e^{-r}. \tag{4.2}$$

Figures 4–6 show the results in an exact parallel to those of the first example. The parameter values taken are

$$Z=-1, \quad \kappa=l=1, \quad \alpha=10^{-4}, \quad \lambda=1, \quad \xi=0,$$
$$C=-\alpha/2, \quad N=30. \tag{4.3}$$

Similarly, the fine-structure parameter is subsequently taken to be large enough ($\alpha=0.2$) to bring out the relativistic effects as shown in Fig. 6.

ACKNOWLEDGMENT

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APPENDIX A: ORTHOGONAL POLYNOMIALS, GAUSS QUADRATURE, AND THE POTENTIAL MATRIX

Let $f(x)$ be an element of a real $L^2[a,b]$ vector space spanned by the complete set of orthonormal basis $\{p_n(x)\}_{n=0}^{\infty}$, where $x\in[a,b]\subset\mathbb{R}$. Orthogonality is defined with respect to a weight function $\rho(x)$ as

$$\int_a^b \rho(x)p_n(x)p_m(x)dx=\delta_{nm}. \tag{A1}$$

$f(x)$ is expandable in this basis as

$$f(x)=\sum_n d_n p_n(x) \tag{A2}$$

and $p_n(x)$ is a polynomial of order n. These polynomials satisfy the symmetric three-term recursion relation

$$xp_n(x)=\hat{a}_n p_n(x)+\hat{b}_{n-1}p_{n-1}(x)+\hat{b}_n p_{n+1}(x), \quad n\geqslant 0, \tag{A3}$$

together with the initial condition $p_0(x)=1$. The recursion coefficients $\{\hat{a}_n,\hat{b}_n\}$ are elements of $\mathbb{R}$. Associated with this space is the following infinite dimensional real tridiagonal symmetric matrix:

$$\begin{pmatrix} \hat{a}_0 & \hat{b}_0 & & & & & \\ \hat{b}_0 & \hat{a}_1 & \hat{b}_1 & & 0 & & \\ & \hat{b}_1 & \hat{a}_2 & \hat{b}_2 & & & \\ & & \hat{b}_2 & \times & \times & & \\ & & & \times & \times & \times & \\ & \underline{0} & & & \times & \times & \times \\ & & & & & \times & \times \end{pmatrix}. \tag{A4}$$

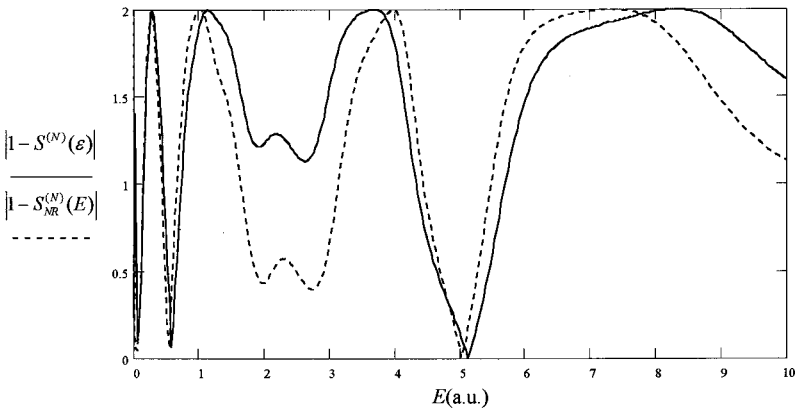

FIG. 6. Superposition of the two plots in Figs. 4 and 5, with the only exception that the fine-structure parameter α is chosen to be large enough ($\alpha=0.2$) so that the relativistic effects become relevant.

For numerical computations, however, the space is truncated to a finite N-dimensional space spanned by $\{p_n(x)\}_{n=0}^{N-1}$. The tridiagonal matrix in Eq. (A4) becomes a finite $N\times N$ matrix H. The real eigenvalues of H, designated as the set $\{\varepsilon_n\}_{n=0}^{N-1}$, are the zeros of the polynomial $p_N(x)$; i.e., $p_N(\varepsilon_n)=0$. In this setting, the Gauss quadrature approximation [11] states that

$$\int_a^b \rho(x)f(x)dx \simeq \sum_{n=0}^{N-1} \omega_n f(\varepsilon_n). \tag{A5}$$

The ''numerical weight'' ω_n is the square of the zero component of the normalized eigenvector of H, $\{\Lambda_{mn}\}_{m=0}^{N-1}$, associated with the eigenvalue ε_n. That is,

$$\omega_n=\Lambda_{0n}^2. \tag{A6}$$

One can also show that

$$P_k(\varepsilon_n)=\Lambda_{kn}/\Lambda_{0n}, \quad n,k=0,1,...,N-1. \tag{A7}$$

The integral approximation of Eq. (A5) becomes exact if $f(x)$ is a polynomial of degree $\leqslant 2N-1$.

For our present work, we consider the case of the normalized Laguerre polynomials

$$p_n(x)\equiv\sqrt{\Gamma(\nu+1)\Gamma(n+1)/\Gamma(n+\nu+1)}L_n^\nu(x) \tag{A8}$$

with the following definition for the density function:

$$\rho(x)\equiv x^\nu e^{-x}/\Gamma(\nu+1). \tag{A9}$$

The recursion coefficients are

$$\hat{a}_n=2n+\nu+1,$$

$$\hat{b}_n=-\sqrt{(n+1)(n+\nu+1)}. \tag{A10}$$

The integrals in Eq. (2.37) for the calculation of the matrix elements of the potential are in one of the following two forms:

$$\int_0^\infty e^{-x}x^\nu L_n^\nu(x)L_m^\nu(x)V(x/\lambda)dx,$$

$$\int_0^\infty e^{-x}x^{\nu+1}L_n^\nu(x)L_m^\nu(x)V(x/\lambda)dx. \tag{A11}$$

Using Eqs. (A5)–(A7), we can define the symmetric tensor

$$\begin{aligned}F_{nm}^\nu &\equiv \sqrt{\Gamma(n+1)\Gamma(m+1)/\Gamma(n+\nu+1)\Gamma(m+\nu+1)}\\ &\times\int_0^\infty e^{-x}x^\nu L_n^\nu(x)L_m^\nu(x)\tilde{V}(x/\lambda)dx\\ &=\int_0^\infty \rho(x)p_n(x)p_m(x)\tilde{V}(x/\lambda)dx\\ &\cong\sum_{k=0}^{N-1}\Lambda_{nk}^\nu\Lambda_{mk}^\nu\tilde{V}(\varepsilon_k^\nu/\lambda)=F_{mn}^\nu,\end{aligned} \tag{A12}$$

where the eigenvalue ε_n^ν and the corresponding normalized eigenvector $\{\Lambda_{mn}^\nu\}_{m=0}^{N-1}$ are associated with the tridiagonal matrix (A4) whose recursion coefficients are defined in Eq. (A10) and parametrized by ν.

Therefore, the first integral in Eq. (A11) is proportional to F_{nm}^ν. The second integral can be evaluated by one of three alternatives: (1) Using the property of the Laguerre polynomials that $L_n^\nu=L_n^{\nu+1}-L_{n-1}^{\nu+1}$, in terms of $F_{nm}^{\nu+1}$, $F_{n,m-1}^{\nu+1}$, $F_{n-1,m}^{\nu+1}$ and $F_{n-1,m-1}^{\nu+1}$; (2) using the recursion property $xL_n^\nu=(2n+\nu+1)L_n^\nu-(n+\nu)L_{n-1}^\nu-(n+1)L_{n+1}^\nu$, in terms of F_{nm}^ν, $F_{n-1,m}^\nu$, and $F_{n+1,m}^\nu$; (3) directly in terms of R_{nm}^ν, where

$$R_{nm}^\nu\equiv\sum_{k=0}^{N-1}\Lambda_{nk}^\nu\Lambda_{mk}^\nu[\varepsilon_k^\nu\tilde{V}(\varepsilon_k^\nu/\lambda)]=R_{mn}^\nu. \tag{A13}$$

The result of calculating the integrals in Eq. (2.37) for $\tilde{V}_{nm}$ along these lines, with extra attention given to the manipulation of indices, is given by Eq. (2.38). The general ansatz is

$$\begin{aligned}&\int_0^\infty e^{-x}x^\sigma L_n^\mu(x)L_m^\nu(x)\tilde{V}(x/\lambda)dx\\ &=\frac{\Gamma(\sigma+1)}{\sqrt{\Gamma(\mu+1)\Gamma(\nu+1)}}\\ &\times\sqrt{\Gamma(n+\mu+1)\Gamma(m+\nu+1)/\Gamma(n+1)\Gamma(m+1)}\\ &\times\int_0^\infty\rho^\sigma(x)p_n^\mu(x)p_m^\nu(x)\tilde{V}(x/\lambda)dx\\ &\cong\frac{\Gamma(\sigma+1)}{\sqrt{\Gamma(\mu+1)\Gamma(\nu+1)}}\\ &\times\sqrt{\Gamma(n+\mu+1)\Gamma(m+\nu+1)/\Gamma(n+1)\Gamma(m+1)}\\ &\times\sum_{k=0}^{N-1}\frac{(\Lambda_{0k}^\sigma)^2}{\Lambda_{0k}^\mu\Lambda_{0k}^\nu}\Lambda_{nk}^\mu\Lambda_{mk}^\nu\tilde{V}(\varepsilon_k^\sigma/\lambda).\end{aligned} \tag{A14}$$

For the general short-range potential with spin-dependent coupling as given by Eq. (2.40), we proceed as follows. Applying the global fixed-point transformation defined by Eqs. (2.3)–(2.6) gives

$$\tilde{V}(r)\to\tilde{W}(r)=\begin{pmatrix}\tilde{W}_+(r) & \tilde{W}_0(r)\\ \tilde{W}_0(r) & \tilde{W}_-(r)\end{pmatrix}, \tag{A15}$$

where

$$\tilde{W}_\pm=\frac{\tilde{V}_{\uparrow\uparrow}+\tilde{V}_{\downarrow\downarrow}}{2}\pm\left(\frac{\alpha Z}{\kappa}\tilde{V}_{\uparrow\downarrow}-\frac{\gamma}{\kappa}\frac{\tilde{V}_{\uparrow\uparrow}-\tilde{V}_{\downarrow\downarrow}}{2}\right),$$

$$\tilde{W}_0=-\frac{\gamma}{\kappa}\tilde{V}_{\uparrow\downarrow}-\frac{\alpha Z}{\kappa}\frac{\tilde{V}_{\uparrow\uparrow}-\tilde{V}_{\downarrow\downarrow}}{2}. \tag{A16}$$

Therefore, the matrix elements of this potential are

$$\tilde{V}_{nm}=\alpha^2\int_0^\infty \theta_n(r)\tilde{W}_-(r)\theta_m(r)dr + \alpha^2\int_0^\infty \phi_n(r)\tilde{W}_+(r)\phi_m(r)dr + \alpha^2\int_0^\infty \theta_n(r)\tilde{W}_0(r)\phi_m(r)dr + \alpha^2\int_0^\infty \phi_n(r)\tilde{W}_0(r)\theta_m(r)dr. \quad \text{(A17)}$$

Here, we give only the results for the case where $\tilde{V}(r)=\tilde{V}_0 f(r)$ and $\tilde{V}_0$ is a constant 2×2 symmetric matrix. The transformed potential matrix in this case is

$$\tilde{V}(r)\to\tilde{W}(r)=\begin{pmatrix}\tilde{W}_+ & \tilde{W}_0\\ \tilde{W}_0 & \tilde{W}_-\end{pmatrix}f(r), \quad \text{(A18)}$$

where the entries $\tilde{W}_\pm,\tilde{W}_0$ are now constant. The resulting potential matrix is

$$\begin{aligned}\tilde{V}_{nm}\cong{}&\frac{\alpha^2\tilde{W}_-}{2}\left[\sqrt{(2\gamma+n+2)(2\gamma+m+2)}G^{2\gamma+2}_{n,m}+\sqrt{nm}G^{2\gamma+2}_{n-1,m-1}-\sqrt{m(2\gamma+n+2)}G^{2\gamma+2}_{n,m-1}-\sqrt{n(2\gamma+m+2)}G^{2\gamma+2}_{n-1,m}\right]\\
&+\frac{(\alpha\lambda C)^2\tilde{W}_+}{2}\left(\frac{1+\xi/\lambda}{2}\right)^2\left\{\sqrt{(2\gamma+n+1)(2\gamma+m+1)}G^{2\gamma}_{n,m}+\left(\frac{1-\xi/\lambda}{1+\xi/\lambda}\right)^2\sqrt{(n+1)(m+1)}G^{2\gamma}_{n+1,m+1}+\left(\frac{1-\xi/\lambda}{1+\xi/\lambda}\right)\right.\\
&\left.\times\left[\sqrt{(m+1)(2\gamma+n+1)}G^{2\gamma}_{n,m+1}+\sqrt{(n+1)(2\gamma+m+1)}G^{2\gamma}_{n+1,m}\right]\right\}+\frac{\alpha^2\lambda C\tilde{W}_0}{4}(1+\xi/\lambda)\left\{\left[(2\gamma+m+1)\right.\right.\\
&\left.-\frac{1-\xi/\lambda}{1+\xi/\lambda}(m+1)\right]G^{2\gamma+1}_{n,m}-\sqrt{m(2\gamma+m+1)}G^{2\gamma+1}_{n,m-1}+\frac{1-\xi/\lambda}{1+\xi/\lambda}\sqrt{(m+1)(2\gamma+m+2)}G^{2\gamma+1}_{n,m+1}\left.\right\}+\frac{\alpha^2\lambda C\tilde{W}_0}{4}(1+\xi/\lambda)\\
&\times\left\{\left[(2\gamma+n+1)-\frac{1-\xi/\lambda}{1+\xi/\lambda}(n+1)\right]G^{2\gamma+1}_{n,m}-\sqrt{n(2\gamma+n+1)}G^{2\gamma+1}_{m,n-1}+\frac{1-\xi/\lambda}{1+\xi/\lambda}\sqrt{(n+1)(2\gamma+n+2)}G^{2\gamma+1}_{m,n+1}\right\}, \quad \text{(A19)}\end{aligned}$$

where

$$G^\nu_{nm}\equiv\sum_{k=0}^{N-1}\Lambda^\nu_{nk}\Lambda^\nu_{mk}f(\epsilon^\nu_k/\lambda)=G^\nu_{mn}. \quad \text{(A20)}$$

APPENDIX B: THE FINITE GREEN'S FUNCTION $g_{N-1,N-1}(\varepsilon)$ IN A NONORTHOGONAL BASIS

Let $\{\psi_n(r)\}_{n=0}^\infty$ be the basis of an L^2 space that supports a Hermitian representation for the reference Hamiltonian H_0. The conjugate orthogonal space is spanned by $\{\overline{\psi}_n(r)\}_{n=0}^\infty$, where $\langle\overline{\psi}_n|\psi_m\rangle=\delta_{nm}$. Given a short-range perturbing potential $\tilde{V}(r)$ whose matrix elements are

$$\tilde{V}_{nm}=\begin{cases}\langle\psi_n|\tilde{V}|\psi_m\rangle, & n,m\leqslant N-1\\ 0 \quad \text{otherwise}\end{cases}, \quad \text{(B1)}$$

the finite Green's function $g_{N-1,N-1}(z)$ is defined by

$$g_{N-1,N-1}(z)=\langle\overline{\psi}_{N-1}|(H-z)^{-1}|\overline{\psi}_{N-1}\rangle, \quad \text{(B2)}$$

where H is the $N\times N$ full Hamiltonian matrix $H_0+\tilde{V}$ and z is a complex number. Manipulation of Green's functions involving the inverse of operators with nonempty null space is done in a basis in which the representation of these operators is diagonal. That is to say, we solve the eigenvalue problem

$$H|\chi_n\rangle=\varepsilon_n|\chi_n\rangle, \quad n=0,1,\ldots,N-1. \quad \text{(B3)}$$

Since the matrix representations of the relevant operators are in the basis $\{\psi_n(r)\}_{n=0}^\infty$ rather than $\{\chi_n(r)\}_{n=0}^\infty$, we can write this equation in the form

$$\sum_{k=0}^{N-1}\langle\psi_m|H|\psi_k\rangle\langle\overline{\psi}_k|\chi_n\rangle=\varepsilon_n\sum_{k=0}^{N-1}\langle\psi_m|\psi_k\rangle\langle\overline{\psi}_k|\chi_n\rangle, \quad n,m=0,1,\ldots,N-1. \quad \text{(B4)}$$

We have used the completeness property of the basis:

$$\sum_k|\psi_k\rangle\langle\overline{\psi}_k|=\sum_k|\overline{\psi}_k\rangle\langle\psi_k|=I \quad \text{(B5)}$$

where I is the identity.

In matrix notation, Eq. (B4) reads

$$\sum_{k=0}^{N-1}H_{mk}\zeta^n_k=\varepsilon_n\sum_{k=0}^{N-1}\Omega_{mk}\zeta^n_k, \quad n,m=0,1,\ldots,N-1, \quad \text{(B6)}$$

where $\{\zeta_k^n\}_{k=0}^{N-1}$ is the normalized eigenvector associated with the eigenvalue ε_n and Ω_{nm} is the overlap matrix element $\langle\psi_n|\psi_m\rangle$. Equation (B6) is a generalized eigenvalue equation in the $\{\psi_n(r)\}$ basis

$$H|\zeta^n\rangle=\varepsilon_n\Omega|\zeta^n\rangle. \tag{B7}$$

Let us define the eigenvector matrix $\Gamma_{nm}\equiv\zeta_n^m=\langle\overline{\psi}_n|\chi_m\rangle$. Then Eq. (B6) reads $(H\Gamma)_{mn}=\varepsilon_n(\Omega\Gamma)_{mn}$, which when multiplied from the left by Γ^T, where $\Gamma_{nm}^T=\langle\chi_n|\overline{\psi}_m\rangle$, gives

$$(\Gamma^T H\Gamma)_{mn}=\varepsilon_n(\Gamma^T\Omega\Gamma)_{mn}, \quad n,m=0,1,...,N-1. \tag{B8}$$

The matrix Γ *simultaneously* diagonalizes H and Ω,

$$(\Gamma^T H\Gamma)_{nm}=\eta_n\delta_{nm} \quad \text{and} \quad (\Gamma^T\Omega\Gamma)_{nm}=\tau_n\delta_{nm}. \tag{B9}$$

Henceforth, we can write $\varepsilon_n=\eta_n/\tau_n$ and Eq. (B2) can be written as

$$\begin{aligned} g_{N-1,N-1}(z)&=\sum_{i,j,n,m=0}^{N-1}\langle\overline{\psi}_{N-1}|\chi_i\rangle\langle\chi_i|\overline{\psi}_n\rangle\langle\psi_n|(H-z)^{-1}\\ &\quad\times|\psi_m\rangle\langle\overline{\psi}_m|\chi_j\rangle\langle\chi_j|\overline{\psi}_{N-1}\rangle\\ &=\sum_{i,j,n,m=0}^{N-1}\Gamma_{N-1,i}\\ &\quad\times\{\Gamma_{i,n}^T[(H-z\Omega)^{-1}]_{nm}\Gamma_{m,j}\}\Gamma_{j,N-1}^T. \end{aligned} \tag{B10}$$

Now

$$\sum_{n,m=0}^{N-1}\Gamma_{i,n}^T[(H-z\Omega)^{-1}]_{nm}\Gamma_{m,j}=\frac{\delta_{i,j}}{\eta_i-z\tau_i}=\frac{1}{\tau_i}\frac{\delta_{i,j}}{\varepsilon_i-z}. \tag{B11}$$

Therefore, we finally obtain

$$g_{N-1,N-1}(z)=\sum_{i=0}^{N-1}\frac{\Gamma_{N-1,i}^2}{\eta_i-z\tau_i}=\sum_{i=0}^{N-1}\frac{1}{\tau_i}\frac{\Gamma_{N-1,i}^2}{\varepsilon_i-z}. \tag{B12}$$

For an orthogonal basis, that is, a self-dual basis where $\psi_n=\overline{\psi}_n$, the overlap matrix is just the identity matrix I; hence $\tau_i=1$, $\eta_i=\varepsilon_i$, and the eigenvectors are orthogonal (i.e., $\Gamma^T\Gamma=\Gamma\Gamma^T=I$). In this orthogonal basis, we can write

$$g_{N-1,N-1}(z)=\sum_{i=0}^{N-1}\frac{\Gamma_{N-1,i}^2}{\varepsilon_i-z} \quad \text{(orthogonal basis)} \tag{B13}$$

Let $\widetilde{H}$ ($\widetilde{\Omega}$) be the submatrix of H (Ω) obtained by deleting the last row and last column, respectively. The eigenvalue and generalized eigenvalue equations in the truncated space, which parallel those of Eqs. (B3) and (B7), are

$$\widetilde{H}|\widetilde{\phi}_n\rangle=\widetilde{\varepsilon}_n|\widetilde{\phi}_n\rangle, \quad n=0,1,\ldots,N-2, \tag{B14}$$

$$\widetilde{H}|\widetilde{\zeta}^n\rangle=\widetilde{\varepsilon}_n\widetilde{\Omega}|\widetilde{\zeta}^n\rangle. \tag{B15}$$

Similarly, we define the corresponding eigenvector matrix $\widetilde{\Gamma}_{nm}\equiv\widetilde{\zeta}_n^m=\langle\overline{\psi}_n|\overline{\phi}_m\rangle$ that simultaneously diagonalizes $\widetilde{H}$ and $\widetilde{\Omega}$,

$$(\widetilde{\Gamma}^T\widetilde{H}\widetilde{\Gamma})_{nm}=\widetilde{\eta}_n\delta_{nm} \quad \text{and} \quad (\widetilde{\Gamma}^T\widetilde{\Omega}\widetilde{\Gamma})_{nm}=\widetilde{\tau}_n\delta_{nm}, \tag{B16}$$

and can also write $\widetilde{\varepsilon}_n=\widetilde{\eta}_n/\widetilde{\tau}_n$. Then, it can be shown that the following is an alternative but equivalent form for $g_{N-1,N-1}(E)$:

$$g_{N-1,N-1}(z)=\frac{|\widetilde{\Omega}|}{|\Omega|}\frac{\prod_{m=0}^{N-2}\overline{\varepsilon}_m-z}{\prod_{n=0}^{N-1}\varepsilon_n-z}=\left(\frac{\prod_{m=0}^{N-2}\widetilde{\xi}_m}{\prod_{n=0}^{N-1}\xi_n}\right)\frac{\prod_{m=0}^{N-2}\widetilde{\varepsilon}_m-z}{\prod_{n=0}^{N-1}\varepsilon_n-z}, \tag{B17}$$

where $\{\xi_n\}_{n=0}^{N-1}$ and $\{\widetilde{\xi}_m\}_{m=0}^{N-2}$ are the eigenvalues of the overlap matrices Ω and $\widetilde{\Omega}$, respectively. In the orthogonal basis, Eq. (B17) can be written as

$$g_{N-1,N-1}(z)=\frac{\prod_{m=0}^{N-2}\widetilde{\varepsilon}_m-z}{\prod_{n=0}^{N-1}\varepsilon_n-z} \quad \text{(orthogonal basis)}. \tag{B18}$$

Combining Eqs. (B12) and (B17), we obtain the following relation:

$$\Gamma_{N-1,k}^2=\tau_k\frac{|\widetilde{\Omega}|}{|\Omega|}\frac{\prod_{m=0}^{N-2}\widetilde{\varepsilon}_m-\varepsilon_k}{\prod_{\substack{n=0\\n\neq k}}^{N-1}\varepsilon_n-\varepsilon_k}. \tag{B19}$$

APPENDIX C: THE MATRIX ELEMENTS OF THE REFERENCE HAMILTONIAN

Using the two components of the basis functions given in Eqs. (2.17) and (2.21) and with the help of Laguerre-polynomial properties [18], we get the following integral formulas which are useful for subsequent calculations:

$$\int_0^\infty \theta_n(r)\,\theta_m(r)dr=(\gamma+n+1)\,\delta_{nm} - \frac{1}{2}\sqrt{n(2\gamma+n+1)}\,\delta_{n,m+1} - \frac{1}{2}\sqrt{(n+1)(2\gamma+n+2)}\,\delta_{n,m-1}, \tag{C1}$$

$$\int_0^\infty \frac{1}{\lambda r}\,\theta_n(r)\,\theta_m(r)dr=\frac{1}{2}\,\delta_{nm}, \tag{C2}$$

$$\int_0^\infty \theta_n(r)\,\frac{d}{dr}\,\theta_m(r)dr=\frac{\lambda}{4}\sqrt{n(2\gamma+n+1)}\,\delta_{n,m+1} - \frac{\lambda}{4}\sqrt{(n+1)(2\gamma+n+2)}\,\delta_{n,m-1} =-\int_0^\infty \theta_m(r)\,\frac{d}{dr}\,\theta_n(r)dr, \tag{C3}$$

$$\int_0^\infty \phi_n(r)\,\phi_m(r)dr=\{(\gamma+n+1)(\lambda C/2)^2[1+(\xi/\lambda)^2] +\lambda\xi\gamma C^2/2\}\,\delta_{nm}+\tfrac{1}{2}\sqrt{n(2\gamma+n+1)} \times(\lambda C/2)^2[1-(\xi/\lambda)^2]\,\delta_{n,m+1} +\tfrac{1}{2}\sqrt{(n+1)(2\gamma+n+2)}(\lambda C/2)^2[1 -(\xi/\lambda)^2]\,\delta_{n,m-1}, \tag{C4}$$

$$\int_0^\infty \theta_n(r)\,\phi_m(r)dr=\frac{\lambda C}{2}\left[(\gamma+n+1)\,\frac{\xi}{\lambda}+\gamma\right]\delta_{nm} + \frac{\lambda C}{4}\sqrt{n(2\gamma+n+1)}\left(1-\frac{\xi}{\lambda}\right)\delta_{n,m+1} - \frac{\lambda C}{4}\sqrt{(n+1)(2\gamma+n+2)} \times\left(1+\frac{\xi}{\lambda}\right)\delta_{n,m-1}, \tag{C5}$$

$$\langle\psi_n|\psi_m\rangle=\int_0^\infty \phi_n(r)\,\phi_m(r)dr+\int_0^\infty \theta_n(r)\,\theta_m(r)dr. \tag{C6}$$

After some manipulations, we obtain the following:

$$(H_0)_{n,n}=(\gamma+n+1)\left\{\frac{\gamma}{\kappa}\left[1-\left(\frac{\lambda C}{2}\right)^2\left(1+\frac{\xi^2}{\lambda^2}\right)\right] -\alpha C\left(\frac{\lambda^2}{2}+\frac{Z\xi}{\kappa}\right)\right\}-\alpha\lambda\left(1+\frac{\gamma C}{\alpha\kappa}\right)(\alpha Z+C\gamma\xi/2),$$

$$(H_0)_{n,n+1}=-\frac{1}{2}\sqrt{(n+1)(2\gamma+n+2)} \times\left\{\frac{\gamma}{\kappa}\left[1+\left(\frac{\lambda C}{2}\right)^2\left(1-\frac{\xi^2}{\lambda^2}\right)\right]+\alpha C\left(\frac{\lambda^2}{2}-\frac{Z\xi}{\kappa}\right)\right\},$$

$$(H_0)_{n,n-1}=-\frac{1}{2}\sqrt{n(2\gamma+n+1)}\left\{\frac{\gamma}{\kappa}\left[1+\left(\frac{\lambda C}{2}\right)^2\left(1-\frac{\xi^2}{\lambda^2}\right)\right] +\alpha C\left(\frac{\lambda^2}{2}-\frac{Z\xi}{\kappa}\right)\right\}. \tag{C7}$$

Thus, the representation of $J=H_0-\varepsilon$ is the tridiagonal matrix defined by

$$J_{n,n}=-(\gamma+n+1)\left\{-2\,\frac{\gamma}{\kappa}+\left(\varepsilon+\frac{\gamma}{\kappa}\right)\left[1+\left(\frac{\lambda C}{2}\right)^2\left(1+\frac{\xi^2}{\lambda^2}\right)\right] +\alpha C\left(\frac{\lambda^2}{2}+\frac{Z\xi}{\kappa}\right)\right\}-\alpha\lambda\gamma C\left(\frac{\xi}{2}+\frac{Z}{\kappa}\right) -\frac{1}{2}\lambda\xi\gamma C^2\left(\varepsilon+\frac{\gamma}{\kappa}\right)-\alpha^2\lambda Z,$$

$$J_{n,n+1}=-\frac{1}{2}\sqrt{(n+1)(2\gamma+n+2)} \times\left\{2\,\frac{\gamma}{\kappa}-\left(\varepsilon+\frac{\gamma}{\kappa}\right)\left[1+\left(\frac{\lambda C}{2}\right)^2\left(-1+\frac{\xi^2}{\lambda^2}\right)\right] +\alpha C\left(\frac{\lambda^2}{2}-\frac{Z\xi}{\kappa}\right)\right\},$$

$$J_{n,n-1}=-\frac{1}{2}\sqrt{n(2\gamma+n+1)}\times\left\{2\,\frac{\gamma}{\kappa}-\left(\varepsilon+\frac{\gamma}{\kappa}\right) \times\left[1+\left(\frac{\lambda C}{2}\right)^2\left(-1+\frac{\xi^2}{\lambda^2}\right)\right]+\alpha C\left(\frac{\lambda^2}{2}-\frac{Z\xi}{\kappa}\right)\right\}. \tag{C8}$$

If, for the sake of simplicity, we choose $\xi=\lambda$ then Eq. (2.21) gives

$$\phi_n(r)=\lambda C a_n(2\gamma+n+1)(\lambda r)^\gamma e^{-\lambda r/2}L_n^{2\gamma}(\lambda r) \tag{C9}$$

and the tridiagonal matrix representation above simplifies to

$$(H_0)_{n,n}=(2\gamma+n+1)\left[\frac{\gamma}{\kappa}\left(1-\frac{\lambda^2C^2}{2}\right)-\alpha C\lambda\left(\frac{\lambda}{2}+\frac{Z}{\kappa}\right)\right] -\alpha^2\lambda Z-\gamma^2/\kappa,$$

$$(H_0)_{n,n+1}=-\frac{1}{2}\sqrt{(n+1)(2\gamma+n+2)}\left[\frac{\gamma}{\kappa}+\alpha C\lambda\left(\frac{\lambda}{2}-\frac{Z}{\kappa}\right)\right],$$

$$(H_0)_{n,n-1}=-\frac{1}{2}\sqrt{n(2\gamma+n+1)}\left[\frac{\gamma}{\kappa}+\alpha C\lambda\left(\frac{\lambda}{2}-\frac{Z}{\kappa}\right)\right]. \tag{C10}$$

Similarly,

$$J_{n,n}=-(2\gamma+n+1)\left[\left(\varepsilon-\frac{\gamma}{\kappa}\right)\left(1+\frac{\lambda^2C^2}{2}\right)+\frac{\gamma\lambda^2C^2}{\kappa}+\alpha\lambda C\left(\frac{Z}{\kappa}+\frac{\lambda}{2}\right)\right]+\gamma\left(\varepsilon-\frac{\gamma}{\kappa}\right)-\alpha^2\lambda Z,$$

$$J_{n,n+1}=\frac{1}{2}\sqrt{(n+1)(2\gamma+n+2)}\left[\left(\varepsilon-\frac{\gamma}{\kappa}\right)+\alpha\lambda C\left(\frac{Z}{\kappa}-\frac{\lambda}{2}\right)\right],$$

$$J_{n,n-1}=\frac{1}{2}\sqrt{n(2\gamma+n+1)}\left[\left(\varepsilon-\frac{\gamma}{\kappa}\right)+\alpha\lambda C\left(\frac{Z}{\kappa}-\frac{\lambda}{2}\right)\right]. \tag{C11}$$

Moreover, the matrix elements of the scalar potential given in Eq. (2.38) simplify to

$$\tilde{V}_{nm}\cong\frac{\alpha^2}{2}[\sqrt{(2\gamma+n+2)(2\gamma+m+2)}F^{2\gamma+2}_{n,m}+\sqrt{nm}F^{2\gamma+2}_{n-l,m-1}-\sqrt{m(2\gamma+n+2)}F^{2\gamma+2}_{n,m-1}-\sqrt{n(2\gamma+m+2)}F^{2\gamma+2}_{n-1,m}+(\lambda C)^2\sqrt{(2\gamma+n+1)(2\gamma+m+1)}F^{2\gamma}_{n,m}], \tag{C12}$$

while those for the potential with spin-dependent coupling constant in Eq. (A19) simplify to

$$\tilde{V}_{nm}\cong\frac{\alpha^2\tilde{W}_-}{2}[\sqrt{(2\gamma+n+2)(2\gamma+m+2)}G^{2\gamma+2}_{n,m}+\sqrt{nm}G^{2\gamma+2}_{n-1,m-1}-\sqrt{m(2\gamma+n+2)}G^{2\gamma+2}_{n,m-1}-\sqrt{n(2\gamma+m+2)}G^{2\gamma+2}_{n-1,m}]+\frac{(\alpha\lambda C)^2\tilde{W}_+}{2}\sqrt{(2\gamma+n+1)(2\gamma+m+1)}G^{2\gamma}_{n,m}+\frac{\alpha^2\lambda C\tilde{W}_0}{2}[(2\gamma+m+1)G^{2\gamma+1}_{n,m}-\sqrt{m(2\gamma+m+1)}G^{2\gamma+1}_{n,m-1}]+\frac{\alpha^2\lambda C\tilde{W}_0}{2}[(2\gamma+n+1)G^{2\gamma+1}_{n,m}-\sqrt{n(2\gamma+n+1)}G^{2\gamma+1}_{m,n-1}]. \tag{C13}$$

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