Nonperturbative dynamical-group approach to screened Coulomb potentials

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In this paper we consider screened Coulomb potentials of the Yukawa type and treat them using a scaling variational method based on the SO(2,1) subgroup of the full SO(4,2) dynamical group of the point Coulomb problem. In this formulation the tilting angle is treated as a variational parameter and the relevant matrix elements of the Yukawa potential can be expressed as matrix elements of an analytically continued finite SO(2,1) transformation of the parabolic type. We calculate the energy eigenvalues, wave functions (essentially scaled Coulomb wave functions), and normalization factors. Our energy eigenvalues are more accurate than those found by the analytic perturbation theory of McEnnan *et al.*, while the normalization factors are less accurate. Thus our method may be considered as complementary to the analytic perturbation theory.

I. INTRODUCTION

The problem of screened Coulomb potentials is of unquestionable importance in the physics of atomic phenomena. Such potentials have been studied using many techniques, both numerical and analytical. These include WKB methods[1] and various types of perturbation theory.[2–4] In particular, McEnnan *et al.*[4] have developed an analytic perturbation theory for screened Coulomb potentials that can be expanded in the form

$$V(r)=-(a/r)[1+V_1\lambda r+V_2(\lambda r)^2+V_3(\lambda r)^3+\cdots], \tag{1.1}$$

where $\lambda\simeq\alpha Z^{1/3}$ is a small parameter characterizing the screening. The coefficients are chosen to give rapid convergence and to give a good approximation to realistic numerical potentials on the interior of atoms where $\lambda r<1$. McEnnan *et al.*[4] consider mainly two types of potentials namely the simple Yukawa potential

$$V(r)=-(a/r)\exp(-\lambda r),$$

where λ is taken as the Thomas-Fermi radius, and the Herman-Skillman[5] potential which is expressed as a sum of Coulombic and Yukawa potentials as

$$V(r)=-\frac{a}{r}[Z^{-1}+\xi e^{-\mu_1 r}+(1-\xi-Z^{-1})e^{-\mu_2 r}]. \tag{1.2}$$

The parameters ξ, μ_1, and μ_2 are obtained from least-squares fits to the Hartree-Fock-Slater data given in Ref. 5. Upon expansion of the exponentials in Eq. (1.2) the coefficients V_k of Eq. (1.1) may be determined so that the perturbation method of Ref. 4 may be applied. We shall follow the authors of Ref. 4 and refer to Eq. (1.2) as the Herman-Skillman (HS) potential and note that the values of the coefficients in Eq. (1.2) may be found for various values of Z in their paper.

In the present work we wish to present an approach to these screened Coulomb potentials based on the well-known SO(4,2) dynamical group of the Coulomb problem.[6] In fact, the dynamical-group method has previously been used to treat the Yukawa potential in the context of algebraic perturbation theory.[7,8] The present method, however, is nonperturbative. It consists of two essential features. First, since the potential is spherically symmetric we need utilize only the SO(2,1) subgroup of SO(4,2) and in this formulation the matrix elements of the Yukawa-type potential can be expressed as a global SO(2,1) group element. The second feature is related to the so-called "tilting" transformation that relates between the physical states and the group states which are the basis of the relevant unitary irreducible representations (UIR) of SO(2,1). In configuration space this transformation amounts to a scale transformation.[9] In the point Coulomb problem, the tilting angle is usually fixed by the requirement that the coefficients of the nondiagonal terms in the eigenvalue problems should vanish. However as we have shown elsewhere,[10] this angle may be treated as a variational parameter. This leads to a group theoretical formulation of what has been called the scaling variational method (SVM).[11] We shall use this method here to obtain the energy eigenvalues, wave functions (essentially scaled Coulomb wave functions) and normalization factors for bound states of both the Yukawa and HS potentials. The continuum states will be discussed elsewhere.

In Sec. II we review the formulation of the Coulomb problem in terms of the generators of the dynamical group SO(2,1) and the relevant representations. We also present our formulation of the SVM. In Sec. III we derive the energy functionals for the screened Coulomb potentials and in Sec. IV our numerical results are given and compared to those of Ref. 4. As will be seen, our calculations for the energy levels are superior to the analytical results of that paper while the normalization factors are somewhat less accurate. A brief discussion concludes the paper and an appendix is included to summarize some results from the theory of SO(2,1) representations as discussed by Bargmann.[12]

II. SO(2,1) THEORY AND THE SCALING VARIATIONAL METHOD

The SO(2,1) lie algebra consist of the generators K_0, K_1, and K_2, the commutation relations

$$[K_1,K_2]=-iK_0 , \tag{2.1a}$$

$$[K_2,K_0]=iK_1 , \tag{2.1b}$$

$$[K_0,K_i]=iK_2 , \tag{2.1c}$$

and the Casimir invariant

$$Q=K_0^2-K_1^2-K_2^2 . \tag{2.2}$$

The eigenvalues of Q we shall denote as $k(k-1)$. The relevant UIR's employed here are the so-called positive discrete series $\mathscr{D}^+(k)$ where $k>0$ and the compact generator K_0 is diagonal as

$$K_0 \mid n,k\rangle = n \mid n,k\rangle \qquad n=k,k+1,k+2,\ldots . \tag{2.3}$$

In the case of the Coulomb problem SO(2,1) generators have the following realization[6]

$$K_0=\tfrac{1}{2}(rp^2+r) , \tag{2.4a}$$

$$K_1=\tfrac{1}{2}(rp^2-r) , \tag{2.4b}$$

$$K_2=\vec{r}\cdot\vec{p}-i . \tag{2.4c}$$

Upon calculating the Casimir operator one finds that

$$\begin{aligned} Q&=K_0^2-K_1^2-K_2^2 \\ &=L_1^2+L_2^2+L_3^2 \\ &=L^2 , \end{aligned} \tag{2.5}$$

where the L_i are simply the generators of the SO(3) symmetry group. Since L^2 has eigenvalues $l(l+1)$, Eq. (2.5) leads to the identification

$$k(k-1)=l(l+1) \tag{2.6}$$

whose solutions are $k=-l$ and $k=l+1$. However only the second root leads to a UIR so the first must be discarded. We therefore may label the group states (basis of the UIR) as $\mid n,l+1\rangle$ but we shall simply write them as $\mid n,l\rangle$. We actually have here a decomposition of the full dynamical group SO(4,2) as $\mathrm{SO(4,2)}\supset\mathrm{SO(3)}\otimes\mathrm{SO(2,1)}$ which may be interpreted as a separation of variables into spherical polar coordinates. We thus shall include the azimuthal quantum number m in our definition of the group state, i.e., $\mid n,l,m\rangle$. It will be demonstrated shortly that the number n is in fact the principle quantum. We must also point out that these states satisfy the orthogonality relation

$$\langle n',l',m' \mid n,l,m\rangle=\delta_{n'n}\delta_{l'l}\delta_{m'm} \tag{2.7}$$

and the completeness relation [in the SO(2,1) subspace]

$$\sum_{n=l+1}^{\infty} \mid n,l\rangle\langle n,l \mid =1 . \tag{2.8}$$

Now for the point Coulomb problem the Hamiltonian is

$$H=\tfrac{1}{2}p^2-a/r , \tag{2.9}$$

where $a=Z\alpha$. To use the generators of Eqs. (2.4) the eigenvalue problem must be written as

$$\overline{\Omega}(E) \mid \overline{\Psi}\rangle=0 , \tag{2.10}$$

where

$$\overline{\Omega}(E)=r(H-E) \tag{2.11}$$

and $\mid\overline{\Psi}\rangle$ is a physical state. Using Eqs. (2.4) we have

$$\overline{\Omega}(E)=\tfrac{1}{2}(K_0+K_1)-E(K_0-K_1)-a . \tag{2.12}$$

To remove the nondiagonal operator K_1, one performs the tilting transformation so that Eq. (2.10) becomes

$$\Omega(E,\theta) \mid \Psi\rangle=0 , \tag{2.13}$$

where

$$\mid\Psi\rangle=e^{-i\theta K_2} \mid \overline{\Psi}\rangle \tag{2.14}$$

and

$$\begin{aligned} \Omega(E,\theta)&=e^{-i\theta K_2}\overline{\Omega}(E)e^{+i\theta K_2} \\ &=\tfrac{1}{2}e^{\theta}(K_0+K_1)-Ee^{-\theta}(K_0-K_1)-a . \end{aligned} \tag{2.15}$$

The transformation of Eq. (2.15) has been accomplished through the use of the Baker-Hausdorff-Campbell formulas

$$e^{-i\theta K_2}K_0e^{i\theta K_2}=K_0\cosh\theta+K_1\sinh\theta \tag{2.16a}$$

$$e^{-i\theta K_2}K_1e^{i\theta K_2}=K_0\sinh\theta+K_1\cosh\theta . \tag{2.16b}$$

Now with the choice of $\theta=\ln(\sqrt{-2E}\,)$, Eq. (2.15) becomes

$$\Omega(E,\theta)=\sqrt{-2E}\,K_0-a \tag{2.17}$$

so with $\mid\Psi\rangle=\mid n,l,m\rangle$ (a group state), one obtains from Eqs. (2.3) and (2.13) $E_n=-a^2/(2n^2)$ the Coulomb energy levels. Note that the tilting angle depends on the level in question and in fact becomes $\theta_n=\ln(a/n)$.

Alternatively we may use the group states $\mid n,l,m\rangle$ and Eq. (2.5) and write

$$\langle n,l,m \mid \Omega(E,\theta) \mid n,l,m\rangle=0 \tag{2.18}$$

to obtain the energy functional

$$E_n(\theta)=\tfrac{1}{2}e^{2\theta}-\frac{a}{n}e^{\theta} . \tag{2.19}$$

Setting $dE_n(\theta)/d\theta=0$ we obtain $\theta_n=\ln(a/n)$ and $E_n(\theta_n)=-a^2/(2n^2)$ as before. This method of treating θ as a variational parameter is just the scaling variational method since K_2 is essentially a generator of scale transformations.

Now the group states $\mid n,l,m\rangle$ are related to the physical states $\mid\overline{n,l,m}\rangle$ via

$$\mid\overline{n,l,m}\rangle=\mathscr{N}_ne^{-\theta_nK_2} \mid n,l,m\rangle , \tag{2.20}$$

where $\mathcal{N}_n$ is a normalization constant. These states are normalized according to[6]

$$\langle \overline{n,l,m} \mid r \mid \overline{n,l,m} \rangle = 1 , \tag{2.21}$$

where $r = K_0 - K_1$. This becomes

$$\begin{aligned} 1 &= \mathcal{N}_n^2 \langle n,l,m \mid (K_0 - K_1) \mid n,l,m \rangle e^{-\theta_n} \\ &= \mathcal{N}_n^2 e^{-\theta_n} n \end{aligned} \tag{2.22}$$

which yields $\mathcal{N}_n^2 = e^{\theta_n}/n$. For $e^{\theta_n} = a/n$ we have $\mathcal{N}_n = a^{1/2}/n$.

In configuration space the group states are realized as

$$\begin{aligned} \Psi_{nlm}(\vec{r}) &= \langle \vec{r} \mid n,l,m \rangle \\ &= \frac{2l+1}{(2l+1)!} \left[\frac{(n+l)!}{(n-l-1)!} \right]^{1/2} r^l e^{-r} \\ &\quad \times {}_1F_1(l+1-n, 2l+2, 2r) Y_{lm}(\vartheta, \varphi) , \end{aligned} \tag{2.23}$$

where ${}_1F_1$ is the confluent hypergeometric function. The physical wave functions will be, by Eq. (2.20), scaled group functions. Scale transformations are generated by $\vec{r} \cdot \vec{\nabla}$ such that

$$\exp[(\ln\beta) \vec{r} \cdot \vec{\nabla}] f(\vec{r}) = f(\beta \vec{r}) . \tag{2.24}$$

Since $iK_2 - 1 = \vec{r} \cdot \vec{\nabla}$ we have, by Eqs. (2.20) and (2.23)

$$\begin{aligned} \overline{\Psi}_{nlm}(\vec{r}) &= \langle \vec{r} \mid \overline{n,l,m} \rangle \\ &= \left[\frac{e^{3\theta_n}}{n} \right]^{1/2} \frac{2^{l+1}}{(2l+1)!} \left[\frac{(n+l)!}{(n-l-1)!} \right]^{1/2} \\ &\quad \times (e^{\theta_n} r)^l e^{-e^{\theta_n} r} {}_1F_1(l+1-n, 2l+2; 2e^{\theta} r) , \end{aligned} \tag{2.25}$$

where we have taken $\mathcal{N}_n = e^{\theta n/2}/n^{1/2}$. If we set $e^{\theta_n} = a/n$ the $\overline{\Psi}_{nlm}(\vec{r})$ are just the hydrogenic wave functions.

III. SCREENED COULOMB POTENTIALS

We consider first the case of the simple Yukawa potential where

$$H = \tfrac{1}{2} p^2 - \frac{a}{r} e^{-\lambda r} . \tag{3.1}$$

With $\overline{\Omega}(E) = r(H - E)$ and with $r = K_0 - K_1$ we have

$$\begin{aligned} \overline{\Omega}(E) &= \tfrac{1}{2}(K_0 + K_1) - E(K_0 - K_1) \\ &\quad - a \exp[-\lambda(K_0 - K_1)] . \end{aligned} \tag{3.2}$$

We perform the tilting transformation to obtain

$$\begin{aligned} \Omega(E,\theta) &= \tfrac{1}{2} e^{\theta}(K_0 + K_1) - E e^{-\theta}(K_0 - K_1) \\ &\quad - a \exp[-\lambda e^{-\theta}(K_0 - K_1)] , \end{aligned} \tag{3.3}$$

where we have used the fact that for any function $f(r)$ which has an expansion polynomial in $r = K_0 - K_1$

$$e^{-i\theta K_2} f(r) e^{i\theta K_2} = f[e^{-\theta}(K_0 - K_1)] . \tag{3.4}$$

We now find the energy functional using the group states to write

$$\langle n,l,m \mid \Omega(E,\theta) \mid n,l,m \rangle = 0 . \tag{3.5}$$

We obtain

$$E_{nl}(\theta) = \tfrac{1}{2} e^{2\theta} - \frac{a}{h} e^{\theta} \langle n,l \mid e^{-\lambda e^{-\theta}(K_0 - K_1)} \mid n,l \rangle , \tag{3.6}$$

where the azimuthal quantum number has been suppressed in the last term. This term may in fact be considered as an analytically continued diagonal matrix element of a finite SO(2,1) transformation. It may be expressed in terms of the Bargmann functions given in the appendix. But first we need to find the corresponding matrix elements α and β of the 2×2 nonunitary representation.

We consider the SO(2,1) transformation

$$\begin{aligned} G &= e^{-i\gamma(K_0 - K_1)} \\ &= \begin{bmatrix} \alpha & \beta \\ \beta^* & \alpha^* \end{bmatrix} . \end{aligned} \tag{3.7}$$

The SO(2,1) algebra has the 2×2 realization $K_1 = i\sigma_2/2$, $K_2 = -i\sigma_1/2$, and $K_0 = \sigma_3/2$ where the σ_3 are Pauli matrices. Thus we have

$$\begin{aligned} K_0 - K_1 &= \tfrac{1}{2}(\sigma_3 - i\sigma_2) \\ &= \tfrac{1}{2} \begin{bmatrix} 1 & -1 \\ 1 & -1 \end{bmatrix} \end{aligned} \tag{3.8}$$

and therefore we easily obtain upon expansion

$$e^{-i\gamma(K_0 - K_1)} = \begin{bmatrix} 1 - i\gamma/2 & i\gamma/2 \\ -i\gamma/2 & 1 + i\gamma/2 \end{bmatrix} . \tag{3.9}$$

This falls into the category of a parabolic SO(2,1) transformation.[13] Upon making the analytic continuation $\gamma \to -i\lambda e^{-\theta}$ we find that

$$\begin{aligned} &\alpha = 1 - \frac{\lambda}{2} e^{-\theta}, \quad \alpha^* = 1 + \frac{\lambda}{2} e^{-\theta} , \\ &\beta = \frac{\lambda}{2} e^{-\theta}, \quad \beta^* = -\frac{\lambda}{2} e^{-\theta} . \end{aligned} \tag{3.10}$$

Therefore the energy functional of Eq. (3.6) may be written in terms of the Bargmann functions as

$$E_{nl}(\theta) = \tfrac{1}{2} e^{2\theta} - \frac{a}{n} e^{\theta} V_{n,n}^{l+1}(\alpha,\beta) , \tag{3.11}$$

where α and β (and α^* and β^*) are given by Eqs. (3.10). As seen from the form of $V_{n,n}^{l+1}$ in the Appendix Eq. (3.11) may be written

$$\begin{aligned} E_{nl}(\theta) &= \frac{1}{2} e^{2\theta} - \frac{a}{n} e^{\theta} \left[1 + \frac{\lambda}{2} e^{-\theta} \right]^{-2n} \\ &\quad \times {}_2F_1(l+1-n, -n-l, 1; \tfrac{1}{4}\lambda^2 e^{-2\theta}) . \end{aligned} \tag{3.12}$$

The energy functional for the HS potential of Eq. (1.1) is determined in an entirely analogous fashion. One has

$$E_{nl}(\theta)=\frac{1}{2}e^{2\theta}-\frac{a}{n}e^{\theta}[Z^{-1}+\xi V_{n,n}^{l+1}(\alpha_1,\beta_1) +(1-\xi-Z^{-1})V_{n,n}^{l+1}(\alpha_2,\beta_2)] , \quad (3.13)$$

where

$$\alpha_{1,2}=1-\frac{\mu_{1,2}}{2}e^{-\theta}, \quad \alpha_{1,2}^{*}=1+\frac{\mu_{1,2}}{2}e^{-\theta} , \quad \beta_{1,2}=\frac{\mu_{1,2}}{2}e^{-\theta}, \quad \beta_{1,2}^{*}=-\frac{\mu_{1,2}}{2}e^{-\theta} . \quad (3.14)$$

Therefore the energy functional of Eq. (3.13) may be written

$$E_{nl}(\theta)=\frac{1}{2}e^{2\theta}-\frac{a}{n}e^{\theta}\left[Z^{-1}+\xi\left[1+\frac{\mu_1}{2}e^{-\theta}\right]^{-2n}{}_2F_1\left[l+1-n,-n-l,1;\tfrac{1}{4}\mu_1^2e^{-2\theta}\right] +(1-\xi-Z^{-1})\left[1+\frac{\mu_2}{2}e^{-\theta}\right]^{-2n}{}_2F_1\left[l+1-n,-n-l,1;\tfrac{1}{4}\mu_2^2e^{-2\theta}\right]\right] . \quad (3.15)$$

Applications will be considered in the next section.

IV. APPLICATIONS

Here we apply the results of Sec. III to the particular cases studied in Ref. 4. That is, we give the energy levels, wave functions, and normalization factors for the $1S$, $2S$, and $2P$ states for both the Yukawa and HS potentials for various Z values.

The energy functionals for these states are given from Eqs. (3.12) and (3.15) for the Yukawa potential as follows:

$$E_{10}(\theta)=\tfrac{1}{2}e^{2\theta}-ae^{\theta}\left[1+\frac{\lambda}{2}e^{-\theta}\right]^{-2} \quad (4.1a)$$

$$E_{20}(\theta)=\tfrac{1}{2}e^{2\theta}-\frac{a}{2}e^{\theta}\left[1+\frac{\lambda}{2}e^{-\theta}\right]^{-4}\left[1-\frac{\lambda^2}{2}e^{-2\theta}\right] \quad (4.1b)$$

$$E_{21}(\theta)=\tfrac{1}{2}e^{2\theta}-\frac{a}{2}e^{\theta}\left[1+\frac{\lambda}{2}e^{-\theta}\right]^{-4} \quad (4.1c)$$

and for the HS potential as follows:

$$E_{10}(\theta)=\tfrac{1}{2}e^{2\theta}-ae^{\theta}\left[Z^{-1}+\xi\left[1+\frac{\mu_1}{2}e^{-\theta}\right]^{-2}+(1-\xi-Z^{-1})\left[1+\frac{\mu_2}{2}e^{-\theta}\right]^{-2}\right] \quad (4.2a)$$

$$E_{20}(\theta)-\tfrac{1}{2}e^{2\theta}-\frac{a}{2}e^{\theta}\left[Z^{-1}+\xi\left[1+\frac{\theta_1}{2}e^{-\theta}\right]^{-4}\left[1+\frac{\mu_1^2}{2}e^{-2\theta}\right]+(1-\xi-Z^{-1})\left[1+\frac{\mu_2}{2}e^{-\theta}\right]^{-4}\left[1+\frac{\mu_2^2}{2}e^{-2\theta}\right]\right] \quad (4.2b)$$

$$E_{21}(\theta)=\tfrac{1}{2}e^{2\theta}-\frac{a}{2}e^{\theta}\left[Z^{-1}+\xi\left[1+\frac{\mu_1}{2}e^{-\theta}\right]^{-4}+(1-\xi-Z^{-1})\left[1+\frac{\mu_2}{2}e^{-\theta}\right]^{-4}\right] . \quad (4.2c)$$

For the case of the Yukawa potential λ is taken as the Thomas-Fermi radius $1.13\alpha Z^{1/3}$ and for the HS potential the μ_1, μ_2, and ξ are taken from Table II of Ref. 4. In Fig. 1 we give some selected examples of the θ trajectories for the energies.

In Table I we give our scaling factors $e^{\theta_{n,l}}$ which minimize the energy functionals of Eqs. (4.1) and (4.2). We have included for the sake of comparisons the point Coulomb scaling factors $e^{\theta_n}=a/n$. In Table II we present our scaling variational results for the energy levels along with the numerical and perturbation analytic results of Ref. 4. We also include results when e^{θ} is set to its point Coulomb value a/n in Eqs. (4.1)–(4.2). The results obtained in this way are in fact what one would obtain by expanding the exponentials, in the potential and doing the equivalent of first-order perturbation theory on each term then summing. Indeed, if we set $e^{\theta}=a$ in Eq. (4.1a) we obtain upon binomial expansion

$$E_{10}=-\frac{1}{2}a^2+\lambda a-\frac{3}{4}\lambda^2+\ldots \quad (4.3)$$

which contains the first two terms of the perturbation series for the ground state.[7,8]

Our results for energies are uniformly more accurate than those from the analytic perturbation theory of Ref. 4. We note however that in both our results and those of Ref. 4, the $2S$ states in general have the highest fractional error.

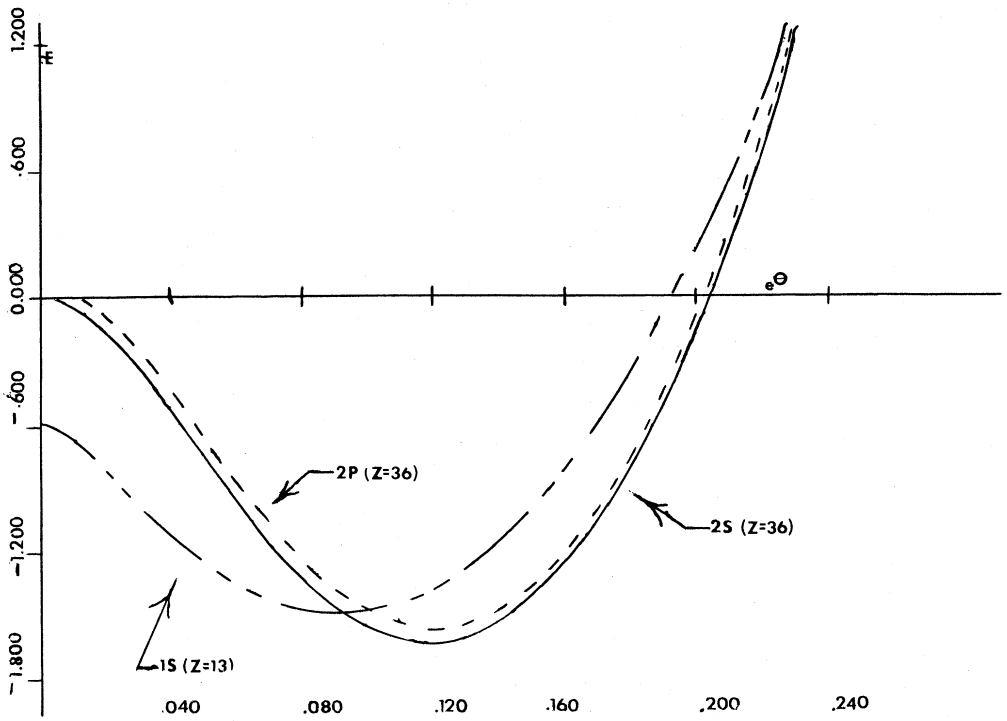

FIG. 1. Examples of energy as a function of e^{θ}. The $1s$ level is for $Z=13$ while the $2s$ and $2p$ are for $Z=36$.

Table III contains our calculated normalization factors. From Eq. (2.25) these factors are

$$N_{nl}=\frac{(2e^{\theta_{nl}})^{(l+3/2)}}{(2l+1)!}\left[\frac{(n+l)!}{2n(n-l-1)!}\right]^{1/2} \tag{4.4}$$

where the point Coulomb factors are

$$N_{nl}^{C}=\left[\frac{2a}{n}\right]^{l+3/2}\frac{1}{(2l+1)!}\left[\frac{(n+l)!}{2n(n-l-1)!}\right]^{1/2}. \tag{4.5}$$

As seen from the tables, our normalization factors calculated from the scaling technique, while exhibiting the proper behavior, do not have the accuracy of those of McEnnan *et al.*[4] They are typically accurate to the second decimal place.

TABLE I. Scaling factors e^{θ} for the point Coulomb and screened potentials.

	Z	n	l	Point Coulomb	Screened Coulomb
Yukawa	13	1	0	0.094 863	0.092 462
	36	1	0	0.262 697	0.260 822
		2	0	0.131 348	0.118 788
		2	1	0.131 348	0.120 335
	79	1	0	0.576 474	0.574 964
		2	0	0.288 237	0.277 692
		2	1	0.288 237	0.279 167
HS	13	1	0	0.094 863	0.092 039
	36	1	0	0.262 697	0.259 860
		2	0	0.131 348	0.115 733
		2	1	0.131 348	0.116 916
	79	1	0	0.576 474	0.573 829
		2	0	0.288 237	0.272 191
		2	1	0.288 237	0.273 958

Finally in Figs. 2 and 3 we note the effect of the scaling on the shape of the unnormalized radial wave functions $u_{nl}(r)=rR_{nl}(r)$ where

$$R_{nl}(r)=r^{l}e^{-e^{\theta_{nl}}r}{}_1F_1(l+1-n,2l+2;2e^{\theta_{nl}}r)\,. \tag{4.6}$$

For the $1s$ and $2s$ states considered these are

$$u_{10}(r)=re^{-e^{\theta_{10}}r}, \tag{4.7a}$$

$$u_{20}(r)=re^{-e^{\theta_{20}}r}(1-e^{\theta_{20}}r)\,, \tag{4.7b}$$

where the $e^{\theta_{nl}}$ are taken from Table I. As seen in the figures, the scaled wave functions have the same general behavior as the perturbed wave functions of Ref. 4.

V. DISCUSSIONS

The method and results given in this paper may be interpreted as complimentary to analytic perturbation theory of McEnnan *et al.* in Ref. 4. That is to say the group theoretical scaling variational method presented here yields generally more accurate energy eigenvalues while the perturbation theory apparently yields more accurate normalization factors.

Our results are actually subject to further improvement by the application of perturbation theory. This may come about in the following way. In forming the energy functionals of Eq. (3.12) only the diagonal matrix elements of the SO(2,1) transformation are used. We may therefore think of the off-diagonal terms as giving rise to perturbations. The first-order correction will of course be zero so

TABLE II. Bound-state energy eigenvalues (in keV) for the Yukawa and HS potentials as a function of n,l,Z. The analytic and numerical results are from Ref. 4. (Quantities in parentheses denote factors of 10.)

	Z	n	l	Numerical	Variational	Coulomb scaled	Analytic	Fractional error
Yukawa	13	1	0	−1.488(0)	−1.488(0)	−1.486(0)	−1.484(0)	0.000 34
	36	1	0	−1.424(1)	−1.424(1)	−1.424(1)	−1.424(1)	0.008 2
		2	0	−1.692(0)	−1.696(0)	−1.662(0)	−1.615(0)	0.002
		2	1	−1.566(0)	−1.561(0)	−1.534(0)	−1.504(0)	0.003 1
	79	1	0	−7.495(1)	−7.495(1)	−7.495(1)	−7.495(1)	0.000 027
		2	0	−1.250(1)	−1.251(1)	−1.248(1)	−1.245(1)	0.000 8
		2	1	−1.225(1)	−1.225(1)	−1.223(1)	−1.221(1)	0.000 24
HS	13	1	0	−1.544(0)	−1.543(0)	−1.541(0)	−1.535(0)	0.000 52
	36	1	0	−1.413(1)	−1.413(1)	−1.413(1)	−1.412(0)	0.0
		2	0	−1.833(0)	−1.840(0)	−1.787(0)	−1.563(0)	0.038
		2	1	−1.676(0)	−1.670(0)	−1.625(0)	−1.479(0)	0.006 1
	79	1	0	−7.404(1)	−7.403(1)	−7.403(1)	−7.403(1)	0.000 12
		2	0	−1.237(1)	−1.238(1)	−1.213(1)	1.212(1)	0.000 8
		2	1	−1.199(1)	−1.198(1)	−1.193(1)	−1.180(1)	0.000 92

the first nonzero correction term is actually second order. As this will be negative our energy eigenvalues will improve and also, we expect, our normalization factors. In Ref. 10, we considered the simpler problem of the Coulomb potential perturbed by the confining potential λr ($\lambda>0$) in just this way. The application of this method to the screened Coulomb potentials will be discussed elsewhere.

Finally, we mention that our method is applicable to more general cases of screened potentials. Consider for instance the potential

$$V(r)=-\frac{e^2}{r}[1+(1+\alpha r)e^{-2\alpha r}] \tag{5.1}$$

for one electron of the helium atom in the field of the other and the nucleus. To apply the dynamical-group method we must multiply by r to get

$$rV(r)=-e^2[1+(1+\alpha r)e^{-2\alpha r}] . \tag{5.2}$$

Applying the tilting transformations, the right-hand side becomes

$$[rV(r)]_T=-e^2[1+(1+\alpha e^{-\theta}r)e^{-2\alpha e^{-\theta}r}] . \tag{5.3}$$

Then we need

$$\langle n,l\,|\,[rV(r)]_T\,|\,n,l\rangle=-e^2(1+\langle n,l\,|\,e^{-2\alpha e^{-\theta}r}\,|\,n,l\rangle +\alpha e^{-\theta}\langle n,l\,|\,re^{-2\alpha e^{-\theta}r}\,|\,n,l\rangle). \tag{5.4}$$

The second term is expressed as a Bargmann function as before while the third term can be evaluated by using the completeness relation of Eq. (2.8) to write

$$\langle n,l\,|\,re^{-2\alpha e^{-\theta}r}\,|\,n,l\rangle = \sum_{n'=l+1}\langle n,l\,|\,r\,|\,n',l\rangle\langle n',l\,|\,e^{-2\alpha e^{-\theta}r}\,|\,n,l\rangle . \tag{5.5}$$

From the Eq. (2.3) and that

$$K_1\,|\,n,l\rangle=a_{nl}\,|\,n+1,l\rangle+b_{nl}\,|\,n-1,l\rangle , \tag{5.6}$$

where

TABLE III. Bound-state normalization factors for the Yukawa and HS potentials as a function of n, l, and Z. (Quantities in parentheses denote factors of 10.)

	Z	n	l	Numerical	Variational	Analytic	Fractional error
Yukawa	13	1	0	5.692(−2)	5.623(−2)	5.711(−2)	0.012
	36	1	0	2.674(−1)	2.644(−1)	2.674(−1)	0.011
		2	0	8.618(−2)	8.188(−2)	8.933(−2)	0.16
		2	1	6.306(−3)	5.800(−3)	6.582(−3)	0.080
	79	1	0	8.731(−1)	8.719(−1)	8.731(−1)	0.0014
		2	0	2.982(−1)	2.926(−1)	2.999(−1)	0.051
		2	1	4.905(−2)	4.755(−2)	4.937(−2)	0.031
HS	13	1	0	5.664(−2)	5.585(−2)	5.699(−2)	0.014
	36	1	0	2.663(−1)	2.649(−1)	2.665(−1)	0.0053
		2	0	8.394(−1)	7.874(−1)	9.200(−2)	0.21
		2	1	6.008(−3)	5.397(−3)	6.628(−3)	0.10
	79	1	0	8.714(−1)	8.694(−1)	8.715(−1)	0.0023
		2	0	2.923(−1)	2.840(−1)	2.981(−1)	0.087
		2	1	4.758(−2)	4.536(−2)	4.861(−2)	0.047

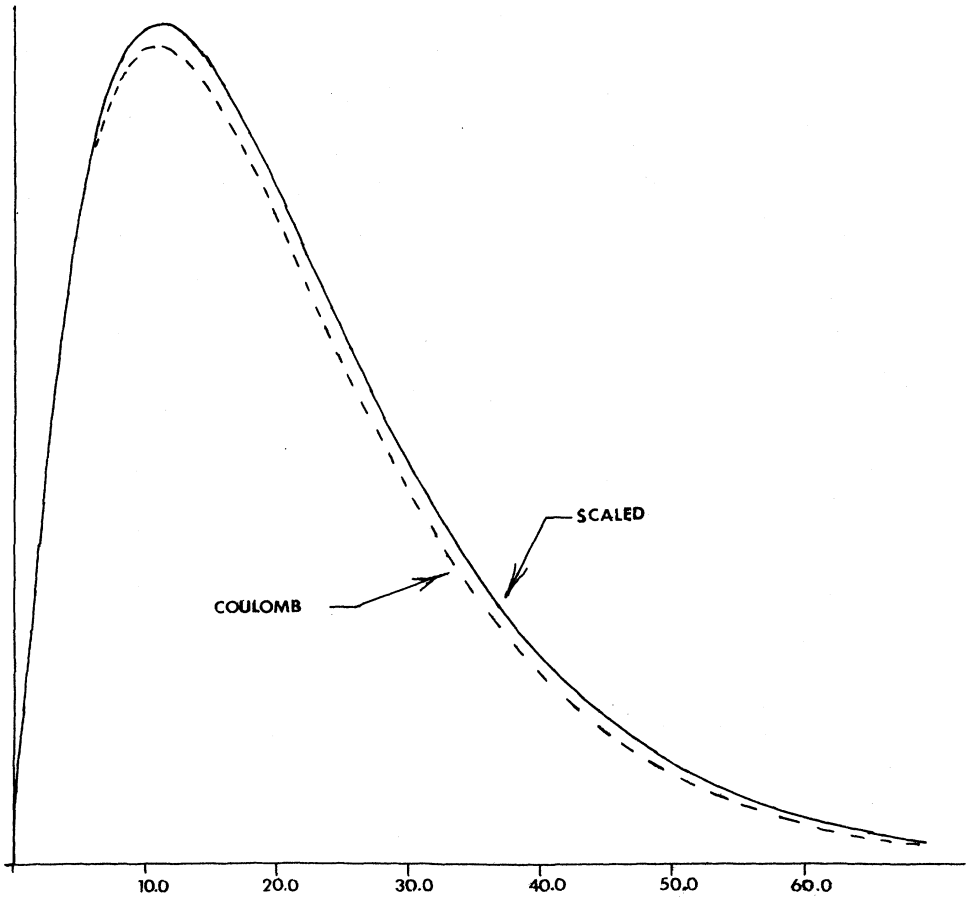

FIG. 2. Unnormalized scaled radial wave function $u(r)=rR(r)$ for the $1S$ state of aluminum ($Z=13$) for the HS potential compared with the point Coulomb wave function.

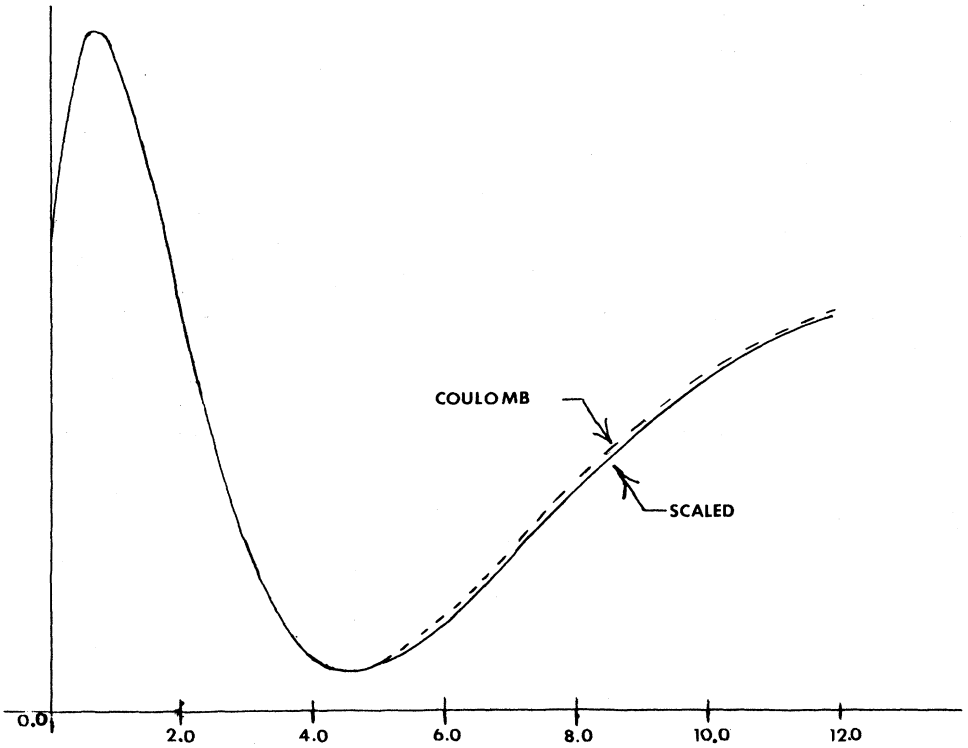

FIG. 3. Unnormalized scaled radial wave for the $2S$ state of gold ($Z=79$) for the Yukawa potential compared with the point Coulomb wave function.

$$a_{nl}=\tfrac{1}{2}[(n-l)(n+l+1)]^{1/2} \tag{5.7a}$$

$$b_{nl}=\tfrac{1}{2}[(n+l)(n-l-1)]^{1/2} \tag{5.7b}$$

we obtain

$$\langle n,l \mid re^{-2\alpha e^{-\theta}r} \mid n,l\rangle = n V_{n,n}^{l+1}-a_{nl}V_{n+1,n}^{l+1}-b_{nl}V_{n-1,n}^{l+1}\ , \tag{5.8}$$

where the $V_{n',n}^{l+1}$ are the appropriate Bargmann functions. Altogether then we have

$$\langle n,l \mid [rV(r)]_T \mid n,l\rangle = -e^2[1+(1+e^{-\theta}\alpha n)V_{n,n}^{l+1} -\alpha e^{-\theta}(a_{nl}V_{n+1,n}^{l+1}+b_{nl}V_{n-1,n}^{l+1})]\ . \tag{5.9}$$

This result may be used in Eq. (3.11) to obtain the corresponding energy functional.

APPENDIX

In the elementary 2×2 representation of the three-parameter group SO(2,1)~SU(1,1) the generators are realized as $K_1=i\sigma_2/2$, $K_2=-i\sigma_1/2$, and $K_0=\sigma_3/2$ where the σ_i are Pauli matrices. In this representation a finite transformation may be written in the form

$$G=\begin{bmatrix}\alpha & \beta\\ \beta^* & \alpha^*\end{bmatrix}, \tag{A1}$$

where

$$\det G=\alpha^*\alpha-\beta^*\beta=1 \tag{A2}$$

for α and β complex numbers. K_1 and K_2 generate hyperbolic subgroups of SO(2,1) while K_0 (the compact generator) generates an elliptic class of subgroups.[13] The combination $K_0\pm K_1$ generates the parabolic subgroup of the form[13]

$$e^{-i\gamma(K_0\pm K_1)}=\begin{bmatrix}1\mp\frac{i\gamma}{2} & \mp i\gamma/2\\ \pm i\gamma/2 & 1\pm\frac{i\gamma}{2}\end{bmatrix}. \tag{A3}$$

Comparison with Eq. (A1) yields α and β.

We have used in this paper only the unitary irreducible representation $\mathscr{D}^+(k)$ where basis states $\mid n,k\rangle$ diagonalize K_0 as is Eq. (2.3) and the eigenvalue of the Casimir operator Q is $k(k-1)$. A transformation G in this space has the action

$$V(G)\mid n,k\rangle=\sum_{n'=k}V_{n'n}^{k}(\alpha,\beta)\mid n',k\rangle\ , \tag{A4}$$

where

$$V_{n'n}^{k}(\alpha,\beta)=\langle n',k\mid V(G)\mid n,k\rangle\ . \tag{A5}$$

For $n'\geq n$ we have

$$V_{n'n}^{k}(\alpha,\beta)=A_{n'n}(\alpha^*)^{-n'-n}\beta^{n'-n}\times {}_2F_1(k-n,1-n-k,1+n'-n;-\beta^*\beta)\ , \tag{A6}$$

where

$$A_{n'n}=\frac{1}{\Gamma(1+n'-n)}\left[\frac{\Gamma(n'+1-k)\Gamma(n'+k)}{\Gamma(n+1-k)\Gamma(n+k)}\right]^{1/2} \tag{A7}$$

and for $n'\leq n$

$$V_{n'n}^{k}(\alpha,\beta)=A_{nn'}(\alpha^*)^{-n'-n}(-\beta^*)^{n-n'}\times {}_2F_1(k-n',1-k-n',n-n'+1;-\beta^*\beta)\ . \tag{A8}$$

[1] L. L. Foldy, Phys. Rev. **111**, 1093 (1958).
[2] M. J. Featon, Mon. Not. R. Astron. Soc. **118**, 504 (1958).
[3] R. H. Pratt and H. K. Tseng, Phys. Rev. A **5**, 1063 (1972).
[4] J. McEnnan, L. Kissel, and R. H. Pratt, Phys. Rev. A **13**, 532 (1976).
[5] F. Herman and S. Skillman, *Atomic Structure Calculations* (Prentice-Hall, Engelwood Cliffs, 1963).
[6] A. O. Barut, *Dynamical Groups and Generalized Symmetries in Quantum Theory* (University of Caterbury, Christchurch, New Zealand, 1971).
[7] M. Bednar, Ann. Phys. (NY) **75**, 305 (1973).
[8] A. Bechler, Ann. Phys. (NY) **108**, 49 (1977).
[9] A. O. Barut, and W. Rasmussen, J. Phys. B **6**, 1695 (1973).
[10] C. C. Gerry and S. Silverman, Phys. Lett. **95A**, 481 (1983); Phys. Rev. A **29**, 1574 (1984).
[11] See, for example, F. M. Fernández and E. M. Castro, Phys. Rev. A **27**, 663 (1982) and references cited therein.
[12] V. Bargmann, Ann. Math. **48**, 568 (1947).
[13] See B. G. Wybourne, *Classical Groups for Physicists* (Wiley, New York, 1974), p. 190.