improves agreement between the theoretical profile and the experimental data, while in the case of the measurements of Boldt and Cooper[14] (Lyα, $n_e = 8.4\times10^{16}$ cm^{-3}, $T_e = 12\,200$ K) the agreement becomes worse.

The main effect of time ordering, as discussed above, appears to be a decrease in intensity at the line center with a corresponding increase in the wings. This behavior was obtained in the S-matrix limit[6,7] for both Lyα and Hα. One may therefore expect a similar behavior for other hydrogen lines (in the case of the recent measurements by Wiese, Kelleher, and Paquette[15] the correction from time ordering improves agreement between the theoretical and experimental profiles).

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Group Properties of Hydrogenic Radial Functions*

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The radial wave functions of hydrogen are put into such a form that they form bases for irreducible unitary representations of an algebra isomorphic to that of $O(2, 1)$. Operators proportional to r^k are found which form bases for the adjoint representations of this algebra. Matrix elements of these operators are evaluated, and selection rules are determined by considering Kronecker products of representations of $O(2, 1)$. Differences between this approach and one previously suggested are discussed.

I. INTRODUCTION

Following Racah,[1] the angular portion of the atomic wave function has been analyzed using the powerful techniques of group theory. The radial atomic function has, on the other hand, been considered simply to be a solution to a differential equation. As a result, calculations involving the radial function lack, in general, the elegance and essential simplicity of calculations involving the angular functions.

The possibility has recently been raised of extending the use of group theory to studies of the radial wave function. Because the techniques necessary for such studies are largely unknown (or unrecognized), work has been centered on the simpler quantum-mechanical systems—the hydrogen-atom (both nonrelativistic[2,3] and relativistic[4]), the harmonic-oscillator,[5] and the generalized Kepler problem.[4] The radial functions of these systems must certainly be completely understood before any significant progress can be made in more complex systems.

In a previous paper,[2] the hydrogenic radial wave functions were analyzed by studying a closely related set of functions. These functions were shown to form bases for representations of the noncompact group $O(2,1)$. On the basis of a study of the transformation properties of these functions, considerable insight was gained into the properties of the hydrogenic functions. It is felt, however, that more information concerning the general group properties of radial parameters would be obtained if this previous work could be related directly to the hydrogenic functions, rather than to this similar set of functions. It is the purpose of this paper to describe the previous work directly in terms of hydrogenic functions.

II. CHOICE OF ALGEBRA

A dynamical group[6] of the H atom is $O(4,2)$. Of interest to us here is not this group, but rather a $O(2,1)\times O(3)$ subgroup of $O(4,2)$. The $O(3)$ group is, in this case, the ordinary rotation group in three dimensions; the $O(2,1)$, called the transition group by Barut and Kleinert,[6] is closely related to the group of interest to us. The three generators of this $O(2,1)$ (B^+, B^-, and N) affect only the principal quantum number of the total wave function for hydrogen, $|nlm)$:

$$N|nlm)=n|nlm), \quad B^{\pm}|nlm)\to|n\pm 1\,lm). \tag{1}$$

Barut and Kleinert[6] have given explicit forms for B^+ and B^- in the position representation, but not for N. A consideration of the properties of this $O(2,1)$ reveals certain characteristics of N, however. Foremost among these properties is the requirement that N must not be defined in the space of the radial function alone. If it were, equations such as

$$NR_{nl}=nR_{nl}\,, \quad CR_{nl}=l(l+1)R_{nl} \tag{2}$$

would result, where C is the Casimir operator for $O(2,1)$, and R_{nl} is the radial wave function of hydrogen. Since both C and N are Hermitian, this indicates that

$$\int R_{n'l'}R_{nl}\,d\Omega=\delta(n',n)\delta(l',l) \tag{3}$$

for some $d\Omega$, i.e., that the states diagonalizing the Hermitian operators are orthonormal. As is well known, however, no relationship such as (3) exists. We must conclude, therefore, that although N satisfies Eq. (1), it does not satisfy Eq. (2).

The $O(2,1)$ subgroup of Barut and Kleinert[6] is therefore not exactly the one of interest to us if we wish to study the radial wave function separately. We can, however, obtain the desired algebra by combining the properties of this algebra with those of the algebra discussed in the previous paper.[2] We first introduce a new variable t, and a new function $f_{ln}(z_n)$. The function $f_{ln}(z_n)$ is simply related to the hydrogenic radial wave function by

$$f_{ln}(z_n)=e^{int}[(2l+1)(2n)/2\pi]^{1/2}(n/2Z)R_{nl}(z_n), \tag{4}$$

where $z_n=2Zr/n$, $Ze=$ nuclear charge. The proportionality factors in (4) are chosen such that

$$(f_{ln}|f_{l'n'})=\int_0^\infty\int_0^{2\pi}f_{ln}{}^*f_{l'n'}\,dt\,dr=\delta(l,l')\delta(n,n'). \tag{5}$$

We can also construct an $O(2,1)$ algebra which acts in the space of the $f_{ln}(z_n)$:

$$\begin{aligned} N_\pm &= D\left(\frac{N\mp 1}{N}\right)e^{\pm it}\left(z_N\frac{\partial}{\partial z_N}\mp i\frac{\partial}{\partial t}+1\mp\frac{z_N}{2}\right), \\ N &= -i\frac{\partial}{\partial t}, \end{aligned} \tag{6}$$

with $z_N=2Zr/N$; $D((N\mp 1)/N)$ is a dilatation operator[6] with the property

$$D((N\mp 1)/N)[e^{iqt}g(r)]=e^{iqt}g((q\mp 1)r/q)$$

for any $g(r)$. This dilatation operator can be expressed in a position representation as $[(N\mp 1)/N]^{r\,\partial/\partial r}$. The operators of Eq. (6) satisfy the appropriate commutation relations for the complexification of an $O(2,1)$ algebra:

$$[N,N_\pm]=\pm N_\pm\,, \quad [N_+,N_-]=2N, \tag{7}$$

and, in the space defined by the f_{ln}, satisfy the equations

$$\begin{aligned} N_\pm f_{ln}(z_n) &= \pm[(n\mp l)(n\pm l\pm 1)]^{1/2}f_{l\,n\pm 1}(z_{n\pm 1})\,, \\ Nf_{ln}(z_n) &= nf_{ln}(z_n). \end{aligned} \tag{8}$$

The operators (6) differ from those of the previous paper[2] by introduction of the dilatation operator and through replacement of z_n by z_N. Equation (8) indicates that the representation formed by the f_{ln} has a lower bound, since $N_-f_{l\,l+1}=0$; there is clearly no upper bound. Equation (8) also indicates that

$(N_\pm)^\dagger = -(N_\mp)$, and that both N_+N_- and N_-N_+ are real and negative definite. The representations of $O(2,1)$ formed using the f_{ln} as bases are therefore unitary.[7] They are obviously irreducible. We conclude then, that the $f_{ln}(z_n)$ with l fixed, $n > l$, form bases for positive discrete unitary irreducible representations of $O(2,1)$. These representations are denoted by D_l^+.

III. OPERATORS

We now wish to search for operators in the radial space which transform like "tensors" with respect to the algebra of Eq. (6). One such operator is

$$T^{(k)}{}_q = e^{iqt} D(N/(N+q))(r/N)^{-k}, \quad k > 0. \tag{9}$$

To evaluate $[N_\pm, T^{(k)}{}_q]$ we consider

$$\begin{aligned}
[N_\pm, T^{(k)}{}_q] f_{ln}(z_n) &= N_\pm e^{iqt} D\left(\frac{N}{N+q}\right)\left(\frac{r}{N}\right)^{-k} f_{ln}(z_n) - e^{iqt} D\left(\frac{N}{N+q}\right)\left(\frac{r}{N}\right)^{-k} N_\pm f_{ln}(z_n) \\
&= D\left(\frac{N\mp 1}{N}\right) e^{\pm it}\left(z_{n+q}\frac{\partial}{\partial z_{n+q}} \mp i\frac{\partial}{\partial t} \mp \frac{z_{n+q}}{2} + 1\right) e^{iqt}\left(\frac{r}{n+q}\right)^{-k} f_{ln}(z_{n+q}) \\
&\qquad \mp [(n\mp l)(n\pm l\pm 1)]^{1/2} e^{iqt}\left[\left(\frac{r}{n+q\pm 1}\right)\right]^{-k} f_{l\,n\pm 1}(z_{n+q\pm 1}) \\
&= -(k\mp q) e^{i(q\pm 1)t} D\left(\frac{N}{N+q\pm 1}\right)\left(\frac{r}{N}\right)^{-k} f_{ln}(z_n)
\end{aligned}$$

or

$$[N_\pm, T^{(k)}{}_q] = -(k\mp q) T^{(k)}{}_{q\pm 1}\,. \tag{10}$$

Clearly, we also have

$$[N, T^{(k)}{}_q] = qT^{(k)}{}_q\,.$$

This operator is obviously the extension of the operator $T^{(k)}$ of the previous papers[2,5] to the new Hilbert space defined on the $f_{ln}(z_n)$.

Matrix elements of the operators $T^{(k)}{}_q$ can be evaluated easily by considering the matrix elements

$$(f_{l'n'}|\,[N_\pm, T^{(k)}{}_q]\,|f_{ln});$$

in this way, recursion relations for the desired matrix elements can be obtained.[1,2,5] One finds in a straightforward manner that

$$\begin{aligned}(f_{l'n'}|\,T^{(k)}{}_q\,|f_{ln}) &= A(kq, ln|l'n') \\ &\quad\times (f_{l'\,l'+1}|\,T^{(k)}{}_{l'-l}\,|f_{l\,l+1}),\end{aligned} \tag{11}$$

where the coefficient $A(kq, ln|l'n')$ is given by[5]

$$\begin{aligned}A(kq, ln|l'n') &= \left(\frac{(2l+1)!\,(2l'+1)!\,(l'+n')!\,(n'-l'-1)!\,(n-l-1)!}{(l+n)!}\right)^{1/2} \\
&\quad\times \delta(n', q+n)\sum_t (-1)^{q+t+l-l'}[(n-l-1-t)!\,(l+l'+q+t+1)!]^{-1}\binom{l-l'-k-1}{q+l-l'+t}\binom{k-q}{t}\,.\end{aligned} \tag{12}$$

In the definition of A, the binomial coefficients are defined as

$$\begin{aligned}\binom{n}{r} &= n!/(n-r)!\,(r)! && \text{if } n \geq 0 \\ &= (-1)^r(r-n-1)!/(-n-1)!\,(r)! && \text{if } n < 0.\end{aligned}$$

A second operator in the radial space which transforms like a "tensor" is given by

$$P^{(k)}{}_q = e^{iqt} D(N/(N+q))(r/N)^{k+1}, \quad k \geq 0. \tag{13}$$

A simple calculation yields

$$\begin{aligned}[N_\pm, P^{(k)}{}_q] &= (k\pm q+1)P^{(k)}{}_{q\pm 1}\,, \\ [N, P^{(k)}{}_q] &= qP^{(k)}{}_q\,,\end{aligned} \tag{14}$$

and[5]

$$\begin{aligned}(f_{l'n'}|\,P^{(k)}{}_q\,|f_{ln}) &= A(-k-1\,q, ln|l'n') \\ &\quad\times (f_{l'\,l'+1}|\,P^{(k)}{}_{l'-l}\,|f_{l\,l+1}).\end{aligned} \tag{15}$$

The matrix elements appearing on the right-hand sides of Eqs. (11) and (15) can easily be evaluated since

$$\begin{aligned}f_{l\,l+1}(z_{l+1}) &= [2Z/(l+1)]^{l+1/2} e^{i(l+1)t} r^l \\ &\quad\times [2\pi(2l)!]^{-1/2} e^{-Zr/(l+1)}\,.\end{aligned}$$

Thus

$$\begin{aligned}(f_{l'\,l'+1}|\,T^{(k)}{}_{l'-l}\,|f_{l\,l+1}) &= (2Z)^k(l'+1)(l+l'-k)! \\ &\quad\times[(2l)!\,(2l')!\,(l+1)(l'+1)]^{-1/2}\end{aligned} \tag{16}$$

and

$$(f_{l'\,l'+1}|\,P^{(k)}{}_{l'-l}\,|\,f_{l\,l+1}) = (1/2Z)^{k+1}(l'+1)(l+l'+k+1)!\times[(2l)!(2l')!(l+1)(l'+1)]^{-1/2}\,. \quad (17)$$

IV. SELECTION RULES

As in the previous papers[2,5] selection rules can be obtained on the matrix elements of Sec. III by considering Kronecker products of representations of $O(2,1)$. If the matrix element is not to vanish, the Kronecker product of the representation of the ket and the representation of the operator must contain the representation of the bra.

The representation labels which describe the operators are easily found.[5] The operators $T^{(k)}{}_q$ with $|q| \leq k$ form bases for finite dimensional irreducible adjoint representation of $O(2,1)$ which we call $D(k)$. The operators $P^{(k)}{}_q$ with $q > k$ form bases for infinite-dimensional irreducible adjoint representations of the type D_k^+; the operators $P^{(k)}{}_q$ with $-q > k$ form bases for infinite-dimensional irreducible adjoint representation of the negative discrete type D_k^-. All other operators form bases for not fully reducible adjoint representations of $O(2,1)$. Kronecker products can easily be evaluated between these irreducible representations and the representations D_l^+ which describe the ket.[2,8] The following selection rules result from consideration of this product[5]: (i) Matrix elements of $T^{(k)}{}_q$ vanish if $|q| \leq k$ and k, l, and l' do not satisfy the triangular condition. (ii) Matrix elements of $P^{(k)}{}_q$ vanish if $q > k$ and $l' < l+k+1$. (iii) Matrix elements of $P^{(k)}{}_q$ vanish if $-q > k$ and $l' > l-k-1$. Other selection rules may exist, of course, for the operators which form bases for the not fully reducible adjoint representations.

V. DISCUSSION

Matrix elements of $T^{(k)}$ and $P^{(k)}$ can be rewritten in the form

$$\int R_{n'l'} D\left(\frac{n}{n'}\right)\left(\frac{r}{n}\right)^{-k} R_{nl}\,dr = \frac{(2Z)^{k+2}}{nn'} A(kn'-n, ln|\,l'n')\times(l'+1)(l+l'-k)!\;2[(2l+2)!(2l'+2)!(2n)(2n')]^{-1/2} \quad (18)$$

and

$$\int R_{n'l'} D\left(\frac{n}{n'}\right)\left(\frac{r}{n}\right)^{k+1} R_{nl}\,dr = \left(\frac{1}{2Z}\right)^{k-1}\left(\frac{1}{nn'}\right) A(-k-1\,n'-n, ln|\,l'n')\times(l'+1)(l+l'+k+1)!\;2[(2l+2)!(2l'+2)!(2n)(2n')]^{-1/2}\,. \quad (19)$$

When $n=n'$, Eq. (18), in conjunction with the selection rules of Sec. IV, explains immediately the selection rules on matrix elements of r^{-k} noted by Pasternack and Sternheimer.[9]

We have described an algebra which has as basis functions the hydrogenic radial functions times e^{int}. Introduction of the variable t is an essential characteristic of this approach, and enables us to study the hydrogenic radial wave function separately from the angular function. Unfortunately, it is somewhat difficult to obtain radial operators which transform as tensors with respect to this algebra. Equations (9) and (13) describe two such operators. Essentially, however, these operators seem to be of interest only when $q=0$. Thus this approach provides no advantage over the previous work[2] in so far as the evaluation of matrix elements or r^k is concerned.

The importance of the present approach is that, since it deals directly with the radial function, it more clearly suggests the types of problems which may be encountered in future studies in which more complicated potentials are used. For example, even if the algebra can be found for which the radial functions of interest form bases, there still remains the significant problem of expressing useful radial operators in a fashion such that they transform as tensors with respect to this algebra. The case of hydrogen demonstrates that expressing even such a simple operator as r^k in the proper form is a quite difficult problem, and one which has not yet been solved in a manner which allows matrix elements off-diagonal in n to be evaluated.

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Correlation Energies and Auger Rates in Atoms with Inner-Shell Vacancies*

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Many-body perturbation theory is used to calculate the correlation energy of an atom with an inner-shell vacancy. Numerical calculations are given for neon with either a 1*s* or a 2*s* vacancy. For the case of the 1*s* vacancy, the energy has an imaginary part which is proportional to the Auger rate. Our results are compared with semiempirical determinations of the correlation energy and with experimental results for the fluorescence yield.

I. INTRODUCTION

The many-body perturbation theory of Brueckner[1] and Goldstone[2] is used to calculate the correlation energy of a neon atom in which there is a 1*s* or 2*s* electronic vacancy. The problem is, in principle, the same as that treated by Köhler in calculating nucleon separation energies by K-matrix theory.[3] However, rather than using the spectrum of single-particle states for the N-particle system,[3] we calculate the single-particle states for the $(N-1)$ system in which the vacancy is already present. In the calculations, we use methods discussed previously[4,5] for applying many-body perturbation theory to atoms. We have found it convenient to employ the Silverstone-Yin[6] and Huzinaga-Arnau[7] potential, which has the desirable property that our unexcited states are represented by Hartree-Fock orbitals, while the excited states are calculated in a V^{N-1} potential.[8]

In Sec. II, we discuss the basic theory and considerations in the choice of potential. In Sec. III, we present numerical results for the correlation energy, Auger rates, and fluorescence yield when there is an initial 1*s* vacancy. Numerical results are also presented for the case where there is an initial 2*s* vacancy. Section IV contains the discussion and conclusions.

II. THEORY

A. Singularities in Diagrams

Consider the second-order energy diagram shown in Fig. 1(a). The expression for this diagram is

$$\sum_{k,k'} |\langle kk'|v|pq\rangle|^2 D^{-1} , \qquad (1)$$

where

$$D = \epsilon_p + \epsilon_q - \epsilon_k - \epsilon_{k'} . \qquad (2)$$

Hole lines p and q refer to unexcited bound states, and k and k' refer to excited single-particle states. The usual two-body interaction is represented by v.

If one of the excited states is a state which normally would have been occupied in the ground state of the atom, the denominator of Eq. (1) may vanish. In this paper, we consider the neon atom with a 1*s* vacancy, and, as a separate case, with a 2*s* vacancy.

In evaluating Eq. (1), sums over bound states are carried out explicitly up to $n = 13$, and the n^{-3} rule[8] is used to obtain the contribution from the rest of the bound states. Sums over continuum states are carried out by numerical integration[8] according to

$$\sum_k \to \frac{2}{\pi} \int_0^\infty dk ,$$

where our continuum states are normalized according to

$$P_{kl}(r) = \cos[kr + \delta_l + (q/k)\ln 2kr - (l+1)\tfrac{1}{2}\pi] , \qquad (3)$$

as $r \to \infty$. The logarithmic term in Eq. (3) arises from the fact that $V(r) \to q/r$ as $r \to \infty$.

When excited state $|k\rangle$ is an inner-shell vacancy, D of Eq. (2) may vanish for a particular excited state $|k'\rangle$. In such a case, the singularity in D^{-1} is treated in the usual manner by introducing a