Brinkman-Kramers approximation gives surprisingly good agreement with the measured cross section. In this approximation, the cross section scales as Z^5 with projectile atomic number and hence these results lend credence to the hypothesis of the importance of electron capture[2] in explaining the departure from Z^2 scaling of the cross section for vacancy production in heavy-ion collisions.[3]

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New Developments in the Application of Hyperspherical Coordinates to Atomic Wave Functions*

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Spin and antisymmetry have been incorporated into a hyperspherical expansion of the many-electron wave function. This new expansion increases the range of exact and approximate results available for atomic systems.

Hyperspherical expansions of wave functions have been used previously for many-body systems of spinless, distinguishable particles.[1] However, work on N-electron atoms has been limited both theoretically[2] and computationally[3] to the case of $N=2$, for which angular momentum, spin, and antisymmetry are trivial to treat. I have incorporated these properties into a general formulation of the hyperspherical expansion for arbitrary N,[4] and have employed this new basis to obtain information about exact wave functions[5,6] and to develop new methods of calculation. These results are summarized in this Letter.

Hyperspherical expansion of N-electron wave functions.—The N electrons in an atom are conveniently described by N radii r_i and N pairs of angles $\omega_i \equiv (\theta_i, \varphi_i)$. The radii can be obtained from a hyperradius r and a set of $N-1$ angles η_j by the relations

$$\begin{aligned} r_N &= r\cos\eta_N, \\ r_{N-1} &= r\sin\eta_N\cos\eta_{N-1}, \\ &\vdots \\ r_2 &= r\sin\eta_N\sin\eta_{N-1}\cdots\sin\eta_3\cos\eta_2, \\ r_1 &= r\sin\eta_N\sin\eta_{N-1}\cdots\sin\eta_3\sin\eta_2, \end{aligned} \tag{1}$$

where

$$\sin^2\eta_j = \sum_{i=1}^{j-1} r_i^2 \Big/ \sum_{i=1}^{j} r_i^2, \tag{2}$$

$$r^2 = \sum_{i=1}^{N} r_i^2. \tag{3}$$

Any configuration in the $3N$-dimensional space of the system is thus described by r and the set of

$3N-1$ "hyperspherical angles" $\Omega=(\eta_2,\ldots,\eta_N,\omega_1,\omega_2,\ldots,\omega_N)$. This definition of the angles is particularly convenient because the usual spherical angles of the electrons are retained. The radius r specifies the overall extent, or size, of the system while the angles Ω describe a scale-independent, relative configuration of the system onto the surface of a $3N$-dimensional hypersphere which we exploit in our approach.

The total Laplacian in these coordinates has the form

$$\nabla^2=\frac{\partial^2}{\partial r^2}+\frac{3N-1}{r}\frac{\partial}{\partial r}-\frac{\Lambda^2(\Omega)}{r^2}, \tag{4}$$

where Λ is a generalized angular momentum operator (see Smith[1] and Delves[1]). The operator Λ^2 has a complete set of eigenfunctions called hyperspherical harmonics,

$$\Lambda^2 S_\mu{}^{L,M_L}(\nu|\Omega)=\lambda_\nu(\lambda_\nu+3N-2)S_\mu{}^{L,M_L}(\nu|\Omega). \tag{5}$$

All variables are separable in this equation, and the functions of the ω_i angles are just the usual spherical harmonics. These have been coupled into eigenstates of total angular momentum, since we anticipate their use in the atomic problem. The eigenfunction of η_j is related to a Jacobi polynomial of order γ_j. The label ν stands for τ, the cycle structure of the azimuthal quantum numbers l_i, and $\beta=2\sum_j\gamma_j$. The eigenvalue λ_ν is $\beta+\sum_i l_i$. The index μ labels the S functions of given L, M_L, τ, and β.

These functions provide a basis for a partial-wave expansion of a spatial function:

$$\psi^{L,M_L}(\vec{r})=\sum_\nu\sum_\mu R_\mu(\nu|r)S_\mu{}^{L,M_L}(\nu|\Omega), \tag{6}$$

having specified L and M_L. We say that the S functions are "normal modes" of behavior of the hypersphere. Contours of S functions describe specifically correlated relative motions of the electrons, and the expansion is a superposition of these normal modes with scale-dependent expansion coefficients. Of course, the radial functions themselves also have some dynamical content.

To incorporate spin and antisymmetry into the total electronic wave function, we use the Kotani-Yamanouchi expansion[7] of a given ^{2S+1}L state in the form

$$\Psi^{L,M_L,S,M_S}(\vec{r},\sigma)=\sum_{\kappa=1}^{f}\psi_\kappa{}^{L,M_L}(\vec{r})\theta_\kappa{}^{S,M_S}(\sigma); \tag{7}$$

the functions θ of the spin variables σ are basis functions for the spin state. In order to satisfy the Pauli principle, the spatial functions are required to transform under electron permutation P as

$$P\psi_\kappa{}^{L,M_L}=\sum_{\kappa'=1}^{f}\psi_{\kappa'}{}^{L,M_L}U_{\kappa',\kappa}(P), \tag{8}$$

where the matrices $\underline{U}(P)$ are determined by the spin basis. Because r is invariant under P, the spatial functions must have a hyperspherical expansion of the form

$$\psi_\kappa{}^{L,M_L}(\vec{r})=\sum_\nu\mathfrak{R}(\nu|r)\mathcal{S}_\kappa{}^{L,M_L}(\nu|\Omega), \tag{9}$$

in which the set of functions $\mathcal{S}_\kappa{}^{L,M_L}(\nu|\Omega)$, $\kappa=1,2,\ldots,f$, transform as in Eq. (8).

We construct such a set of basis functions from the hyperspherical harmonics. The labels L, M_L, τ, and β of those functions are invariant under P. Thus, the functions $S_\mu{}^{L,M_L}(\nu|\Omega)$, $\mu=1,2,\ldots,g$, for a given L, M_L, and ν form a representation (generally reducible) of the permutation group. If this representation contains the irreducible representation $\underline{U}(P)$, we can (by Schur's lemma[8]) construct linear combinations,

$$\mathcal{S}_\kappa{}^{L,M_L}(\nu|\Omega)=\sum_\mu^{g}c_{\mu\kappa}{}^{\nu}S_\mu{}^{L,M_L}(\nu|\Omega), \tag{10}$$

having the desired transformation properties. By taking functions from each invariant subspace ν (since L and M_L are constants of motion) we obtain the expansion in Eq. (9). These new functions $\mathcal{S}$ are called *configurational normal modes;* they are intrinsic to the N-fermion system in a given ^{2S+1}L state and form a basis for describing its relative configuration Ω.

Applications to N-electron atoms.—The atomic Hamiltonian has a striking appearance in these coordinates:

$$\mathcal{H}=-\frac{1}{2}\left(\frac{\partial^2}{\partial r^2}+\frac{3N-1}{r}\frac{\partial}{\partial r}\right)+\left[\frac{\Lambda^2(\Omega)}{2r^2}+\frac{W(\Omega)}{r}\right]. \tag{11}$$

In parentheses is the "kinetic energy of extension," which depends explicitly on the number of electrons. The next term is a "kinetic energy of configuration" on the hypersphere. It contains all of the ordinary angular momenta, in addition to relative radial momenta in terms of the angles η_j. The

electrostatic potential is a homogeneous function of the coordinates of degree -1. Here, the distinction between extension and configuration is most apparent; the hyperradius factors completely from the configuration to give the potential $r^{-1}W(\Omega)$.

Using the expansions in Eqs. (7) and (9), and the Hamiltonian in Eq. (11), we obtain coupled equations for the $\mathfrak{R}$ functions:

$$\left[\frac{d^2}{dr^2}+\frac{3N-1}{r}\frac{d}{dr}-\frac{\lambda_\nu(\lambda_\nu+3N-2)}{r^2}+2E\right]\mathfrak{R}(\nu|r)=\frac{2}{r}\sum_{\nu'}W(\nu|\nu')\mathfrak{R}(\nu'|r), \tag{12}$$

where

$$W(\nu|\nu')=f^{-1}\sum_\kappa\int\mathcal{S}_\kappa^{\dagger}(\nu|\Omega)W(\Omega)\mathcal{S}_\kappa(\nu'|\Omega)d\Omega \tag{13}$$

is the matrix element of the configurational part of the potential over the unit hypersphere. It is important that the symmetries of the functions only require us to do the integrals of r/r_1 and r/r_{12}, since no other electron-electron repulsion is separable in these coordinates. Closed formulas for $W(\nu|\nu')$ can be derived, but one-dimensional numerical integration over η is sometimes more useful.

For a truncation of the expansion over ν, we have studied the resulting finite set of coupled differential equations,[5] and have shown that the solutions may be expanded[6] around $r=0$ as

$$\mathfrak{R}(\nu|r)=\sum_{n=k}^{\infty}\sum_{m=0}^{m^*(n)}A_{n,m}^{(\nu)}r^n\ln^m r, \tag{14}$$

where k is the smallest λ_ν for which $\mathcal{S}_\kappa(\nu|\Omega)$ can be constructed. The limit m^* is less than, or equal to, the greatest integer in $n/2$.[6] Our results on k and m^* correct those of Demkov and Ermolaev[2] to account for spin and indistinguishability of the electrons.[9] The coefficients $A_{n,m}^{(\nu)}$ satisfy a simple, algebraic, triangular recursion in n and m. For fixed n and m, all coefficients can be determined, except for the important coefficients $A_{\lambda_\nu,0}^{(\nu)}$. These, and the energy, are fixed by the boundary condition that ψ vanish as r goes to infinity.

Certain properties of ψ may be determined immediately. For example, the ground-state wave function of ^1S helium has the expansion

$$\begin{aligned}\psi&=1-r\textstyle\sum_\nu 2\pi^{3/2}[(\lambda_\nu-1)(\lambda_\nu+5)]^{-1}W(\nu|\nu_\omega)\mathcal{S}(\nu|\Omega)+\frac{1}{4}\pi^{3/2}Q_2r^2\ln r\mathcal{S}(\nu_2|\Omega)+O(r^2)\\&=1+(-zr_1-zr_2+\tfrac{1}{2}r_{12})+\tfrac{1}{2}Q_2r_1r_2\cos\theta\ln(r_1^2+r_2^2)+O(r^2),\end{aligned} \tag{15}$$

where

$$Q_2=-(16Z/\pi)\int_0^{\pi}d\theta\int_0^{\pi/2}d\eta(\sin\eta+\cos\eta)\left[\frac{1}{1-\sin2\eta\cos\theta}+\frac{1-\sin2\eta\cos\theta}{\sin2\eta}\right]\sin^3\eta\cos^3\eta\sin\theta\cos\theta.$$

This corrects the logarithmic coefficient obtained from perturbation theory by White and Stillinger.[2]

With our development of the $\mathcal{S}$ functions, techniques developed for the two-electron problem can now be used for N electrons. We mention particularly variational calculations with the trial function

$$\tilde{\psi}=\textstyle\sum_\nu\sum_n\sum_m D_{n,m}^{(\nu)}e^{-\zeta r}r^n\ln^m r\mathcal{S}(\nu|\Omega). \tag{16}$$

Also, the "adiabatic" method of Macek can be used, with diagonalization of the operator $(\frac{1}{2}\Lambda^2+rW)$ performed in the angular basis.[10] Finally, there are numerical approaches based on recursion[11] and on integration of coupled differential and integral equations.[12]

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Conversion of Electromagnetic Waves to Electrostatic Waves in Inhomogeneous Plasmas*

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Propagation of electromagnetic waves in a large plasma reveals that refraction effects are much more siginificant than the amplitude swelling commonly predicted from the reduction in group velocity. Near electromagnetic wave cutoff, direct conversion into short-wavelength electron plasma waves is observed. Strong resonant enhancement of the electric field parallel to the density gradient is measured.

Recently considerable attention has been focused[1] on the propagation of electromagnetic (EM) waves in nonuniform plasmas near the cutoff region where the incident frequency ω is close to the local electron plasma frequency ω_p. Near cutoff the conversion[2] to large-amplitude electrostatic (ES) electron plasma waves of short wavelengths can take place, which can effectively transfer energy to plasma particles. The basic understanding of these processes is crucial to the study of laser-plasma interactions as well as the large-scale modification of the ionosphere by EM waves. In this paper, we present experimental data on such processes obtained in a plasma whose dimensions are much larger than the free-space EM wavelength. Measurements of the electric field reveal approximately a 60 dB enhancement of the ES fields over the evanescent EM field at regions near the critical density, $\omega_p(z_c) = \omega$.

The experiment is performed in a space chamber[3] of approximately 2 m diameter and 4 m length in which a quiescent, steady-state, magnetic-field–free plasma is produced by a dc discharge in argon at 10^{-3} Torr. The plasma is contained by multimirror confinement with 10 000 permanent magnets at the interior chamber walls.[4] An axial density gradient ($1 < n_0/|\nabla n_0| < 10$ m) is produced by generating the plasma preferentially near one end of the device and by adjusting the mean free path with neutral pressure; radial gradients are avoided by azimuthally symmetric plasma generation and gas feeds. S-band microwaves ($f \simeq 2\,000$ MHz, $\lambda_0 \cong 15$ cm) are launched from antennas[5] at the low-density end of the device and propagate in the direction of the density gradient toward cutoff, $\omega = \omega_p$. In order to reduce multiple reflection the chamber walls are partly covered with microwave absorbers (fine-wire steel wool). The diagnostics consist of axially and radially motor-driven probes with a shielded coaxial magnetic loop for detection of EM waves $[\vec{H}(\vec{r}, t)]$, a coaxially fed short-wire dipole antenna for detecting electric fields $[\vec{E}(\vec{r}, t)]$, plane Langmuir probes for determining $n_e(\vec{r})$ and kT_e, and a nonlinear scattering dipole for absolute EM field-strength measurements.[6]

The axial density profile and the typical electric field pattern of the EM wave are shown in Figs. 1(a) and 1(b). Effective free-space propagation measurements in the far-field region have been achieved by propagating fast-rise, phase-