

ACKNOWLEDGMENTS

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¹³The thermodynamic expressions following from (2.1) and (2.2) can be generalized to multicomponent systems.

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Griffiths for his interest and for many valuable discussions, and Professor M. E. Fisher for several stimulating conversations.

Hamiltonian to describe a He³-He⁴ mixture is somewhat different than the one to be used in the present context.

¹⁵M. Wortis and D. Saul, in *AIP Conference Proceedings No. 5—Magnetism and Magnetic Materials* (AIP, New York, 1972); and M. Wortis (private communication).

¹⁶Certain nonordering fields have been studied exactly in the context of symmetry-preserving decorations of the $S = \frac{1}{2}$ Ising model. See, for example, M. E. Fisher [Phys. Rev. **176**, 257 (1968)] for further discussion.

¹⁷We note that thermodynamic arguments which use the Griffiths-Wheeler hypothesis (Ref. 7) and which generalize the one-component fluid case (Ref. 6) can be constructed. These indicate (with the same degree of strength as for the one-component fluid) that the above-mentioned derivatives have an asymmetric part diverging at least as strongly as $|t|^{-4-\delta}$.

¹⁸We do not consider here the question of a wave-number-dependent viscosity which has been suggested in recent derivations of (4.1); K. Kawasaki (unpublished).

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²²See the article by P. N. Pusey and W. I. Goldberg quoted in Ref. 1.

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Odd-Parity D States in He

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Positions of the lowest odd-parity 1^3D states in He have been calculated variationally. The trial wave function of Hylleraas type with four nonlinear parameters has been used. The results for the lowest 1^3D states obtained by using 112 terms in the wave function are lower than the previous results. The mass-polarization correction has been also calculated. The transition $2^3P^e \rightarrow 3^3D^0$ is of wavelength 3014.16 Å, which agrees well with the previous calculation and the experimental result. The 1^3D^0 states of H⁻ were also investigated, but no states of odd parity were found in this calculation.

In a previous paper,¹ the positions of the even-parity D states were given. These states decay through autoionization. In this paper the positions

of the lowest 1^3D states of odd parity are presented. These states lie below the $n=2$ threshold of He⁺ and decay radiatively to the lower states.

The odd-parity states, unlike the even-parity D states, are stationary states of the Hamiltonian and therefore the eigenvalues are given by the expectation value of the Hamiltonian, i. e. ,

$$E = \langle \Phi H \Phi \rangle / \langle \Phi \Phi \rangle . \quad (1)$$

The most general D -state wave function of odd parity of two electrons is

$$\begin{aligned} \Phi = & \sin \theta_{12} \\ & \times \{ [(f \mp \tilde{f}) \cos(\frac{1}{2} \theta_{12}) \mathfrak{D}_2^{\frac{1}{2}+} + (f \pm \tilde{f}) \sin(\frac{1}{2} \theta_{12}) \mathfrak{D}_2^{\frac{1}{2}-}] \\ & + [(5 \cos \theta_{12} - 1)(g \mp \tilde{g}) \cos(\frac{1}{2} \theta_{12}) \mathfrak{D}_2^{1+} \\ & + (5 \cos \theta_{12} + 1)(g \pm \tilde{g}) \sin(\frac{1}{2} \theta_{12}) \mathfrak{D}_2^{1-}] \} , \quad (2) \end{aligned}$$

where the \mathfrak{D} are the rotational harmonics, depending on the symmetric Euler angles θ , ϕ , ψ .² These functions are eigenfunctions of exchange and satisfy the following property:

$$\epsilon_{12} \mathfrak{D}_i^{k\pm} = \pm (-1)^{i+k} \mathfrak{D}_i^{k\pm} . \quad (3)$$

The trial wave function is of the Hylleraas type when radial functions $f = f(r_1, r_2, r_{12})$ and $g = g(r_1, r_2, r_{12})$ are given by

$$\begin{aligned} f(r_1, r_2, r_{12}) = & e^{-(r_1 r_1 + \delta_1 r_2) r_1^2 r_2} \\ & \times \sum_{l \geq 0} \sum_{m \geq 0} \sum_{n \geq 0} C_{lmn}^{(1)} r_1^l r_2^m r_{12}^n , \quad (4) \end{aligned}$$

$$\begin{aligned} g(r_1, r_2, r_{12}) = & e^{-(r_2 r_1 + \delta_2 r_2) r_1^3 r_2^2} \\ & \times \sum_{l \geq 0} \sum_{m \geq 0} \sum_{n \geq 0} C_{lmn}^{(2)} r_1^l r_2^m r_{12}^n . \quad (5) \end{aligned}$$

It is implied that

$$\tilde{f} = f(r_2, r_1, r_{12}) , \quad \tilde{g} = g(r_2, r_1, r_{12}) . \quad (6)$$

The upper sign in Eq. (1) corresponds to the singlet states and the lower sign to the triplet states. The first term in the wave function corresponds to the configuration (pd) and the second term corresponds to the configuration (df) for two electrons with total angular momentum equal to 2. This separation then is suggested by the configuration-interaction description and allows the use of four nonlinear parameters, which facilitates the convergence of the eigenvalues with respect to the number of terms in the wave function.

In Table I we present our results, optimized with respect to all the four nonlinear parameters for 112 terms, as a function of the Pekeris number¹ for D states. The comparison of the results with those of Doyle *et al.*³ and McCavert and Rudge⁴ is also given. The latter results seem to be uncertain in the fourth decimal place. The first singlet and triplet states are seen to be lower than the variational results, but above the $1/z$ ex-

TABLE I. $1,3D^0$ energies (in units of Ry) as a function of N , and comparison with previous calculations.

$N(\omega)$	Singlet states			Triplet states		
	$-E_1$	$-E_2$	$-E_3$	$-E_1$	$-E_2$	$-E_3$
8(1)	1.12532412	1.05913105	1.03805286	1.11771762	1.06310965	1.03403110
20(2)	1.12746759	1.06696647	1.04248828	1.11858950	1.06508558	1.04118071
40(3)	1.12759249	1.06901105	1.04378339	1.11865157	1.06533917	1.04136409
70(4)	1.12760047	1.06912539	1.04320504	1.11865632	1.06534945	1.04138773
112(5)	1.12760081	1.06915203	1.04328554	1.11865650	1.06535615	1.04138773
Doyle <i>et al.</i> (Ref. 3) variational results	1.12760046			1.11865608		
$1/z$ expansion results	1.127602			1.1186570		
McCavert and Rudge (Ref. 4)	1.1272	1.0692	1.0440	1.1182	1.0652	1.0414
$E_H \times 10^5$	-0.60762	-0.20116	-0.03775	0.83163	0.44142	0.16376
Position in eV with respect to ground state of He	63.6694	64.4647	64.8166	63.7913	64.5164	64.8425
						65.0182

TABLE II. Explicit comparison with experimental ${}^3P^e-{}^3D^0$ transitions.

Level(n)	λ (Å)	
	Calculated	Observed (vac.)
1	3014.46	3014.6 ± 3
2	2562.71	2561.76 ± 1
3	2400.91	2402.71 ± 1
4	2321.91	2319.69 ± 1

pansion results of Doyle *et al.*³ Careful optimization of the energy with respect to four nonlinear parameters still did not allow us to approach the $1/z$ results and we believe those results are too low.

The mass-polarization correction

$$E_M = - (2/M) \langle \Phi \vec{\nabla}_1 \cdot \vec{\nabla}_2 \Phi \rangle$$

is given for all the states in Table I. Finally, the positions of the D states, including the reduced mass and the mass-polarization corrections, with respect to the ground state of He are given in Table I.

Combining the ${}^3D^0(1)$ results with the position of ${}^3P^e$ state,⁵ we find the wavelength of the transition ${}^3P^e - {}^3D^0$ is equal to 3014.16 Å. This agrees with the results of Doyle *et al.*³ and also with the recent experimental results of Berry *et al.*⁶ An explicit comparison with the experimental ${}^3P^e - {}^3D^0$ transitions is given in Table II.

No ${}^1,{}^3D^0$ states in H^- were found in this calculation.

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ERRATUM

Electronic Transmission Spectroscopy: Core-Excited Resonances in Diatomic Molecules, L. Sanche and G. J. Schulz [Phys. Rev. A **6**, 69 (1972)]. Figure 10 has the band designations incorrectly labeled. Below we show the corrected Fig. 10.

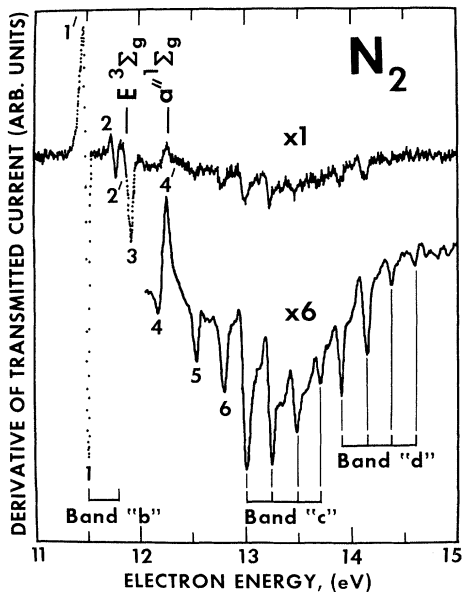


FIG. 10. Derivative of transmitted current vs electron energy in N_2 . The giant resonance 1-1' is a ${}^2\Sigma_g^+$, N_2^- state whose parents are the $E^3\Sigma_g^+$ and $a''\Sigma_g^+$ Rydberg states of N_2 . The grandparent of the structures 1-4 is the ground state of N_2^+ . The other resonances, including bands "c" and "d" which appear on the higher-sensitivity run at the bottom of the figure, have the $A^2\Pi_u$ state of N_2^+ as grandparent.