both the stored energy model and the scattering model are inadequate for small n.

It is seen that for sizable clusters of 10^2 or more vacancies, the resistivity per unit stored energy is about 3 times greater than for isolated vacancies. Thus if vacancies cluster as the sample is warmed from low temperatures we may expect to remove a larger fraction of the stored energy than of the excess resistivity. At sufficiently high temperatures we expect the vacancies to evaporate from the clusters and diffuse away, the excess over the equilibrium figure characteristic of the temperature leaving the crystal, annealing of the vacancies becoming complete.

Unquestionable evidence that the vacancies formed at low temperatures actually cluster in the form treated here does not seem to exist. If it were not for the arguments at the beginning of this section, it would seem plausible on geometrical grounds that they tend to cluster in platelets, which form collapsed vacancy disks. However, in this event they would scatter much less effectively for a given energy storage. That vacancies are created both by cold-work and by high energy bombardment at low temperatures seems inescapable; that they cluster in some form or another, upon warming the crystal, likewise appears so. A number of experiments of the type proposed by Seitz[7] seem capable of deciding in detail the fates of the vacancies created by radiation damage and by cold-work. Most of the crucial experiments have either not been performed or have been carried out on alloy systems which introduce additional complexity into the interpretations. An imperfection similar to the type discussed here would seem to be required if, for a given stored energy, there is a relatively large excess resistivity, a relatively large volume increase in the sample, and a large amount of small angle x-ray or neutron scattering.

ACKNOWLEDGMENTS

The writer is grateful to Dr. F. J. Blatt for inspection of his results before their publication, and to Mr. Charles A. McCarthy for assistance with the numerical computations.

PHYSICAL REVIEW VOLUME 103, NUMBER 1 JULY 1, 1956

Ground-State Solution of the Nonrelativistic Equation for Helium*

H. M. SCHWARTZ
Department of Physics, University of Arkansas, Fayetteville, Arkansas
(Received March 29, 1956)

By the inclusion of half-integral powers in the Hylleraas functions for the ground state of the helium atom, it is possible to obtain more rapid convergence in the Ritz variational method applied to the nonrelativistic Schrödinger equation (for infinite nuclear mass), as shown by results of calculations involving from four to thirteen parameters. The energy obtained with 13 parameters, -2.903719 a.u., is the lowest so far published. The coefficients for the normalized wave functions are given.

THE recent remeasurement[1] of the ionization potential of the helium atom with an accuracy of perhaps a few parts per million,[2] is making it possible to undertake a meaningful check on the relativistic theory for this state.[3] To that end, one requires the solution of the nonrelativistic helium wave equation to a corresponding accuracy. The recent calculations by Chandrasekhar and Herzberg[4] using the Ritz-Hylleraas method may perhaps have yielded such results. Uncertainty arises from present ignorance as to the rapidity of convergence of the Ritz-Hylleraas method.[5] The determination of an upper bound on the error for the energy by using the best method available for finding a lower bound to the energy,[6] is handicapped by the rather poor approximation of this lower bound to the true energy.[6,7] Under these circumstances it seemed worth while to explore modifications in the Hylleraas type solutions that may lead to improvement in convergence. A simple modification consisting in the introduction of half-integral powers in the Hylleraas poly-

* This work is supported in part by the U. S. Atomic Energy Commission.

[1] By G. Herzberg and R. Zbinden (as reported by S. Chandrasekhar and G. Herzberg, Phys. Rev. **98**, 1050 (1955), reference 12).

[2] The experimental result, I.P.(He) = 198 310.$_5$ ± 1 cm^{-1}, quoted in reference 4, is termed "provisional."

[3] Ta-You Wu and G. E. Tauber, Phys. Rev. **100**, 1767 (1955), and references therein to earlier work on the relativistic solution. For preliminary calculations on lowest order radiative corrections see M. Günther, Physica **15**, 675 (1949); H. E. Håkansson, Arkiv Fysik **1**, 555 (1950); P. K. Kabir and E. E. Salpeter, Bull. Am. Phys. Soc. Ser. II **1**, 46 (1956).

[4] S. Chandrasekhar and G. Herzberg, Phys. Rev. **98**, 1050 (1955).

[5] Some uncertainty still exists even with regard to convergence. The proof given by A. S. Coolidge and H. M. James [Phys. Rev. **51**, 855 (1937)] can be shown to be valid in what concerns the completeness of the Hylleraas set, but the part dealing with convergence involves an unproven assumption.

[6] L. Wilets and I. J. Cherry, Phys. Rev. **103**, 112 (1956).

[7] A. F. Stevenson and M. F. Crawford, Phys. Rev. **54**, 375 (1938).

TABLE I. Nonrelativistic wave functions of Hylleraas type with fractional exponents for the He ground state. $\psi=e^{-\frac{1}{2}ks}(c_{000}+c_{00\frac{1}{2}}u^{\frac{1}{2}}+c_{020}t^2+\cdots)$; $s=r_1+r_2$, $t=r_2-r_1$, $u=r_{12}$ (normalized function; atomic units).

k | input	3.614	3.5	3.5	3.5	3.5	3.5
$-E$ |	2.90277	2.9033807	2.9035502	2.903639	2.903660	2.9037135
k | from	3.61529	3.500706	3.498814	3.498639	3.498779	3.500070
$-E$ | variational	2.90277	2.903381	2.903551	2.903639	2.903660	2.903719
| formulas[a]						
c_{lmn}						
000	1.22323	1.401276	1.409473	1.444384	1.487603	1.396898
$00\frac{1}{2}$	0.22927	0.380444	0.312906	0.199743	−0.018836	0.176205
020	0.17392	0.153910	0.226558	0.375122	0.344291	0.329913
001	0.25168	0.144767	0.158258	0.250348	0.648979	0.518561
$\frac{1}{2}00$		−0.366021	−0.337711	−0.347380	−0.354477	−0.232078
100		0.051416	0.026374	0.026178	0.025919	0.007720
$\frac{1}{2}0\frac{1}{2}$			0.037595	0.050218	0.059514	−0.172997
$02\frac{1}{2}$			−0.053238	−0.276125	−0.230744	−0.255175
002				−0.017173	0.059567	0.023661
021				0.080784	0.064742	0.066023
$00\frac{3}{2}$					−0.300762	−0.244214
$\frac{1}{2}01$						0.136027
$\frac{1}{2}20$						0.030960

[a] See formulas (8) in reference 4; or, H. A. Bethe, *Handbuch der Physik* (Verlag Julius Springer, Berlin, 1933), Vol. 24, Part 1, p. 357.

nomials yielded the results summarized in Table I.[8] Comparison of these with the corresponding results in reference 4, shows that there is indeed a substantial improvement of the type sought, especially as no attempt was made to choose the optimum scaling factor k. The following immediate questions remain: (1) Will the energy be pushed substantially lower by suitable increase in the number of parameters? (2) Inasmuch as this method proved less satisfactory for $Z=1$,[9] does it actually improve with increasing Z? (3) What can be expected from the employment of more general fractional powers? (4) What restrictions, if any, in the applicability of the present functions, result from their having singular derivatives on the planes $s=0$ and $u=0$? Some work on these questions is continuing, but any significant progress relative to (1) would involve computational facilities not presently available to the author.

The assistance of Veronica C. Fink, who was in charge of all the numerical work on this problem, is gratefully acknowledged.

[8] The suitable introduction of negative powers has been explored successfully by Dr. T. Kinoshita (private communication).

[9] The result of Levitt, Tauber, and Wu [Phys. Rev. **99**, 1659(A) (1955)] needed revision [G. E. Tauber (private communication)]