COMMENTS AND ADDENDA

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Ground-State Binding Energy of the ^{4}He Trimer

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Through a variational calculation, the ground-state binding energy of the ^{4}He trimer is computed using the *ab initio* potential of Bertoncini and Wahl. These results indicate a stable trimer bound by 0.3 °K.

In a recent letter, Kruger[1] reported the results of a Faddeev-type calculation of the ground-state binding energy of the ^{4}He trimer. The calculation was performed in the three-boson quasiparticle approximation of Alt, Grassberger, and Sandhas[2] using a Morse-potential fit to the *ab initio* He-He interaction of Bertoncini and Wahl.[3] Kruger found a stable trimer bound by 0.4 °K. Unfortunately, Kruger's curve for the binding energy falls below the lower bound, computed through the Hall-Post[4] method, when ϵ, the potential well depth, lies between 9.8 and 10.2 °K. Clearly, this must be the consequence of some numerical error, most likely arising from the truncation of the biorthonormal series of Weinberg states in the expansion for the two-body transition operator $T_\gamma(z)$ which appears in the quasiparticle theory.

As the trimer problem is of some importance in physics, an attempt was made to check on Kruger's calculation using the variational approach of Ohmura *et al.*[5] Originally formulated for the three-nucleon problem where the nucleon-nucleon interaction has a hard core, the method is both accurate and simple since the expression for the energy is analytic.

The variational binding energy E, which is an upper bound, is given by

$$E=\langle\psi|H|\psi\rangle, \tag{1}$$

where the trimer Hamiltonian is

$$H=-\frac{\hbar^2}{2m}\sum_{k=1}^{3}\nabla_k^2+\sum_{i<j=1}^{3}V(r_{ij}) \tag{2}$$

and ψ is a suitable trial function. The Morse fit to the Bertoncini-Wahl potential is

$$V(r_{ij})=\epsilon P(x),\quad x r_m=|\vec{r}_{ij}|, \tag{3}$$

where

$$P(x)=e^{-2\alpha(x-1)}-2e^{-\alpha(x-1)}, \tag{4}$$

with

$$r_m=3.0\ \text{Å},\quad \alpha=6.0,\quad \epsilon=10.48\ ^\circ\text{K}. \tag{5}$$

However, to use the Ohmura expression for E, it was assumed that

$$P(x)=\infty\quad\left(x<\frac{D}{r_m}=x_D\right)$$
$$=e^{-2\alpha(x-1)}-2e^{-\alpha(x-1)}\quad(x>x_D). \tag{6}$$

D is defined by taking $P(x_D)\approx 4\epsilon$ and is about 2.4 Å. This "hard-core" approximation should be reasonable, as the true potential curve is extremely steep at He-He separations less than 2.4 Å (see Fig. 1).

The Ohmura trial function is of the form

$$\psi=\prod_{i<j=1}^{3}g(r_{ij}), \tag{7}$$

$$g(r_{ij})=0\quad(r_{ij}<D)$$
$$=e^{-\mu(r_{ij}-D)}f(r_{ij})\quad(r_{ij}>D). \tag{8}$$

The correlation function $f(r_{ij})$ is given by

$$f(r_{ij})=1-e^{-\nu(r_{ij}-D)}. \tag{9}$$

From the experience of Schmid *et al.*,[6] the variational constants μ and ν were obtained by con-

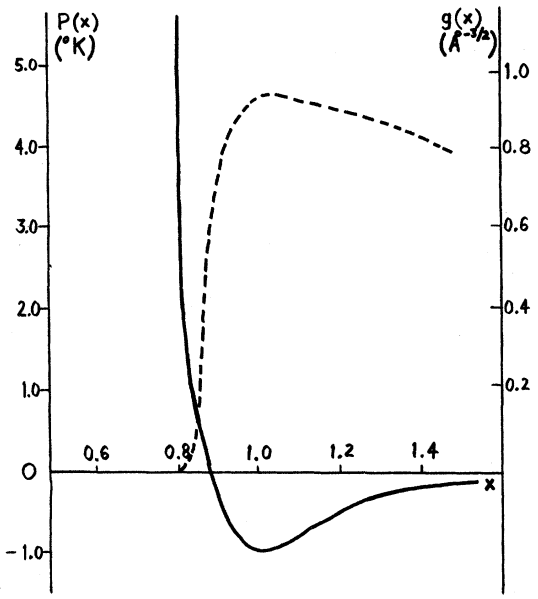

FIG. 1. He-He potential and trial function $g(r_{ij})$.

straining $g(r_{ij})$ to peak at the minimum in the potential and taking the rms radius[7] of the trimer to be about 6.5 Å. The function $g(r_{ij})$ is shown in Fig. 1. The accuracy of this procedure was checked by redoing Schmid's calculation with an appropriate Morse-potential fit to their Lennard-Jones interaction. Their published results were almost reproduced.

The hard-core radius D can be considered a variational parameter. Indeed, the present procedure for selecting its magnitude was a fortuitous choice; other values of D gave poorer results. The explanation for this is fairly obvious. For higher values, a substantial portion of the interaction is neglected; for smaller values, the wave function is inadequate to handle the repulsive core.

For the ^{4}He trimer interacting through the Bertoncini–Wahl potential, the best variational solution corresponds to

$$\mu = 0.100 \text{ Å}^{-1}, \quad \nu = 7.25 \text{ Å}^{-1}, \tag{10}$$

$$\text{rms radius} = 6.75 \text{ Å}$$

and

$$E = -0.256 \text{ °K}. \tag{11}$$

Ohmura *et al.* have estimated the accuracy of their calculation in the three-nucleon case to be within 10% of the result of the most realistic wave function. If the same accuracy is assumed here, then the best upper bound to the binding energy of the trimer is about 0.28 °K. Thus, since it is expected that the true eigenvalue lies closer to this upper bound than to the Hall–Post lower bound, one may conclude that the true binding energy is near 0.3 °K.

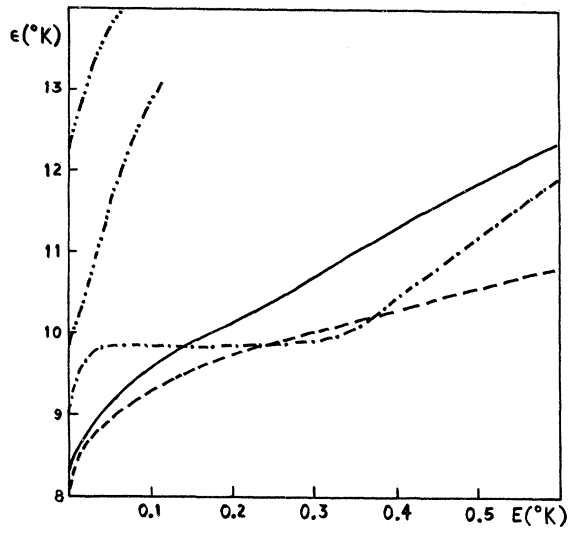

FIG. 2. Binding energy E vs ϵ, the potential well depth. The solid curve is the variational result, the dashed line is the Hall–Post lower bound, while the dash-dot line is Kruger's result. The dash-double-dot and dash-triple-dot lines represent the excited-state curve and the two-body curve, respectively, from Ref. 1.

The E-vs-ϵ curve from this work is shown in Fig. 2 together with Kruger's results. It is worth noting that the excited state found by Kruger may be a manifestation of the "Efimov effect," which predicts that two-body forces which almost lead to

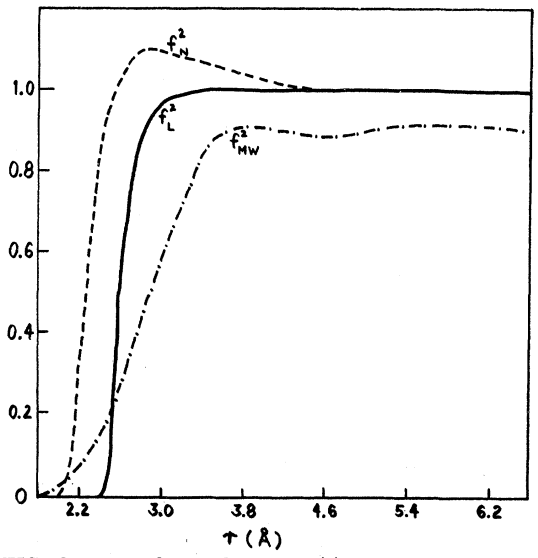

FIG. 3. Correlation function $f(r)$. The solid line is the result of this work, the dashed and dash-dot lines are those of Nosanow and Massey.

bound two-body systems can give rise to a series of excited states in the corresponding three-body systems.[8]

If one assumes for the ^{3}He trimer the same wave function and interaction, its ground-state binding energy can likewise be calculated. It is found to be unbound by 0.127 °K, a result in agreement with Stenschke's.[9]

Of some interest is the form of the correlation function; $f(r_{ij})$ resembles closely those derived by Nosanow[10] and Massey and Woo[11] from their variational calculations for solid ^{3}He. This is shown in Fig. 3.

In summary, the following conclusions can be drawn: (i) The *ab initio* potential of Bertoncini and Wahl leads to a bound trimer of ^{4}He. Other realistic interactions should lead to the same result. (ii) The trimer of ^{3}He is probably unbound. If the ^{3}He-^{3}He potential is deeper than the ^{4}He-^{4}He potential, as suggested by Bennewitz *et al.*,[12] a bound trimer could result. (The author is at present studying this.) (iii) The correlation function derived in this paper is similar to those obtained in solid-^{3}He calculations. (iv) The behavior of the E-vs-ϵ curve from this work indicates inaccuracies in the Kruger calculations.

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High-Energy K-Shell Ionization by Heavy Projectiles*

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The ionization of K-shell electrons by heavy particles is examined in the energy region where the projectile is moving faster than the orbiting electron. An explanation suggested for the rise of the experimental results above the Born approximation is the mechanism of "charge exchange to the continuum." An estimate of the effect shows reasonable agreement with experiment.

At sufficiently high energies, one expects that the K-shell ionization cross section of an atom by a charged projectile would be well described by the first Born approximation. This approximation predicts a cross section proportional to Z_1^2 (Z_1 is the projectile charge number), so that the ratio $R = \sigma(Z_1)/Z_1^2\sigma(1)$ is expected to be unity where the projectile velocities are the same. In fact, experimental results for projectiles of protons and α particles show significant deviations from unity.[1] Attempts have been made[2] to explain these deviations in both the low- and high-velocity regions of the curve. We discuss only the high-energy end here.

Two mechanisms[2,3] have been proposed to explain the deviation of R from unity at higher energies based on initial-state polarization of the K-shell electron by the projectile. The first[2] corresponds to a second-order correction in the standard perturbation expansion in Z_1e^2/hv which, it is expected, extends over a region comparable to the size of the K-shell electric orbit. Since this initial-state polarization is the adiabatic response of the bound electron to the projectile, we suggest that this effect is more appropriate for the low-velocity region. The second initial-state polarization effect[3] extends over projectile impact parameters larger than the atomic radius and could contribute at moderately high projectile velocities where the target still has time to adjust.

In this paper we propose another mechanism to explain the experimental deviations at the higher energies. It has been called[4] "charge exchange to the continuum," or polarization of the final state. When an electron is ionized by the projectile, it can correlate strongly with the projectile in the final state, but still not be bound to it. Even at high velocities the polarization at the final state