SMALL CLUSTERS OF PURE AND ADMIXED H⁺, 3He⁺, T⁺, AND 4He ATOMS

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INTRODUCTION.- The physics of small clusters of rare-gas atoms has received well-deserved attention recently. ¹⁻⁴ We have participated fully in this resurgence of interest in this area of research using as tools a variational technique called ATMS and Faddeev theory. Thus we have already treated the 3-, 4- and 5- atom systems of pure and admixed 3He and 4He, and established the existence of a number of these molecules when they interact pairwise through recently proposed phenomenological helium-helium potentials. ²⁻³ Now with the realization that systems of spin-polarized hydrogen and 3He atoms exhibit quantum behavior even more pronounced than 4He ⁵⁻⁶ we have decided to turn our attention to the study of these spin-polarized quantum systems. In this paper we report the results of our calculations to determine the existence of small clusters of admixed and pure H⁺, 3He⁺, T⁺, and 4He atoms in two and three dimensions. Our study of these molecules in reduced dimensions stems from the suggestion of Lantto and Nieminen ⁷⁻⁸ that 2D systems be investigated more thoroughly since wall-surface effects of the containment vessel may be significant in determining the stability of H⁺.

THE ATMS METHOD AND FADDEEV-UPE THEORY.- We lay out here short descriptions of the two methods we have used in our investigations. The ATMS Method: This variational method was devised by two of us (Akaishi and Tanaka) with other collaborators for use in the study of the few-body systems of nuclear physics. ²⁻⁶ The technique, labelled ATMS by us, differs from traditional ways of constructing trial functions in that its modus operandi includes the derivation of two-body correlation functions which are incorporated explicitly into the final variational wavefunction. Used with the Temple formula, ATMS can yield an accurate lower bound for the binding energy. The integrals which appear in our evaluation of the energy expectation value are computed with a quasirandom method after a suitable transformation of variables. We took 50 000 sam-

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pling points to be sure that the integrals are converged.

The Faddeev-UPE Method: In this method the coupled integral equations arising from the Faddeev formulation of the few-body problem are solved through the device of representing the two-body local potential by a series of separable terms. In principle, this technique is exact. However, truncation of the partial-wave expansion and of the number of terms in the separable expansion as well as the limitations on the number of quadrature points in the computation of integrals render Faddeev-UPE less than exact.

RESULTS. Our results can be summarized as follows:

i) We have performed a detailed and systematic calculation of the \((^4\text{He})_n (^1\text{H})\) systems and searched, in particular, for the maximum value of \(\eta = \frac{\sqrt{m}}{a} \), for which each of these systems has a bound state. Table 1 illustrates our results for Lennard-Jones potentials.

<table>
<thead>
<tr>
<th>N</th>
<th>(\eta_{\text{max}}(^1\text{H})) in KÅ²</th>
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<tbody>
<tr>
<td>4</td>
<td>18</td>
</tr>
<tr>
<td>6</td>
<td>18.21</td>
</tr>
<tr>
<td>8</td>
<td>18.42</td>
</tr>
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It is obvious that as N increases, there is little change in the value of \(\eta_{\text{max}}(^1\text{H})\) in 2D. In 3D, the change is barely discernible. The extracted values of \(\eta_{\text{max}}(^1\text{H})\) are very far from the physical value of 47.73 KÅ². The trend in our results leads us to believe that N has to be at least 20 before a bound molecule will appear. Our calculations indicate that this conclusion is not altered by the inclusion of more atoms of \(^1\text{H}\).

ii) \((^4\text{He})_n\) systems exist for \(n\) as small as 3. In fact, for 3D, we have found binding energies of 0.042 K and 0.243 K for the ground states of the \(n = 3\) and \(n = 4\) systems respectively. In addition, there is an excited state in \((^4\text{He})_3\) which we originally suspected to be an Efimov state.\(^8/\) However it fails to manifest the characteristics expected of one.

iii) When we assume that \((^3\text{He})_n\) systems in 3D are bosonic, we find that at \(n = 8\), there is a bound molecule with an energy of 0.38 K. It appears to us as if a bound molecule may be formed at \(n = 7\). What this suggests to us is that the fermionic \((^3\text{He})_n\) systems will not be bound for \(n\) any less than about 12.

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References


