

Minimal mass-size of a stable ${}^3\text{He}$ cluster

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The minimal number of ${}^3\text{He}$ atoms required to form a bound cluster has been estimated by means of a Diffusion Monte Carlo procedure within the fixed-node approximation. Several importance sampling wave functions have been employed in order to consider different shell-model configurations. The resulting upper bound for the minimal number is 32 atoms.

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Helium clusters are unique systems for studying the properties of finite sized quantum objects. The first systematic microscopic calculation of their ground state properties was carried out by Pandharipande and coworkers [1] eighteen years ago. One interesting finding is that, contrary to the ${}^4\text{He}$ case, a minimum number of ${}^3\text{He}$ atoms is required to create a stable cluster, as a consequence of the large zero-point motion and the Pauli effect. The calculations of Ref. [1] were based on an optimized trial wave function, where the fermions are assumed to fill harmonic oscillator single-particle states $1s^2 1p^6 1d^{10} 2s^2 1f^{14} 2p^6 \dots$. The outcome was that twenty atoms are not enough to form a bound system, but forty atoms are bound, and in between a *critical* or *threshold* number exists for having stable clusters. From the experimental point of view, there is only indirect evidence of such a critical number, since the smaller ${}^3\text{He}$ systems detected insofar contains thousand of atoms.

The critical number was calculated in Ref. [2], by using a non-local finite-range density functional approach. The usual Kohn-Sham procedure provided the residual interaction required to perform a configuration interaction calculation. The obtained critical number was 29 atoms. Afterwards, we carried out [3, 4] a variational microscopic study based on the two-body He-He interaction known as HFD-B(He) interaction [5], which reproduces accurately the properties of both ${}^4\text{He}$ and ${}^3\text{He}$ liquid. The trial wave function contained a Jastrow-correlated part and a self-adjustable translationally invariant configuration interaction part, including up to three particle-hole excitations. Due to the variational character of the computational procedure, only an upper bound was obtained, and we concluded that the critical number is less or equal to 34 atoms.

In order to improve this estimate we have carried out several calculations within the fixed-node Diffusion Monte Carlo (DMC) procedure [6, 7], for selected systems near the previously determined critical number. The importance-sampling wave functions have been constructed in a similar way to the variational forms previously used in Refs. [3, 4], but with some modifications. First of all, the confining part of the two-body Jastrow correlation used here has an exponential shape, instead of a gaussian one. Because of the longer range of the exponential shape one may expect to be more appropriate for systems near the binding threshold. Apart from this, the same backflow correlation was used, but the configuration interaction part has not been included, with the objective of having a fast diffusion Monte Carlo algorithm.

The other relevant modification is related to the antisymmetric part of the wave function. The fermionic antisymmetry is considered by means of the product of two Slater determinants, one for each spin orientation. In the present calculation we have assumed several shell-model orderings for these determinantal parts, and not simply the ordering related to the harmonic-oscillator single-particle potential previously considered. Actually, nothing is known about the ordering of shells. The only indirect information comes from the study of a single ${}^3\text{He}$ atom tied to a core of ${}^4\text{He}$ atoms, where calculations indicate an order based on the orbital angular momentum, namely $1s 1p 1d 1f \dots$, with probably the $2s$ level being interleaved between the $n = 1$ levels [8, 9]. Therefore, we have considered configurations with a fixed occupancy $1s^2 1p^6 1d^{10}$, the $N = 18$ major shell, and several distributions of the remaining particles between the $2s$ and the $1f$ shell, which are classified by the value of the total spin S .

The actual calculations have been carried out with a time slice $\tau = 0.00025 \text{ K}^{-1}$, with an average population of 1000 walkers and for 10000 time steps, plus 1000 previous steps in order to reach the stability. To obtain an estimate of the variance, the sampling steps were grouped into blocks of 100 moves.

The obtained results are presented in Table I. The $N = 34$ cluster appears clearly bound, as well as one of the configurations chosen for $N = 33$. This last result has the interest of suggesting the $2s$ shell to be deeper bound than

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TABLE I: Ground state energies E (in K) obtained for several clusters near the critical binding number. For a given number N of atoms, the shell-model configuration and the value of the total spin S are indicated.

N	Config.	S	E (K)
31	$2s^2 1f^{11}$	3/2	Unbound
31	$2s^2 1f^{11}$	1/2	Unbound
32	$2s^2 1f^{12}$	0	-0.27 ± 0.03
32	$2s^2 1f^{12}$	1	-0.23 ± 0.03
32	$2s^0 1f^{14}$	0	Unbound
33	$2s^1 1f^{14}$	1/2	Unbound
33	$2s^2 1f^{13}$	1/2	-0.86 ± 0.04
34	$2s^2 1f^{14}$	0	-1.52 ± 0.04

the $1f$ shell.

Regarding the $N = 32$ cluster we had an initial guess in favor of the configuration $1s^0 1f^{14}$, because it would correspond to a closed shell. However the actual calculations show that this configuration does not result in a bound state, preferring instead to complete the $2s$ shell. This is not surprising once it has been established the shell ordering in the $N = 33$ case. Note that the total spin of the configuration $2s^2 1f^{12}$ can have the two values $S = 0$ and 1 . Taking into account the statistical errors, one may conclude that these states are bound with the same binding energy. Either these states are degenerate or the difference in energy is smaller than our statistical errors, i.e. of the order of ten mK. Given that the obtained energies are very close to zero, the imaginary time evolution was carried out for these two cases for as much as 40000 time steps.

Finally we have considered the $N = 31$ cluster, with two spin states ($S = 1/2$ and $S = 3/2$) of the $2s^2 1f^{11}$ configuration. It turns out that neither of these states is bound, their energy being close to zero but positive.

In conclusion, we have find $N = 32$ as an upper bound to the minimal mass-size of a stable ${}^3\text{He}$ cluster. The various configurations here considered correspond in practice to probe different nodal surfaces. It is worth stressing that our results indicate that, within the computational statistical errors, the binding energy is independent of the spin coupling, depending only on the chosen configuration. Finally, it should also be mentioned that the separation energy for $N = 34$ (0.66 ± 0.06 K) is almost the same as that of $N = 33$ (0.59 ± 0.05 , 0.64 ± 0.05 K), thus suggesting a single-particle structure of these fermionic clusters, with a residual interaction compatible with zero. The determination of the precise critical number should require a calculation beyond the variational fixed-node approximation, and it is not excluded that the result could depend on the He-He interaction employed in the practical calculation.

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