

density profiles show that the cluster size grows when the number of atoms in the cluster increases, and that the central densities of the largest clusters are very similar to the bulk equilibrium density $\rho_0 = 0.007466(7) \text{ \AA}^{-3}$.

The increase of cluster size with increasing number of atoms can also be seen from the pair distribution function $P(r)$ shown in Fig. 5 for the same clusters. $P(r)$ is normalized such that $\int P(r)r^2 dr = 1$. A significant decay of the peak height for the largest clusters, as well as the growing probability for larger interparticle distances in large clusters, is a clear evidence of the size spreading tendency.

The surface thickness of clusters s_t can be estimated from the density profiles as a difference of radii at which the central density $\rho_c = \rho(r=0)$ has decreased from 90% to 10% of its value. From the plotted density profiles in Fig. 4 it is obvious that the density error bars are large for small distances. In order to determine the central density as precisely as possible we have tried to fit the density profile with the function used in Ref. 27

$$\rho(r) = \frac{\rho_0}{(1 + e^{\beta(r-r_0)})^\delta}, \quad (11)$$

where ρ_0 , β , r_0 and δ are fitting parameters and r is the distance to the centre of mass of the cluster. We find that for $T\downarrow$ clusters Eq. (11) can be employed to model density profiles of small clusters, while for greater clusters the same model reproduces poorly the calculated density profiles at small distances. Since the small distances are important for our calculation, we have decided to fit the calculated density profiles to a constant function for distances up to some value r_1 . We have varied the value of r_1 from 2 \AA to 4 \AA , increasing it with the growing size of the cluster. We have considered the constant obtained with the fit as a central density value and used it in further estimation of the clusters' surface thickness. The results for the surface thickness are reported in Table I. We can compare our results with the surface thickness of ^4He clusters [24, 28]. Using the VMC method Pandharipande *et al.* [24] showed that in ^4He clusters the surface thickness is $\sim 7\text{\AA}$ for clusters $N \geq 112$. In the case of $T\downarrow$ clusters, for $N \geq 100$, the surface thickness is significantly greater than in ^4He (Table I). This is expected due to the evidently greater interparticle distances in $T\downarrow$ clusters, which is a direct consequence of the shallow attractive part of $T\downarrow$ - $T\downarrow$ interaction potential. With the density functional approach, Stringari *et al.* [28] calculated the surface thickness of several ^4He clusters and we can compare those results with our results for $T\downarrow$ clusters having 20, 40 and 240 atoms. The reported surface thickness for clusters $^4\text{He}_{20}$, $^4\text{He}_{40}$ and $^4\text{He}_{240}$ are respectively 8.8 \AA , 9.0 \AA and 9.3 \AA . A comparison with $(T\downarrow)_N$ reveals larger surface thickness of $^4\text{He}_N$ for $N=20,40$ and smaller surface thickness for $N=240$. Also, it can be noticed that the surface thickness reported by Stringari *et al.* is not a linear function of the number of atoms. Contrary, in the

case of $T\downarrow$ clusters, we observe that the surface thickness is almost a linear function of N , up to $N=320$ atoms. We have tried to predict the surface thickness of clusters having more than 320 atoms by fitting our data with the function used in Ref. 27 to predict the width of a free surface. However, with the present results we have not been able to determine the asymptotic value of the surface thickness. Saturation should be probably seen with results for clusters having more than $N=320$ atoms, but the DMC calculations are already difficult with 320 atoms.

CONCLUSIONS

General characteristics of large spin-polarized tritium $T\downarrow$ clusters have been investigated using the DMC approach. The ground-state energies of clusters consisting of up to 40 $T\downarrow$ atoms have been compared with previously published results. For clusters having more than 40 atoms the ground-state energies, as well as the structure description, are determined for the first time. This prediction relies on the use of a very precise potential of interaction between $T\downarrow$ - $T\downarrow$ atoms. The present results for the ground-state clusters' energy are also used to extract the energy per particle of liquid $T\downarrow$ at equilibrium density using a liquid-drop model. The extrapolation using a liquid-drop formula gives a value $E_v = -3.66(3) \text{ K}$ for the energy per particle in the equilibrium bulk system, which is in very good agreement with the result from a recent DMC calculation of the bulk, $e_0 = -3.656(4) \text{ K}$ [6].

The radii of clusters are calculated with pure estimators and those results are used to estimate the interval in which the unit radius of the liquid is expected. The result for the unit radius from the bulk calculation lies in the estimated interval. The latter value of the bulk unit radius has been employed to estimate the surface tension t of bulk $T\downarrow$, $t=0.08 \text{ K}\text{\AA}^{-2}$. In addition, the surface thickness of clusters has been estimated from the clusters' density profiles.

As it is already shown for clusters consisting of up to 40 $T\downarrow$ atoms [1], it is concluded that large spin-polarized tritium clusters are less bound and are more diluted than ^4He clusters with the same number of atoms, i.e., interparticle distances are significantly greater in the corresponding $T\downarrow$ clusters.

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