Quantized Vortices in Mixed ^{3}He-^{4}He Drops

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Using density functional theory, we investigate the structure of mixed $^3\mathrm{He}_{N_3}$-$^4\mathrm{He}_{N_4}$ droplets with an embedded impurity (Xe atom or HCN molecule) which pins a quantized vortex line. We find that the dopant + vortex + $^4\mathrm{He}_{N_4}$ complex, which in a previous work [F. Dalfovo *et al.*, Phys. Rev. Lett. **85**, 1028 (2000)] was found to be energetically stable below a critical size N_{cr}, is robust against the addition of ^{3}He. While ^{3}He atoms are distributed along the vortex line and on the surface of the ^{4}He drop, the impurity is mostly coated by ^{4}He atoms. Results for $N_4 = 500$ and a number of ^{3}He atoms ranging from 0 to 100 are presented, and the binding energy of the dopant to the vortex line is determined.

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Helium nanodroplets have recently attracted considerable interest. A major reason is the possibility of using them as an inert, ultracold matrix for molecular spectroscopy studies [1]. They also allow one to address superfluid phenomena at a microscopic scale [2], and constitute an ideal testing ground for quantum many-body theories. An interesting perspective in this direction is the investigation of quantized vortices in finite systems. Key experiments have been carried out in the past two years on vortices in Bose-Einstein condensed gases of rubidium and sodium atoms confined in magnetic traps [3], where vortical states are created by acting with external perturbations in different ways. These states turn out to be more robust than expected on the basis of qualitative arguments. In principle, analogous vortical configurations are also possible in superfluid ^{4}He droplets, where the external perturbation could be a moving and/or rotating impurity. Although the presence of vortices in superfluid ^{4}He drops is not energetically favorable [4], we have argued that they can be stabilized by molecules hosted in the bulk of the drop [5], and that their existence could be inferred from the changes they induce in the molecular spectrum [6].

The aim of this paper is to extend our previous analysis [5] to the case of mixed ^{3}He-^{4}He droplets. The addition of ^{3}He atoms to doped ^{4}He droplets has significant consequences in current experiments, since it lowers the temperature of the droplet from about 0.4 to 0.15 K, and their presence can be used as another source of information for characterizing the interaction of the dopant with the superfluid environment [7]. In this context, an accurate description of the first solvation layers of ^{4}He and/or ^{3}He around the impurity is important. The presence of ^{3}He in a droplet hosting a quantized vortex would display several interesting features, since (i) ^{3}He atoms behave as a normal component in the superfluid, providing a friction mechanism for the motion of vortex lines; (ii) ^{3}He atoms occupy surface states, known as Andreev states, which are energetically favored by the lighter mass and the larger zero point motion of ^{3}He compared to ^{4}He; (iii) some ^{3}He atoms will be attached to the vortex core, where they are expected to have a binding energy of the order of 2–3 K [8]. We investigate the effects (ii) and (iii) by using a density functional method to calculate the structure and the energetics of these systems, also including dopant atoms and molecules. In the calculations we use Xe or HCN embedded in droplets with $N_4 = 500$ atoms of ^{4}He and a number of ^{3}He atoms N_3 ranging from 0 to 100.

Our starting point is a density functional previously developed for mixed ^{3}He-^{4}He systems, which allows one to write the energy of the mixture as $E = \int d\mathbf{r}\, \mathcal{H}[\rho_3(\mathbf{r}), \rho_4(\mathbf{r})]$, where $\rho_3(\mathbf{r})$ [$\rho_4(\mathbf{r})$] is the ^{3}He [^{4}He] particle density (see [9,10], and references therein). To keep the already cumbersome calculations at an affordable level, here we use a slightly simplified version of the same functional; namely, we take the core of the screened Lennard-Jones He-He potentials as in the original Orsay-Paris functional [11], and drop the gradient-gradient term which appears in the Orsay-Trento functional [12] for ^{4}He. We checked that these changes have negligible effects on the relevant results, while they drastically reduce the numerical effort. As discussed in [9,10], the density functional contains a set of parameters which is fixed to reproduce static properties of pure and mixed He systems at zero temperature, such as the equation of state, surface tension of the different interfaces, the osmotic pressure, and maximum solubility of ^{3}He into ^{4}He [13].

As in [5], the vortex line is included through the Feynman-Onsager *ansatz,* i.e., by adding an extra centrifugal energy associated with the velocity field of ^{4}He, which is singular on the vortex axis, thus forcing its density to vanish. For doped droplets, one has to include the helium-impurity interaction, which acts as an external potential in

which the helium density adjusts to minimize the energy. The potential for Xe has been taken from [14], and that of HCN from [15]. Combining all terms, the total energy can be written in the form

$$E = \int d\mathbf{r} \left\{ \mathcal{H}[\rho_3(\mathbf{r}), \rho_4(\mathbf{r})] + \frac{\hbar^2}{2m_4 r_\perp^2} \rho_4(\mathbf{r}) + V_I(\mathbf{r})[\rho_3(\mathbf{r}) + \rho_4(\mathbf{r})] \right\}, \quad (1)$$

where V_I is the helium-impurity potential and $r_\perp$ is the distance from the vortex axis. The energy minimization is performed in axial symmetry by mapping the densities on a spatial mesh, putting the vortex line along the z axis and the dopant in the center, at $\mathbf{r} = 0$.

We consider two rather simple configurations: (*i*) a mixed droplet with a dopant, but no vortex and (*ii*) a mixed droplet with a vortex, but no dopant. In the former case we just reobtain the results of [9,10], namely, that the amount of ^{3}He atoms in the bulk of the drop is negligible, and the dopant is coated by ^{4}He. The structure of the drop is "onionlike," with ^{3}He distributed in the outer shell and ^{4}He inside, surrounding the embedded impurity. In contrast, in the latter case ^{3}He atoms can funnel through the vortex dimple created at the ^{3}He-^{4}He interface and eventually the vortex core is filled with ^{3}He.

An example of a mixed droplet with a vortex is shown in Fig. 1. The ^{4}He and ^{3}He density profiles in the radial direction, at $z = 0$, are shown in Fig. 2 for different values of N_3. It can be seen that ^{3}He fills the vortex core even for $N_3 = 20$, and that the dependence of the central density on N_3 is weak, as expected for a close-packed linear chain of atoms. The remaining ^{3}He atoms occupy the available surface states, whereas ^{4}He stays in the bulk. A comparison with the case of pure ^{4}He droplets (solid line in Fig. 2) shows that ^{3}He atoms push the superfluid ^{4}He component away from the vortex axis, thus lowering the kinetic energy associated with the vortex flow [16,17].

Placing a dopant in the center of the droplet significantly distorts the ^{3}He and ^{4}He densities. In Fig. 3 we show the same densities as in Fig. 1, but with an embedded HCN molecule. The strong helium-impurity attraction, which is the same for ^{3}He and ^{4}He, favors the formation of a layered structure of ^{4}He atoms near the molecule, since they have a smaller zero point motion than ^{3}He atoms and can be localized more easily in the local minima of the potential. In the vicinity of the dopant, ^{3}He atoms remain only at the pinning points on the vortex axis, where ^{4}He is excluded by the high kinetic energy of the vortex flow. The net effect is that the structure of the complex dopant + vortex near the dopant is very similar to that of pure ^{4}He droplets. It is worthwhile to see that the dopant also produces a modulation of the ^{3}He density along the vortex line.

Let us denote with subscripts X and V the energies, E, of mixed droplets doped with an impurity X and/or

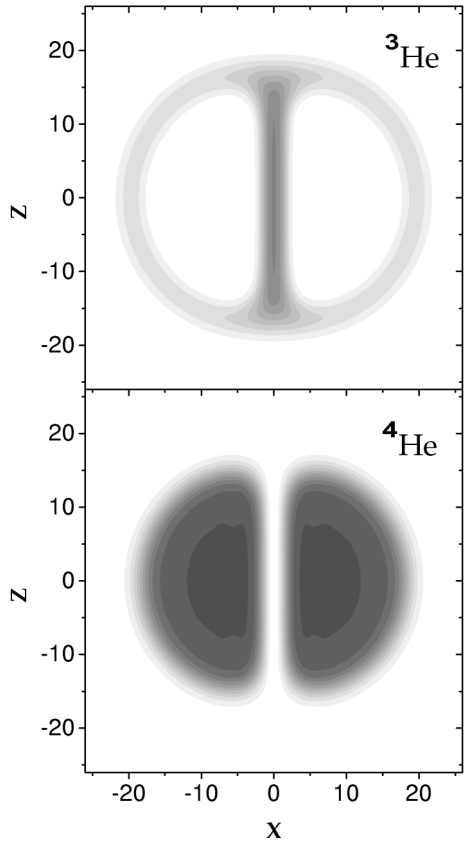

FIG. 1. Density distributions of ^{3}He (top) and ^{4}He (bottom) in the xz plane for the $^4\mathrm{He}_{500} + {}^3\mathrm{He}_{100}$ droplet hosting a vortex line along the z axis. Lengths are in units of Å. Darker regions are high density regions.

containing a vortex line. The energetics of these droplets can be studied by introducing, for a fixed value of N_4, the following functions of N_3 [5]:

$$\Delta E_V(N_3) = E_V(N_3) - E(N_3), \quad (2)$$

$$\Delta E_V^X(N_3) = E_{X+V}(N_3) - E_X(N_3), \quad (3)$$

$$S_X(N_3) = E_X(N_3) - E(N_3), \quad (4)$$

$$S_{X+V}(N_3) = E_{\mathrm{X+V}}(N_3) - E(N_3), \quad (5)$$

$$\delta_X(N_3) = \Delta E_V^X(N_3) - \Delta E_V(N_3). \quad (6)$$

The quantities ΔE_V and ΔE_V^X correspond to the energy associated with the vortex flow in a droplet without dopant and with dopant X, respectively. The quantity S_X is the solvation energy of impurity X in the mixed cluster, while S_{X+V} is the solvation energy of the dopant + vortex complex. When the quantity δ_X is negative, its absolute value represents the binding energy of the dopant to the vortex in the mixed cluster.

In Ref. [5] we studied the above energies in the $N_3 = 0$ case, finding that $S_{X+V}(N_3 = 0)$ is negative and hence the ^{4}He + X + vortex complex is stable for values of N_4 smaller than a critical number, N_{cr}, of the order of 8000 for both Xe and HCN. The effect of a nonzero N_3 value

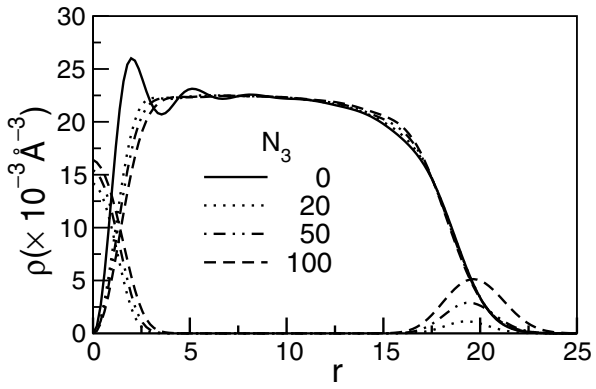

FIG. 2. Density profiles of ^{4}He and ^{3}He in the radial direction, at $z = 0$, for droplets with a vortex line along the z axis and with $N_4 = 500$ and $N_3 = 0$, 20, 50, and 100. The ^{3}He density profiles appear in two disconnected parts separated by the corresponding ^{4}He density profile. For $N_3 = 100$, the dashed lines correspond to a cut at $z = 0$ of the densities in Fig. 1. Lengths are in units of Å.

comes from a delicate interplay between different energy contributions, which are sensitive to the distribution of ^{3}He atoms in the vortex and near the dopant. The crucial question is whether ^{3}He may depin the impurity from the vortex core, i.e., $\delta_X(N_3)$ becomes positive for a certain N_3.

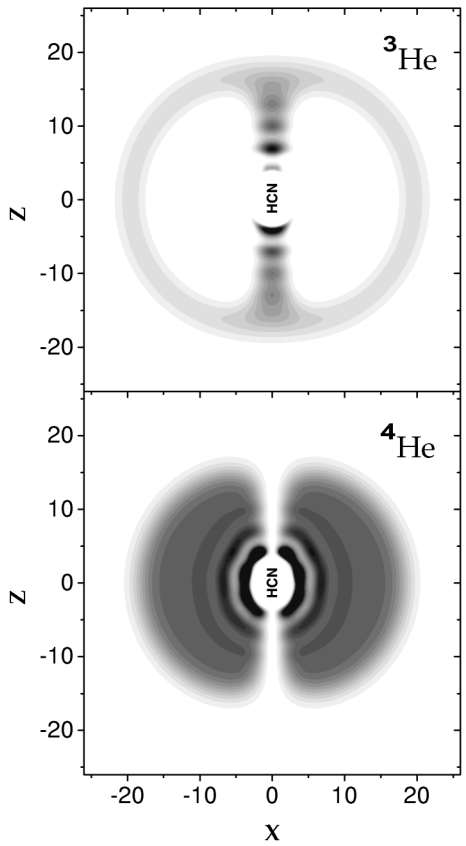

FIG. 3. Same as in Fig. 1 but with a dopant HCN molecule in the center of the droplet.

The relevant energies are plotted in Fig. 4. The top panel shows how the vortex energy decreases with N_3 in droplets without dopant, with a Xe atom, and with a HCN molecule. This behavior is consistent with a reduction of the kinetic energy of the vortex flow when normal ^{3}He atoms displace superfluid ^{4}He atoms away from the vortex core. The two middle panels show the solvation energy of the impurity and of the dopant + vortex complex; both are negative for these droplets. The main result of this analysis is shown in the bottom panel, where one may see the effect of ^{3}He on the binding energy of the dopant to the vortex. The binding energy $|\delta_X|$ of the dopant decreases when N_3 increases, but the dopant is still pinned to the vortex. The initial slope of the curve is steeper than for large N_3. This is consistent with the first ^{3}He atoms occupying states along the vortex line close to the dopant, thus affecting δ_X in a more significant way. In the intermediate region for

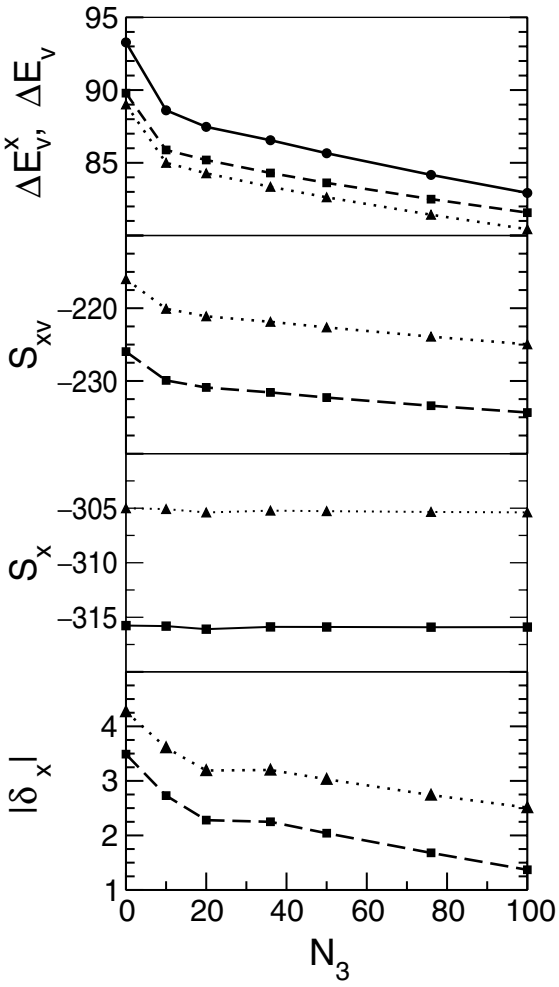

FIG. 4. From top to bottom panel: Vortex energy of the $^4\mathrm{He}_{500} + {}^3\mathrm{He}_{N_3}$; solvation energy of the dopant + vortex complex; solvation energy of Xe and HCN dopants; binding energy $|\delta_X|$. The triangles represent results for Xe, the squares for HCN, and the circles in the top panel are the results for undoped droplets. The energies are in units of K, and the lines have been drawn to guide the eye.

$N_3 = 20-40$, the binding energy exhibits a plateau. In this range, the presence of the dopant is expected to affect the distribution of ^{3}He atoms both in the vortex line and at the surface. One can see in Fig. 2 that in the same range of N_3 values the mixed droplet starts to develop a ^{3}He "skin," i.e., an outer shell where the ^{3}He density is larger than the ^{4}He density. Whereas its effect is imperceptible at the scale of the energies defined in Eqs. (2)–(5), it shows up in δ_X, which is about 2 orders of magnitude smaller [18].

We conclude that the dopant + vortex + $^4\mathrm{He}_{N_4}$ complex is robust against the addition of moderate amounts of ^{3}He atoms. This may offer some experimental advantages. On the one hand, mixed droplets reach lower temperatures than pure ^{4}He droplets; on the other hand, adding a variable amount of the normal component will result in a variable damping for the vortex motion, without losing the characteristics that make ^{4}He drops appealing for molecular spectroscopy, since the dopant environment essentially consists of ^{4}He atoms as in pure drops.

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[18] We want to point out that the four energies involved in the evaluation of δ_X are of the order of 2500–3000 K. This makes its accurate determination a very demanding numerical task.