Ground state properties of liquid ^{3}He injected in a carbon nanotube: A variational approach

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Introduction: Liquid ^{3}He injected in a carbon nanotube is of high interests due to different behavior of the liquid helium in the quasi-one dimensional systems. In this work, a variational approach based on the cluster expansion of energy has been performed to calculate some thermodynamic properties of this quantum system. In order to do so, a single-walled carbon nanotube (SWCN) containing liquid ^{3}He is considered, applying the Lennard-Jones and Stan-Cole potentials for ^{3}He-^{3}He and ^{3}He-C interactions, respectively. We have done our calculations for density range 0.1 - 1.0 nm^{-1} and radii R=0.3, 0.48 and 0.8 nm.

Cluster expansion method:

Based on the cluster expansion, the total energy is obtained as follows

$$E = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} = E_1 + E_2 + ...$$

where E_1 is the one-body cluster energy, E_2 is the two body cluster energy, etc. E_1 is made up of two parts. The first is summation of ^{3}He atoms kinetic energies, whereas they do not feel the presence of each other and the second is summation of potential energies related to the interaction of each ^{3}He atom with the carbon nanotube. E_2 shows the energy contribution related to the interaction between ^{3}He atoms.

$$E_2 = \frac{1}{2}\sum_{i,j} \langle ij | \omega(12) | ij - ji \rangle \qquad \omega(12) = \frac{\hbar^2}{m}[\nabla f(r)]^2 + f^2(r)V(r)$$

where ω(12) is the two-body effective potential, In above equation, V (r) is the inter-particle potential and f (r) is the two-body correlation function. We have considered the Lennard-Jones potential (V_{LJ}) for ^{3}He-^{3}He interaction, and Stan-Cole potential (V_{SC}) for ^{3}He -C interaction.

$$V_{SC}(\rho : R) = 3\pi\theta\epsilon_2\sigma^2\left[\frac{21}{32}\left(\frac{\sigma}{R}\right)^{10} M_{11}(x) - \left(\frac{\sigma}{R}\right)^4 M_5(x)\right]$$

$$V_{LJ}(r) = 4\epsilon_1\left[\left(\frac{\lambda}{\rho}\right)^{12} - \left(\frac{\lambda}{\rho}\right)^6\right]$$

Results and Discussions : At first, we have calculated the one-body (E_1) and the two-body (E_2) energies, then the total energy ($E=E_1+E_2$) has been obtained. Our results show that the one-body energy has negative values while the two-body energy has positive values, although both of them increase by increasing density. To compare our results with other works, we have calculated single particle energy states $\varepsilon(k_{\rho,\varphi})$ for a single ^{3}He atom in a SWCN in ground state n_ρ =1 , n_φ =0 equal (-231.671 K) for radius R=0.48 nm, where there is a good agreement between our results and Vranjes et. Al [1]. The total energy is negative for all densities. We have calculated the equation of state for the system, and have found out that the pressure increases by increasing the density and nanotube radius. Our results for incompressibility show that the system can have a liquid state for higher densities (higher than 1.0 nm^{-1}) for R=0.48 and 0.8 nm whereas for R=0.3 nm can not have a liquid-gas phase transition. These transition points occur in densities about 1.2 and 2.1 nm^{-1} for 0.8 and R=0.48 nm^{-1} radii respectively, which are very low densities. In other words, liquid ^{3}He in a carbon nanotube is the lowest density liquid one ever seen. This help us to make ^{3}He liquid in very low densities in comparison with three dimensional systems.

[1] L. Vranjes, S. Kilic and E. Krotscheck, J. Low Temp. Phys. 134, 73 (2004).

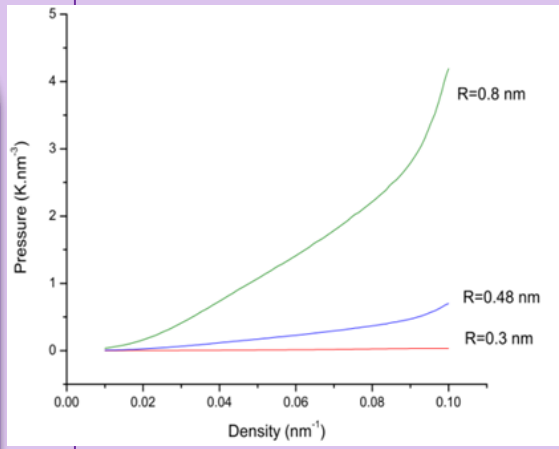

TABLE I: The energy contribution of ^{3}He-C interaction (Potential energy per particle), kinetic energy per particle and total one-body energy per particle for three different radii ($R_1 = 0.3\ nm\ R_2 = 0.48\ nm\ R_3 = 0.8\ nm$).

Density (nm^{-1})	Potential energy (K)			Kinetic energy (K)			One-body energy per particle (K)		
	R_1	R_2	R_3	R_1	R_2	R_3	R_1	R_2	R_3
0.1	-243.376	-231.524	-161.412	0.00255	0.00263	0.00275	-243.373	-231.521	-161.40925
0.2	-243.373	-231.513	-161.401	0.0102	0.01051	0.01102	-243.3628	-231.50249	-161.38998
0.3	-243.369	-231.506	-161.396	0.02295	0.02364	0.02479	-243.34605	-231.48236	-161.37121
0.4	-243.364	-231.498	-161.393	0.0408	0.04202	0.04406	-243.3232	-231.45598	-161.34894
0.5	-243.358	-231.492	-161.391	0.06375	0.06566	0.06885	-243.29425	-231.42634	-161.32215
0.6	-243.354	-231.488	-161.386	0.0918	0.09455	0.09914	-243.2622	-231.39345	-161.28686
0.7	-243.347	-231.484	-161.381	0.12495	0.1287	0.13495	-243.22205	-231.3553	-161.24605
0.8	-243.341	-231.478	-161.376	0.1632	0.1681	0.17626	-243.1778	-231.3099	-161.19974
0.9	-243.335	-231.472	-161.372	0.20655	0.21275	0.22307	-243.12845	-231.25925	-161.14893
1.0	-243.328	-231.463	-161.367	0.255	0.26265	0.2754	-243.073	-231.20035	-161.0916