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

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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 system. 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. 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 $n_\rho=1$, $n_\varphi=0$ equal (-231.671 K) for radius R=0.48 nm, where there is a good agreement between our results and Vranjes *et al.* The total energy is negative for all the 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 cannot 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 has ever seen. This helps us to make ^{3}He liquid in very low densities in comparison with three dimensional systems.

Biography

M A Rastkhadiv has completed BS and MS from Shiraz University and now is finalizing his PhD from Shiraz University, School of Science. He is interested in statistical mechanics and is researching on quantum many body systems in nano dimensions.

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