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Superfluid ^4He density functional theory in 2-D cylindrical coordinates¹ JUSSI ELORANTA, SEAN FRENCH, Department of Chemistry and Biochemistry, California State University at Northridge, STEVEN FIEDLER, Department of Chemical Engineering, The University of Michigan — Bosonic density functional theory describing superfluid ^4He is formulated in 2-D cylindrical coordinates and a numerical implementation of the model using a regular spatial grid basis is presented. The 2-D formulation has many important applications as the 1-D treatment cannot, for example, describe translational motion of atoms and molecules solvated in the liquid and the 3-D theory is usually computationally too expensive, especially when describing dynamics in bulk superfluid ^4He . The theory is implemented in both real and imaginary time forms for allowing solution of both time-dependent and time-independent problems. Two test cases for the developed method are presented and the results are compared against the previously published results. Finally, the method is applied to describe solvation of single wall carbon nanotubes in superfluid ^4He at 0 K and the implications of the results to dynamic liquid response are discussed.

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- Prefer Oral Session
 Prefer Poster Session

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