Calculations For Understanding a Possible Supersolid State

Authors: B.K. Clark and D.M. Ceperley
arXiv.org/cond-mat/0512547

and

M. Boninsegni, N. Prokofev, B.Svistunov
arXiv.org/ cond-mat/0512103

Recommended with a Commentary by P.W. Anderson, Princeton University

The recent report[1] by Chan et al. of the observation of non-classical inertia possible associated with a co-existing solid and superfluid of vacancies phase (a supersolid) has naturally excited considerable theoretical and calculational interest. The two papers discussed here are both very sophisticated Monte Carlo calculations by groups which have a long history of successful simulations of the properties of He^4, and one is inclined to trust them to do the calculations they describe skillfully; in fact, when calculating the off-diagonal element of the density matrix for the perfect solid they seem to get identical results. The paper by Ceperley in particular includes a lengthy review of the theoretical considerations which bear on ODLRO, Bose condensation and nonclassical rmoment of inertia, and makes the dilemma of Chan et al's results quite evident. They explain quite clearly that any wave function containing only purely local correlations, like a Jastrow function or any generalization thereof, necessarily is superfluid; yet the best numerical results depend on introducing a long-range lattice structure into the wave function, which destroys superfluidity of all forms. The path integral Monte Carlo they use does not depend on any assumed variational function, and seems to reliably give no BEC, the atoms being exponentially tied to their sites.

There are two comments I would make that may be relevant. The first is that the experimental results do not, in fact, imply BEC at the temperature of the measurement, as pointed out by D Huse et al[2]; they only require that there be a finite vortex string tension in the sense of Nguyen and Sudbo[3], and that vortices move sluggishly relative to the measuring frequency. Phase fluctuations would probably average out ODLRO.

The second is that calculations following individual atoms may find it very difficult to pick out the effects of incommensurability. There is no question that every site in a supposed lattice must be identical: there can be no localized vacancies or interstitials in the ground state. What may be true is that simply the counts of atoms and of sites do not match, and that the local state must be a coherent superposition of atom and no atom[4] ; and to my knowledge no one has tested that directly. I note that Ceperley and Clark use a box suited to commensurability for their number of atoms. Could that have prejudiced their results? Also, they seem to assume that the atoms not explicitly in the polymer that represents their path are behaving classically.

The Boninsegni et al paper makes the suggestion that a glassy phase may be responsible for the superfluid behavior. While there have been reports of strange optical behavior by some authors, one would expect that defects would find it extremely easy to diffuse out of solid He.; also, a metastable glassy state that is identical in two sizes of pores and in the bulk is hard to credit. I think it is safe to assume that what Chan et al. see is a bulk property of the crystalline state.

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[1] E.Kin and M.H.Chan, Science, 305, 1941 (2004)

[2]D Huse et al, Science 310, 1164 (2005)

[3]A Sudbo and K Nguyen, Phys Rev B 60, 15307 (1999)

[4]P. Anderson, arXiv.org/cond-mat/0504731