Imaginary Time Path Integral Calculations of Supersolid Helium

David Ceperley

Dept. of Physics and NCSA
University of Illinois Urbana-Champaign, Urbana, IL, 61801, USA

In 1953 Feynman, introduced imaginary-time path integrals to understand superfluid ^{4}He. Path integrals are an exact "isomorphism" between quantum systems and the classical statistical mechanics of ring "polymers" allowing one to understand Bose condensation from the point of view of classical statistical mechanics and to calculate many of its properties. Bose symmetry of the wave function implies that the polymers are allowed to “cross-link" or exchange. Superfluidity (coupling to the boundaries) is proportional to the mean squared flux of polymers through a surface. Bose condensation is equivalent to the delocalization of the end-end distance of a cut polymer. We have developed specialized simulation methods (Path Integral Monte Carlo) based on the Metropolis Monte Carlo method, to simulate boson systems[1].

Andreev, Lifshitz, Chester, and Leggett suggested in about 1970 that a quantum crystal such as bulk helium-4 under pressure might show both crystallinity and superfluid behavior. Experiments by Kim and Chan within the last two years have found indications for such a supersolid phase. The theoretical explanation of superflow in a crystal assumed vacancies, however, they have not been seen experimentally and computer simulations do not find stable vacancies. The path integral picture allows one to address the question[2] of whether a highly fluctuating quantum crystal is “insulating” or “metallic”. We and others have done Path Integral Monte Carlo calculations of exchange frequencies[3], superfluid density and the condensate fraction[4]. We do not find superfluid response, but calculations are limited to equilibrium samples of small crystals. Hence, there is a possible discrepancy between the best computer simulations and the interpretation of experiments. Recent experimental results support the view that defects such as grain boundaries, dislocations or impurities are an essential part of the mechanism leading to the observations.

References:

1. Ceperley, D. M., Path Integrals in the Theory of Condensed Helium , Rev. Mod. Phys. **67**, 279 (1995).
2. N. Prokof’ev and B. Svistunov, Phys. Rev. Lett. **94**, 155302 (2005).
3. Ceperley D. M. and B. Bernu, Ring exchanges and the supersolid phase of 4He, Phys. Rev. Letts. **93**, 155303: 1-4 (2004): cond-mat/0409336.
4. Khairallah, S. A. and D. M. Ceperley, Superfluidity of Dense 4He in Vycor, Phys. Rev. Letts. **95**, 185301 (2005); physics/0502039.
5. lark, B. and D. M. Ceperley, Off-Diagonal Long-Range Order in Solid 4He, Phys. Rev. Letts. **96**,105301 (2006); cond-mat/0512547.