Vacancies in solid Helium-4

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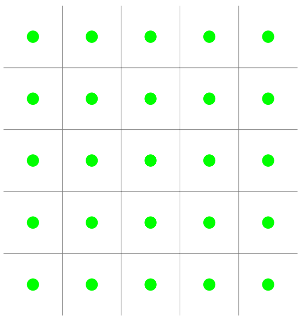
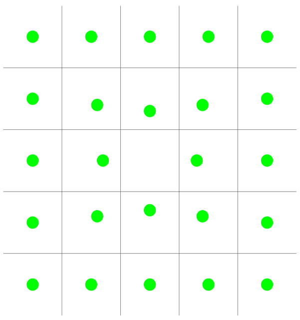
Introduction

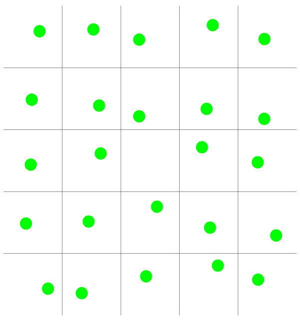
solid He, a quantum crystal: Lindemann ratio ≈ 0.3 even at $T \to 0$



pure class. crystal

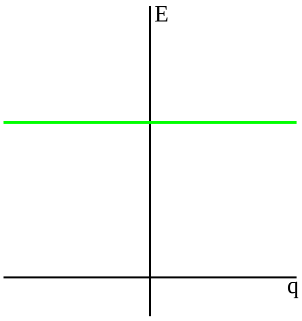


classical vacancy
elasticity theory

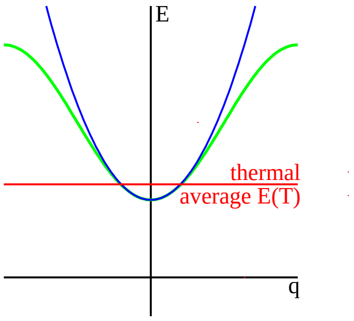


quantum vacancy
microscopic theory

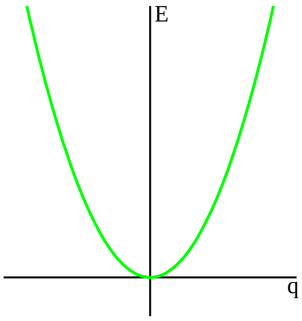
general definition: # vacancies = # lattice sites - # atoms



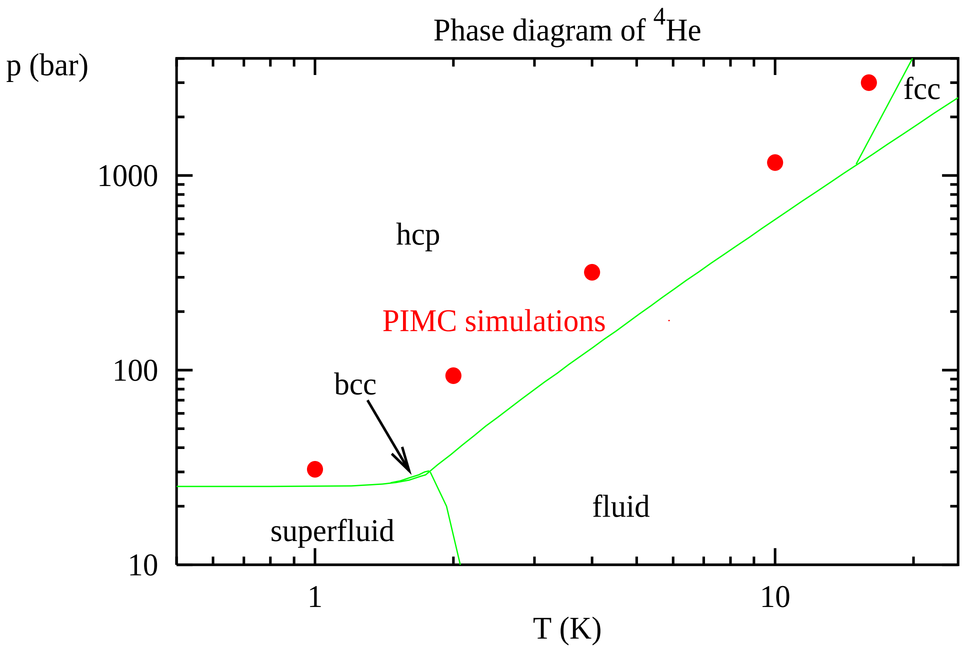
localized vacancy



wide band vacancy



ground state vacancy

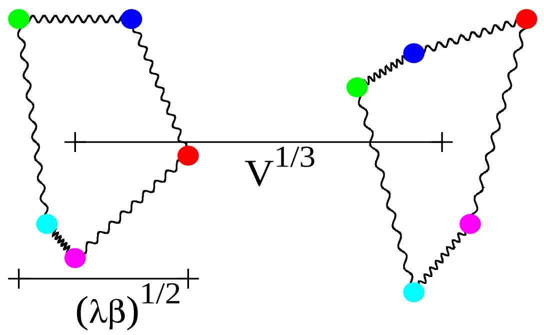


Method

Path Integral Monte Carlo (PIMC)

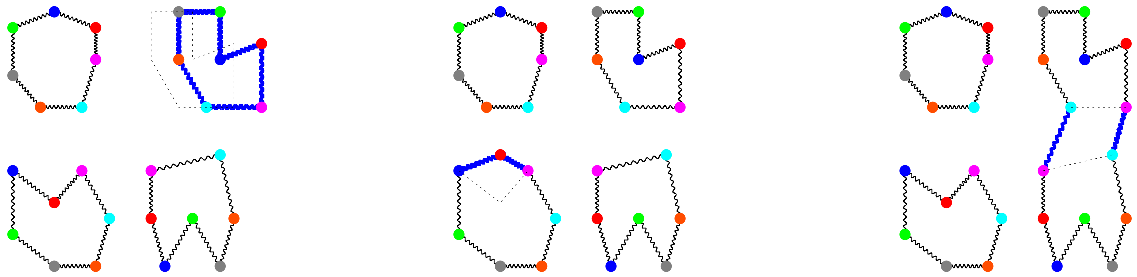
quantum system $\xrightarrow{\text{path integral}}$ classical ensemble of (ring) polymers

for distinguishable particles:



finite number of points: "discretization of imaginary time"

Monte Carlo sampling: moves of polymers



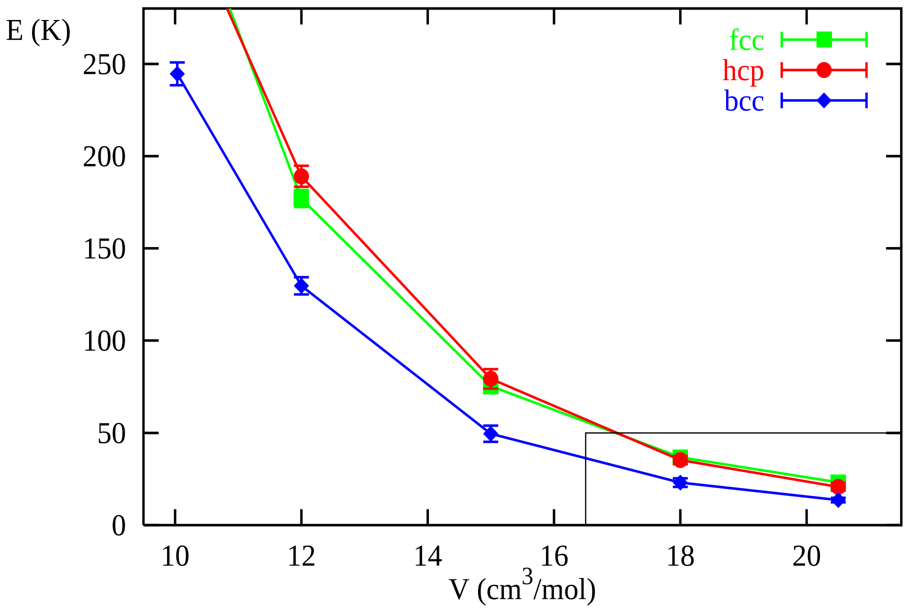
"classical" single-particle exchange

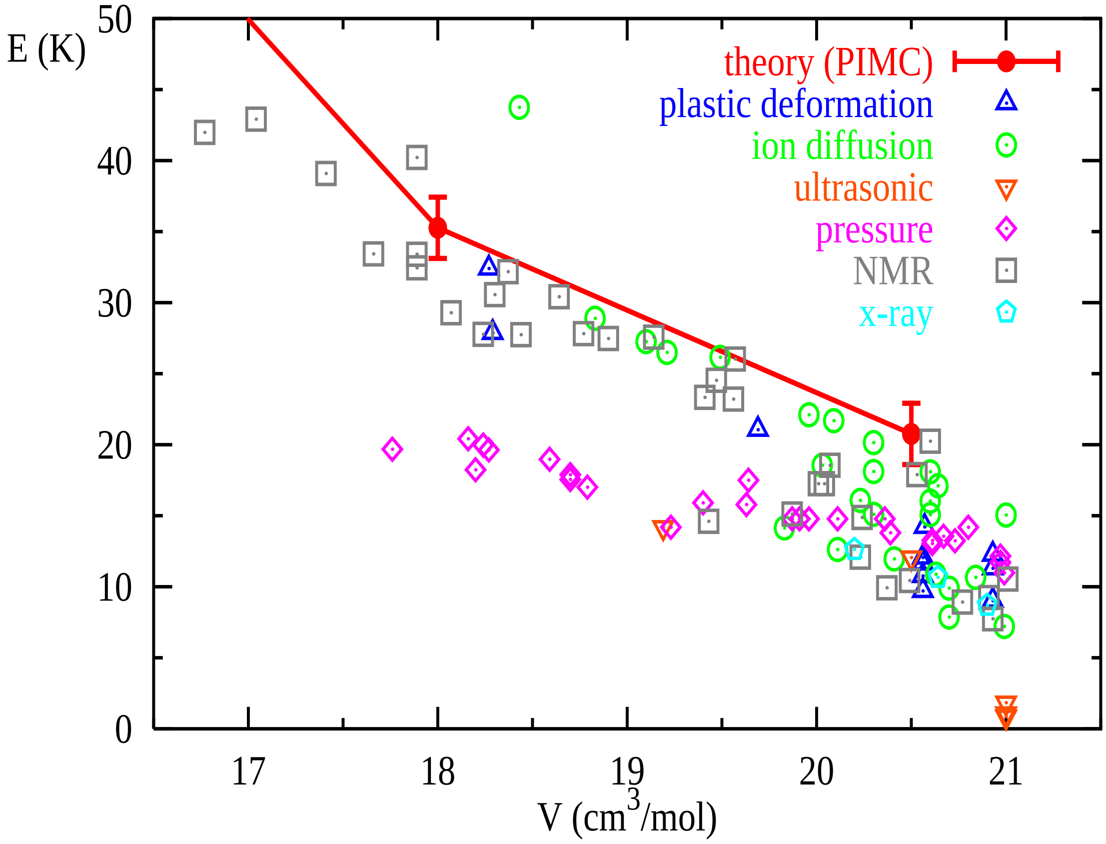
observables:
- energy E
- free energy difference $F_{\text{boson}} - F_{\text{dist}}$
- pair correlation function
- superfluid density

simulated systems:
- 100-200 particles
- periodic boundary conditions

Results

^{4}He: vacancy energy E vs. atomic volume V





Comparison to experiment for hcp ^{4}He

- large vacancy energy of formation
- weak temperature dependence ($\Rightarrow F \approx E$)

No indications for
- ground state vacancies
- supersolid