

Vacancies in solid Helium-4

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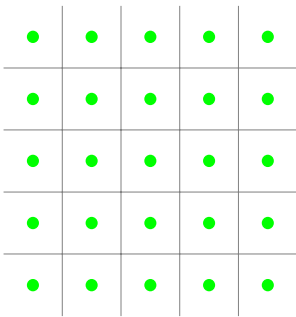
Introduction

Method

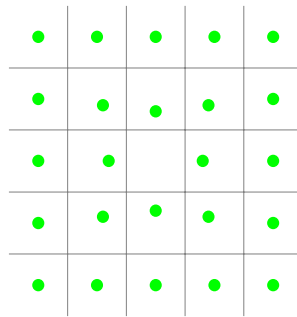
Results

Introduction

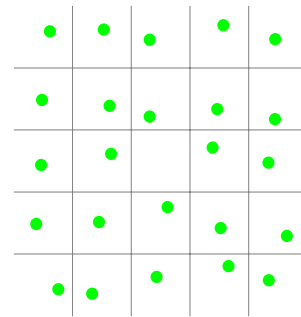
solid He, a **quantum crystal**: Lindemann ratio ≈ 0.3 even at $T \rightarrow 0$



pure class. crystal

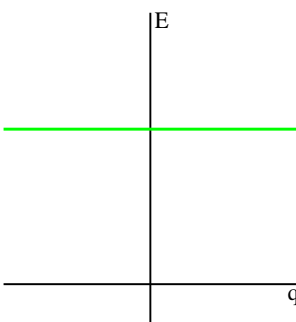


classical vacancy
elasticity theory

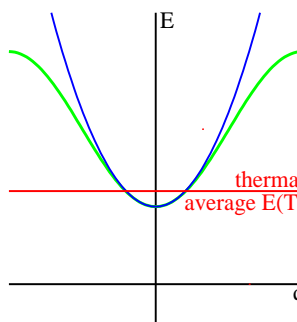


quantum vacancy
microscopic theory

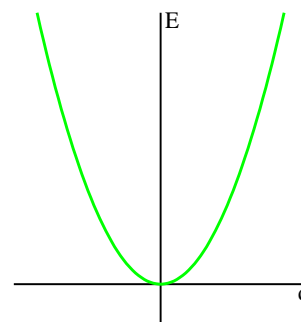
general definition: $\# \text{ vacancies} = \# \text{ lattice sites} - \# \text{ atoms}$



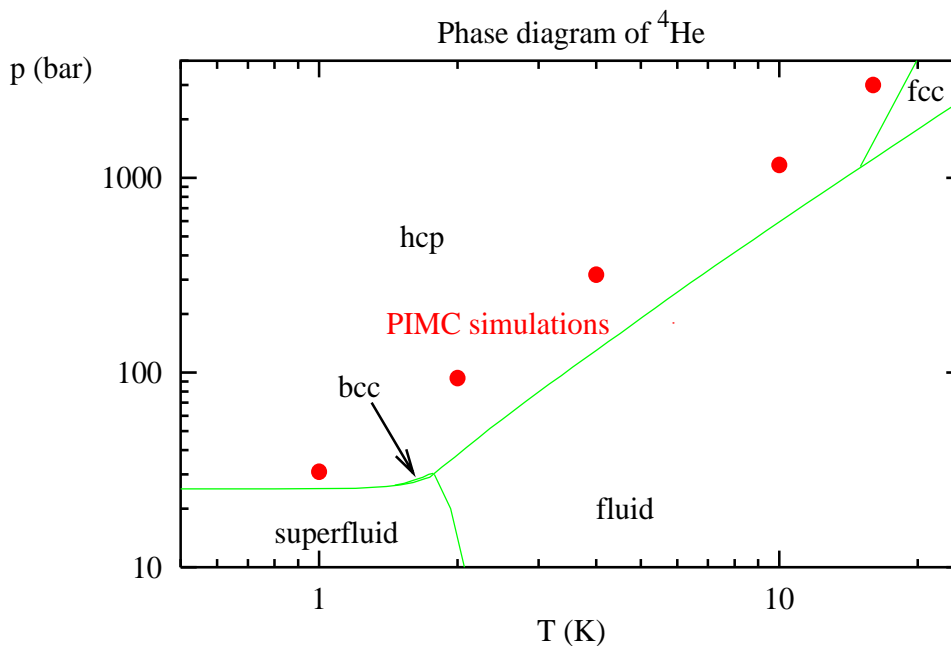
localized vacancy



wide band vacancy



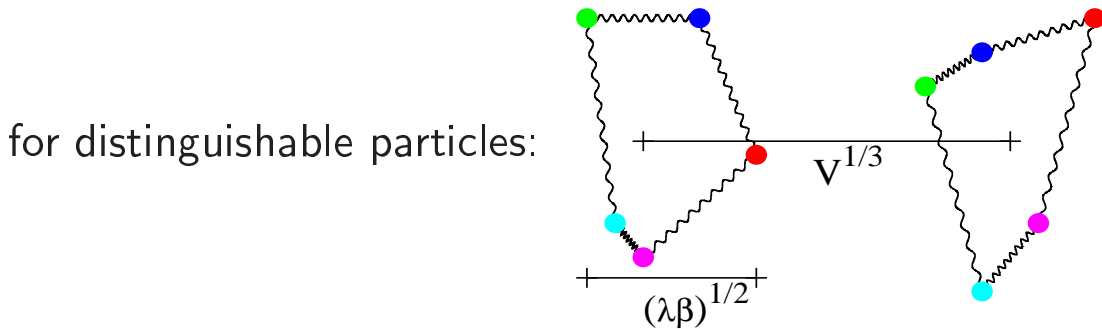
ground state vacancy



Method

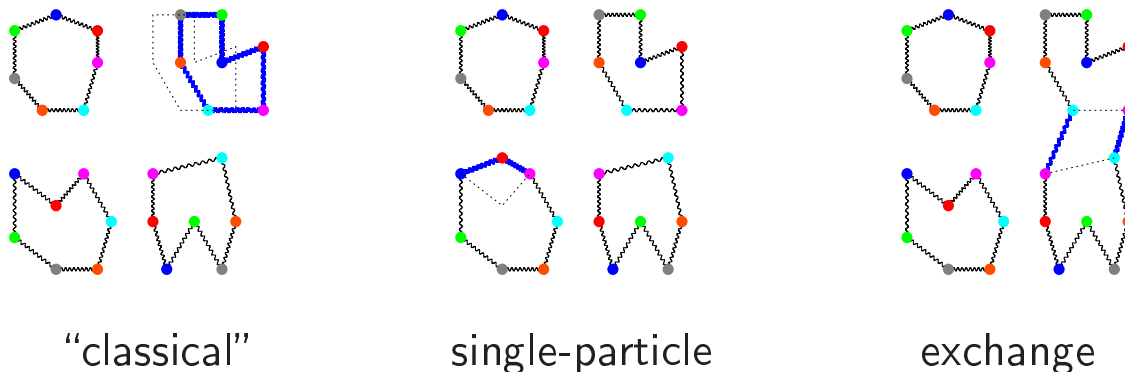
Path Integral Monte Carlo (PIMC)

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



finite number of points: “discretization of imaginary time”

Monte Carlo sampling: moves of polymers

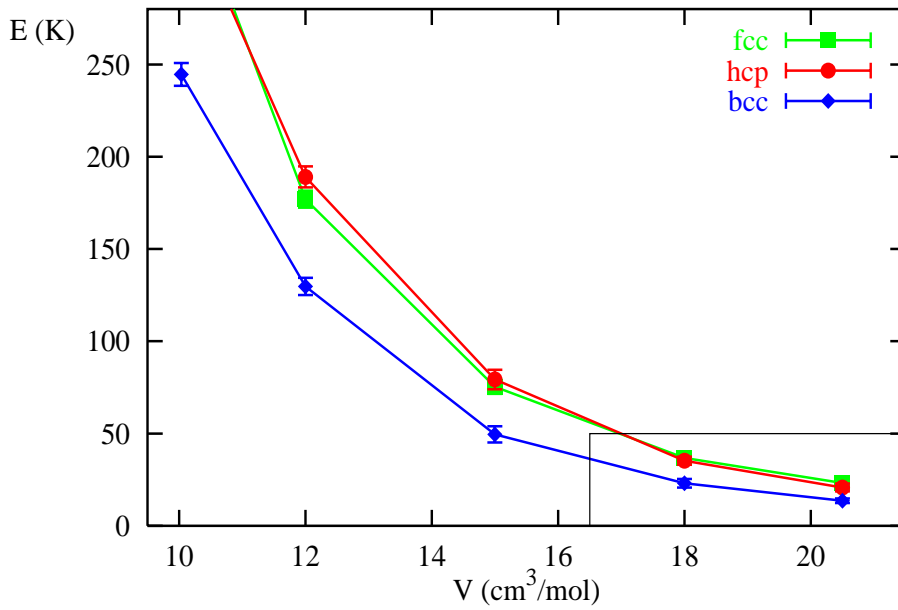


- observables:
- energy E
 - free energy difference $F_{\text{boson}} - F_{\text{dist}}$
 - pair correlation function
 - superfluid density

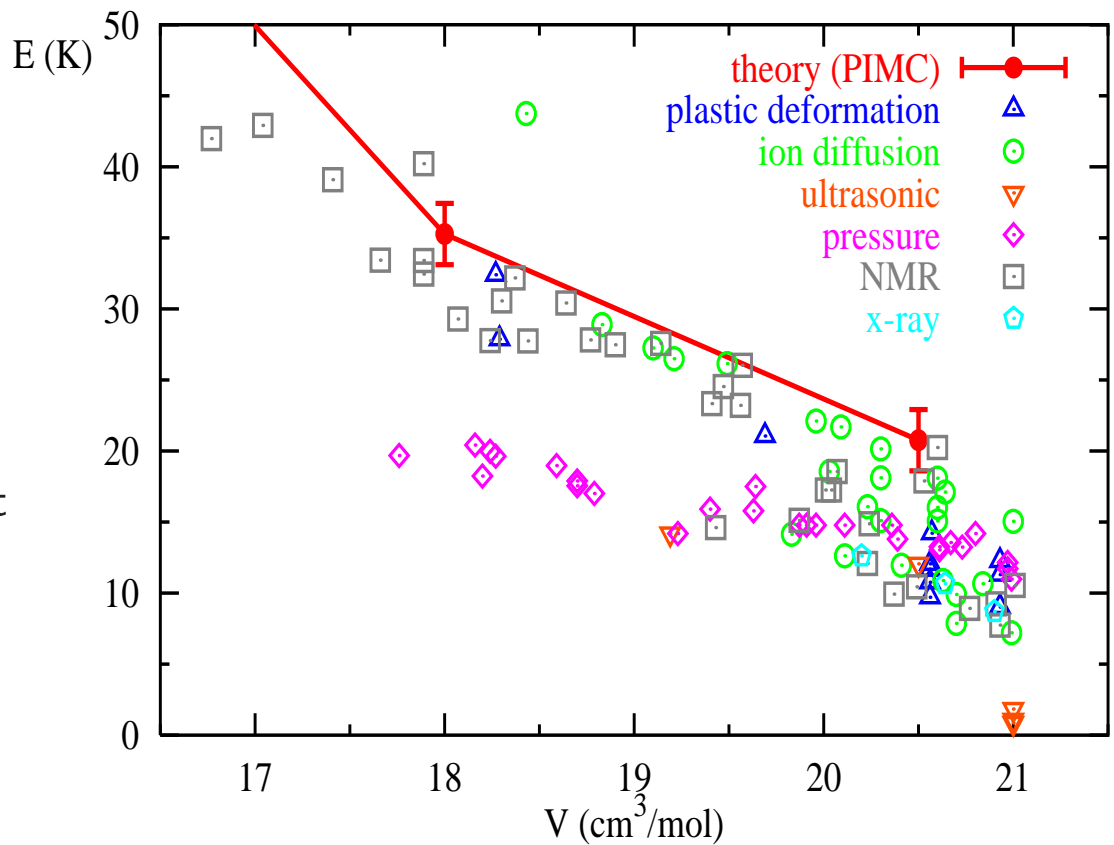
- simulated systems:
- 100-200 particles
 - periodic boundary conditions

Results

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



Comparison to experiment for hcp ^4He



- large vacancy energy of formation
 - weak temperature dependence ($\Rightarrow F \approx E$)
- No indications for
- ground state vacancies
 - supersolid