

Abstract Submitted  
for the MAR08 Meeting of  
The American Physical Society

**Rotational spectrum of small, doped  $^3\text{He}$  clusters** TATJANA SKRBIC, SISSA - DEMOCRITOS (Trieste, Italy), SAVERIO MORONI, DEMOCRITOS - SISSA (Trieste, Italy), STEFANO BARONI, SISSA - DEMOCRITOS (SISSA) — In recent years, symmetry-adapted imaginary-time correlation functions have been extensively used to study the rotational spectrum of doped  $^4\text{He}$  clusters within the frame of the reptation quantum Monte Carlo method. The success of this approach relies on the choice of suitable correlation functions, whose spectral resolution is dominated by few, well separated eigenvalues of the Hamiltonian. Under these conditions, reliable excitation energies can be extracted by inverse Laplace transform. This method has been tailored for bosons, due to the positivity of the ground-state wave-function and to the distinctive scarcity of low-lying states. For sufficiently small systems, however, the states of the discrete spectrum can be calculated in the same manner also with Fermi statistics, using appropriate generalizations of the correlation functions. We present rotational spectra for small  $^3\text{He}$  clusters doped with molecules –such as  $\text{CO}_2$  and  $\text{OCS}$ – whose effective moments of inertia, in  $^4\text{He}$  clusters, feature a non-trivial dependence on the system size, with a pronounced turnaround for less than 10 atoms.

Stefano Baroni  
SISSA - DEMOCRITOS

Date submitted: 29 Nov 2007

Electronic form version 1.4