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Dynamic structure factor of a monoatomic crystal with vacancies

Inelastic scattering experiments are commonly used to measure the spectral functions in solids. The energy transfer between the scattered particles and the atoms in the material leads to resonances in the spectral functions. The frequencies of the resonances give the speeds of the propagating modes (e.g. acoustic waves) while their widths reflect how quickly these waves lose energy, i.e. the damping of the modes, which in turn depend on the transport coefficients such as the heat conductivity or the viscosities. The transport properties of a material can be extracted from inelastic scattering experiments providing that a theory leading to the analytical expressions for the spectral functions exists.

The dynamical structure factor corresponds to the spectral function characterizing the fluctuations of mass densities and is obtained from the hydrodynamic equations ruling the slow modes of the system. In a monoatomic crystal, there are eight modes, fives coming from the fundamental conservation laws of mass, energy and momentum and three Goldstone modes coming from the breaking of the continuous translational symmetry. These eight hydrodynamic modes split into six acoustic modes and two diffusing modes corresponding to the conduction of heat and of vacancies.

In the last few years, a microscopic statistical-mechanical theory leading to the hydrodynamics of crystals has been developed [1, 2]. Based on these results, the dynamic structure factor of a perfect monoatomic crystal has been deduced analytically and computed numerically by means of a molecular dynamics simulation of hard spheres (MDHS), shoving excellent agreement [3]. In a perfect crystal, all the lattice sites are occupied and there are no vacancies. Very recently, an hydrodynamic theory for a crystalline solid with vacancies has been established [4]. The aim of this internship is first to first compute the dynamical structure factor of a monoatomic crystal with vacancies from the hydrodynamic equations deduced in [4] and following the method of [3]. In a second step, the dynamical structure factor is computed numerically with a MDHS simulation to challenge the analytical result.

This internship could be followed by a thesis on first-principles approaches to hydrodynamics in systems with broken symmetries with applications to ordered and amorphous solids, active matter and interfaces.

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[4] J. Mabillard and P. Gaspard, *Vacancy diffusion and the hydrodynamics of crystals*, arXiv :2408.07399 (2024).