

A non-perturbative approach to freezing of superfluid He-4 in density functional theory

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It is known that density functional theory (DFT) fails to describe the freezing of superfluid He-4. In fact, DFT gives too stable solid phase and the superfluid phase does not exist at finite pressures within a second order perturbation. In this paper we try a non-perturbative version of DFT, that is modified weighted density approximation (MWDA) to go beyond second order perturbation for the freezing of superfluid He-4.

By utilizing a recently introduced analytic continuation method (GIFT method), which enables us to extract information on real time dynamics from quantum Monte-Carlo (QMC) imaginary time correlation functions, we obtain the compressibility and the density response function at various densities of superfluid He-4 at zero temperature. Contrary to second order perturbation, by employing these QMC data as DFT input we find a 'too stable superfluid phase', preventing freezing around the experimentally observed freezing pressure. We find the same pathological behavior by using another model energy functional of superfluid He-4 (Orsay-Trento model). We conclude that the straightforward MWDA calculation gives poor result when liquid-gas transition is present.