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Is there a stable commensurate solid phase in the second ⁴He layer on graphite? - path integral Monte Carlo study JEONGHWAN AHN, HOONKYUNG LEE, YONGKYUNG KWON, KonKuk Univ — Existence of a stable commensurate structure in the second ⁴He layer on graphite has been a subject of intensive experimental and theoretical studies because of its implication in the possible realization of two-dimensional supersolidity. Earlier path-integral Monte Carlo (PIMC) calculations of Pierce and Manousakis predicted a stable $C_{4/7}$ commensurate structure above the first-layer ⁴He atoms fixed at triangular lattice sites [1], but Corboz et al. later showed that no commensurate phase was stable when quantum dynamics of the first-layer ⁴He atoms was incorporated in the PIMC calculations [2]. On the other hand, recent heat capacity measurements of Nakamura et al. provided a strong evidence for a commensurate solid in the second ⁴He layer over an extended density range [3]. Motivated by this, we have performed new PIMC calculations for the second helium layer on graphite. Unlike previous PIMC calculations where a laterally-averaged one-dimensional substrate potential was used, we here employ an anisotropic ⁴He-graphite potential described by a sum of the ⁴He-C pair potentials. With this fully-corrugated substrate potential we make more accurate description of quantum dynamics of the first-layer ⁴He atoms and analyze its effects on the phase diagram of the second layer.

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