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Approximate Wannier functions using discrete variable representation for asymmetric optical lattices SAURABH PAUL, Joint Center for Quantum Information and Computer Science, Joint Quantum Institute and University of Maryland, College Park, EITE TIESINGA, Joint Quantum Institute, National Institute of Standards and Technology and University of Maryland, Gaithersburg, Maryland — We propose a numerical method using discrete variable representation (DVR) for constructing real-valued approximate Wannier functions localized in a unit cell for both symmetric and asymmetric periodic potentials in the context of optical lattices. For a symmetric lattice with inversion symmetry, we construct Wannier functions for the lowest two bands as eigen states of the position operators. To ensure that the Wannier functions are real valued, we numerically obtain the band structure and real-valued eigen states using a uniform Fourier grid DVR. We then show by a comparison of tunneling energies, that the Wannier functions are accurate to better than ten significant digits when using double-precision arithmetic. The calculations are performed for a periodic double-well optical lattice having double-wells per unit cell with tunable asymmetry along the x axis and a single sinusoidal potential along the perpendicular directions. Localized functions at the two potential minima within each unit cell are similarly constructed, but using a superposition of solutions from the two lowest bands. We finally use these localized basis functions to determine the two-body interaction energies in the Bose-Hubbbard (BH) model, and show the dependence of the BH model on lattice asymmetry.

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