CONVERGENCE OF THE PLANEWAVE APPROXIMATIONS FOR QUANTUM INCOMMENSURATE SYSTEMS

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ABSTRACT

We study the numerical approximations of the spectrum distribution of Schrodinger operators for incommensurate systems. We provide rigorous analysis to characterize the quantitative of interests, i.e. the density of states, and develop numerical methods to approximate them based on planewave discretizations. In particular, we (i) justify the thermodynamic limit of the density of states in the real space formulation; (ii) propose a planewave approximation for the problem with some novel energy cutoffs specified for incommensurate systems, and provide a convergence analysis and error estimates with respect to the cutoffs; (iii) design an efficient algorithm to evaluate the density of states by sampling the reciprocal space. We present numerical simulations of some typical incommensurate systems to support the reliability and efficiency of our numerical algorithms.

References

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