Localization in the Incommensurate Systems: A Plane Wave Study via Effective Potentials

Ting Wang^{1,*}, Yuzhi Zhou^{3,4} and Aihui Zhou^{1,2}

 ¹ LSEC, Institute of Computational Mathematics and Scientific/Engineering Computing, Academy of Mathematics and Systems Science, Chinese Academy of Sciences, Beijing 100190, P.R. China.
² School of Mathematical Sciences, University of Chinese Academy of Sciences,

- School of Mathematical Sciences, University of Chinese Academy of Sciences, Beijing 100049, P.R. China. ³ CAEP Sciences Country for High Parlimentary Neuropical Sciences Pailing 100

³ CAEP Software Center for High Performance Numerical Simulation, Beijing 100088, P.R. China.

⁴ *Institute of Applied Physics and Computational Mathematics, Beijing 100094, P.R. China.*

Received 1 August 2023; Accepted (in revised version) 8 March 2024

Abstract. In this paper, we apply the effective potentials in the localization landscape theory (Filoche et al., 2012, Arnold et al., 2016) to study the spectral properties of the incommensurate systems. We uniquely develop a plane wave framework for the effective potentials of the incommensurate systems. And utilizing the effective potentials represented by the plane wave, the location of the electron density can be inferred. Moreover, the spectral distribution can be obtained from the effective potential version of Weyl's law. We perform some numerical experiments on some typical incommensurate systems, showing that the effective potential provides an alternative tool for investigating the localization and spectral properties of the incommensurate systems, without solving the eigenvalue problem explicitly.

AMS subject classifications: 35J10, 35P15, 35Q40

Key words: Incommensurate systems, localization, effective potential, plane wave method.

1 Introduction

Localization in the non-periodic media has garnered interest due to its significant effects on many physical properties of condensed matter [2,21]. Incommensurate systems are one typical class of the non-periodic media, and the localization of particle/waves

http://www.global-sci.com/cicp

©2024 Global-Science Press

^{*}Corresponding author. *Email addresses:* ting_wang@lsec.cc.ac.cn (T. Wang), zhou_yuzhi@iapcm.ac.cn (Y. Zhou), azhou@lsec.cc.ac.cn (A. Zhou)

in them has recently been widely observed in modern optical, mechanical, and lowdimensional material systems [12, 24, 25, 27], due to the advances in experimental technologies nowadays. In [12, 24], the localization and its interplay with quantum manybody effects of the cold atomic gases were studied by adjusting incommensurate potentials through lasers, as well as by tuning repulsive interactions between atoms. On the other hand, the localization of certain electrons in the twisted multilayer two-dimensional materials could lead to drastic changes in the electronic, transport and magnetic properties [21], such as the quantum Hall effect [11], the enhanced carrier mobility [16], and the unconventional superconductivity [7]. Despite the fruitful results listed above, the mechanism of localization and its connection to these emergent properties have not been fully understood yet. A better understanding of this subject would definitely be helpful for the studies of the relevant unconventional phenomena and their practical application in the future.

Theoretical interests in the localization mechanism of disordered or incommensurate systems have been raised in the physics and mathematics communities recently [5, 6, 18, 20], and references therein. Here we briefly review the literature that is directly relevant to this paper. In [8], the localized-extended transitions in the one-dimensional incommensurate systems were studied through a scattering picture under the plane wave discretization. Alternatively, a new mathematical technique was proposed to approximate the eigenstates as proposed in [13]. The landscape concept was introduced for the first time, whose authors provided a novel sight to predict the location of the low energy eigenfunctions by the relevant Dirichlet problem. In [19,26], some mathematics consequences were presented. Further, in [4,6], effective potential defined as the reciprocal of landscape function was proposed. It contains abundant information on localized eigenpairs, providing a wealth of insights into their localization properties with the advantage of reduced computational cost. Recently, considerable applications of this theory have been presented [1,3,9,14,22,23]. In [14,22], the localization properties in systems of ultracold atoms gases and disordered semiconductor alloys were addressed by these prediction methods. In [3,23], the localization was studied for tight-binding Hamiltonians in two-dimensional materials employing the localization landscape theory. Yet, to our best knowledge, this framework has not been applied to the incommensurate systems.

On the other hand, spectral properties play a central role in determining the physical behaviors of incommensurate systems. Through the evaluation of the spectral distribution, we can in principle derive the system's conductivity, specific heat, magnetism, and superconductivity, among other relevant properties. The density of states is a powerful tool in this respect, as it allows us to compute the spectral distribution by quantifying the number of accessible energy states per unit of energy in a more or less mean-field context, and as an intermediate quantity to further calculate other physical properties. The integrated density of states, essentially an accumulation of the density of states, offers a broader perspective by accounting for the number of states with energies less than a certain threshold. A crucial aspect of this process is the application of Weyl's law. This fundamental mathematical principle offers an asymptotic estimation of the integrated