

# H-wave: A quantum lattice solver using Wavenumber-Space Mean Field Approximation and Random Phase Approximation

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In a project for Advancement of Software Usability in Materials Science (PASUMS) [1] in FY2022, **H-wave** [2] has been developed to perform unrestricted Hartree-Fock (UHF) approximation in wavenumber space and random phase approximation (RPA) for itinerant electron systems. UHF and RPA correspond to simple approximations that deal with fluctuations up to first order and enable analyses of electron correlation effects in materials at a low computational cost. The input files describing the one-body and two-body interactions are based on the `Wannier90` [3] format. This allows smooth connection for the software packages that derive the effective models from first principles calculations, such as `RESPACK` [4], to the analyses of the effective model with **H-wave**.

**H-wave** is implemented in Python3 and is available from PyPI package repository. The source archive can be obtained from the GitHub site<sup>1</sup>. To use **H-wave**, we must prepare an input parameter file written in the TOML format which specifies calculation conditions and file names of the definition files for the geometry and Hamiltonian. The Hamiltonian is defined through the input files of the transfer integrals and the interactions denoted by `CoulombIntra`, `CoulombInter`, `Hund`, `Ising`, `Exchange`, and `PairLift`. In UHF mode, a `PairHop` term can also be specified. To learn

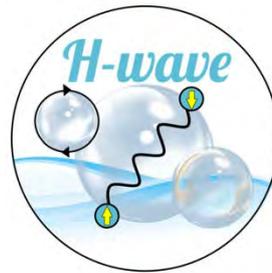


Figure 1: A logo of H-wave designed by T. Kawamura.

details of the input files, the readers may refer to the manual [2]. Once these input files are prepared, the calculation will be performed by typing the following command:

```
$ hwave input.toml
```

where `hwave` is the executable file of **H-wave** and `input.toml` is the name of the input file. After the calculations are completed, the following physical quantities are obtained:

in UHF mode: energy, eigen values and vectors, and one-body Green's functions.

in RPA mode: irreducible susceptibilities

A brief tutorial is included in the manual, and several application examples have been uploaded to the ISSP data repository [5]. For the UHF calculations, we provide examples such as the band and density of state plots, and the finite temperature calculations. In addition, a more applied example analysis of the

<sup>1</sup><https://github.com/issp-center-dev/h-wave>

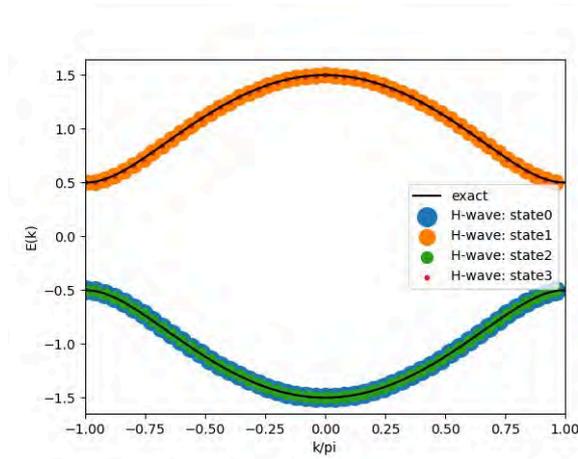


Figure 2: The band dispersion of SSH model.

Su–Schrieffer–Heeger (SSH) model [6] which is one of the well-known platforms for the emergence of the topological insulator is also provided. In this sample, the scripts to obtain the band dispersion (shown in Fig.2) and the Zak phase [7] of the lowest band, which corresponds to the topological number, are also provided. For RPA calculations, we provide examples for calculating charge and spin susceptibility that reproduce the results of Refs. [8, 9]. Figure 3 shows the static charge and spin susceptibilities ( $\chi_s(q, 0)$  and  $\chi_c(q, 0)$ ) for one-orbit two-dimensional extended Hubbard model on the square lattice at  $(U, V) = (3.7, 0)$  and  $(0, 0.8)$  examined in Ref. [8].

In this report, we introduced the features and examples of H-wave developed through PASUMS. In the future, we would like to develop functions such as follows; (a) providing calculation scripts for quantities corresponding to dynamic susceptibility measured in experiments, (b) evaluating the instability of superconducting transition by solving the linear Eliashberg equation considering charge and spin fluctuations as pairing interactions, and (c) adding more samples such as the calculation with spin-orbit interactions. We believe that H-wave is useful for a wide range of materials scientists and can contribute to the promotion of the computational materials design.

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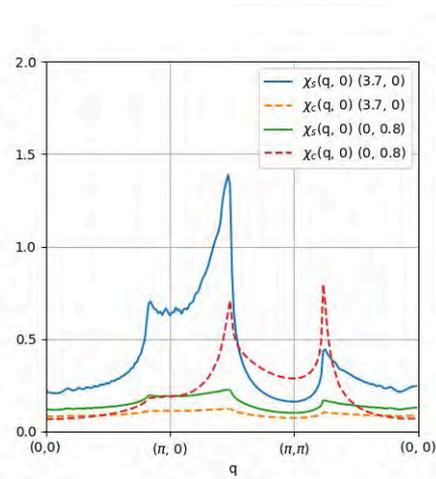


Figure 3: The charge and spin susceptibilities at  $(U, V) = (3.7, 0)$  and  $(0, 0.8)$  in Ref. [8].

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