Generating Hubbard Model Solutions from Anderson Impurity Model Solutions

Abhirup Mukherjee, Dr. Siddhartha Lal

August 1, 2021

1 Introduction

This is an attempt to obtain solutions of the Hubbard model (groundstate wavefunction and ground state energy) using the solutions of the simpler single-impurity Anderson model (SIAM) (the models will be defined later). Broadly speaking, the method involves first solving the SIAM using a unitary renormalisation group approach, to get the ground state wavefunction and energy eigenvalue, and then combining these wavefunctions in a symmetrized fashion to get the wavefunction for the Hubbard model lattice. It is quite similar to dynamical mean-field theory (DMFT) in essence, but differs in practice. The similar part is the involvement of an impurity-solver. The difference, however, lies in the following points:

- While DMFT primarily works with Green's functions and self-energies, this method involves Hamiltonians and wavefunctions.

- The impurity-solver in DMFT provides an impurity Green's function (which is then equated with the local Green's function of the bath), while the impurity-solver in this method actually provides a wavefunction.

- The final step of DMFT is the self-consistency equation, where the impurity and bath-local quantities are set equal. This ensures all sites, along with the impurity site, have the same self-energy, something which is required on grounds of translational invariance. The present method, however, brings about the translational invariance in a different way. It symmetrizes the wavefunctions and Hamiltonians itself, such that all quantites then derived from the Hamiltonian or wavefunction are then guaranteed to have the symmetry.

The meaning of each of these statements will become clearer when we describe the method in more detail.