Hubbard model Hamiltonian

The Hubbard Hamiltonian

The Hamiltonian is a two-electron site-interaction model, with one orbital per site. It is equivalent to the Hückel model, with the addition of an on-site repulsion that tends to prevent multiple electrons from occupying the same site ($U > 0$) or models effective attractive interactions between electrons as in superconductivity ($U < 0$).

$$\hat{H}_{\text{Hubbard}} = \sum_{pq} h_{pq} a_p^\dagger a_q + \sum_p U_p \hat{n}_{p\alpha} \hat{n}_{p\beta}$$

Traditionally there are two parameters: - an α_{pp} parameter for the diagonal terms h_{pp}, representing the energy associated with an electron on the site p. This is usually zero in Hubbard models. - a $t_{pq} = t_{qp}$ parameter for the off-diagonal terms $h_{p \neq q}$, this is the resonance/hopping/bond term between sites p and q. - a U_p parameter that is the onsite interaction (generally repulsion).

> Note: Traditionally Hubbard models work by assuming that orbitals on different sites do not overlap. Hubbard Hamiltonians are always restricted but we do support the imposition of an external magnetic field.

Input Formats

API

- Connectivity can be provided in the usual way, as a lattice, an adjacency matrix, a distance matrix, or explicit connectivity specification.
- Parameters can be specified as constants (all sites equal) or as dictionaries.
- Proposed Calling Sequence:

```
modelh.Hubbard(connectivity, alpha=0.0, t=1.0, U=1.0, atom_types=None, atom_dictionary=

"""Compute the 1- and 2-electron integrals associated with the Hubbard Hamiltonian.

Parameters
----------
connectivity
    an object specifying molecular connectivity
alpha
    If alpha is a float, it specifies the site energy if all sites are equivalent.
t
```

```
    Specifies the resonance/hopping term if all bonds are equivalent.
U
    Specifies the on-site interaction; usually repulsive.
atom_types
    A list of dimension equal to the number of sites specifying the atom type of each s
    If a list of atom types is specified, the values of alpha and beta are ignored.
atom_dictionary
    Contains information about alpha and U values for each atom type.
bond_dictionary
    Contains information about beta values for each bond type.
Bz
    External magnetic field in atomic units.

Returns
-------
integrals_1el
    One-electron integrals.
integrals_2el
    Two-electron integrals.
```