Philosophies of Diagonalization

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We discuss the formalisms and models and functionalities of the functions developed for Qutip for Google Summer of Code 2019.

I. INTRODUCTION

From elementary theory of crystals, a crystal can be completely specified with the knowledge of a basis and a set of lattice translation vectors. The repetition of the basis with the aid of lattice vectors produces the entire crystal. In the QuTip functions developed individual bases can be produced with instances of the object 'Qbasis'. Its inputs are the onsite energies, intra-hoppings, positions of the orbitals(or a hardcore fermion or boson) in the basis.

II. CLASS QBASIS(QOBJ):ORBITALS AND INRA HOPPING MATRIX ELEMENTS

Qbasis is a subclass ('child-class') of qutip.Qobj which can completely specify a lattice basis. For the orbitals $orb_0, orb_1, ..., orb_n$ in a basis and their ${}^nC_2$ intra hopping terms $t^i_{0,1}, t^i_{0,2}, ...$, the Hamiltonian in real space assuming the basis makes up the entire crystal (i.e. no other unit cells existing nor inter-coupling between them),H_{basis} would be

$$H_{basis} = \begin{bmatrix} a_0^\dagger & a_1^\dagger & ..a_n^\dagger \end{bmatrix} \begin{bmatrix} \epsilon_0 & t^i_{0,1} & t^i_{0,2} & .. & t^i_{0,n} \\ t^i_{1,0} & \epsilon_1 & t^i_{1,2} & .. & t^i_{1,n} \\ t^i_{2,0} & t^i_{2,1} & \epsilon_2 & .. & t^i_{2,n} \\ .... & .... & .... & .. & \vdots \\ t^i_{n,0} & t^i_{n,1} & t^i_{n,1} & .. & \epsilon_n \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix}$$

where $\epsilon_0, \epsilon_1, ...\epsilon_n$ are respectively the onsite energies of $orb_0, orb_1, ..., orb_n$.

In the code, the Hamiltonian in Eq. 1 is formed with the call $Qbasis.basis\_Hamiltonian()$.

$$\begin{bmatrix} \epsilon_0 & t^i_{0,1} & t^i_{0,2} & .. & t^i_{0,n} \\ t^i_{1,0} & \epsilon_1 & t^i_{1,2} & .. & t^i_{1,n} \\ t^i_{2,0} & t^i_{2,1} & \epsilon_2 & .. & t^i_{2,n} \\ .... & .... & .... & .. & \vdots \\ t^i_{n,0} & t^i_{n,1} & t^i_{n,1} & .. & \epsilon_n \end{bmatrix} \tag{1}$$

III. HONEYCOMB LATTICE: BASIS VECTORS AND RECIPROCAL LATTICE VECTORS

Basis vectors for the honeycomb lattice:

$$\mathbf{a_1} = (\sqrt{\mathbf{3}}\mathbf{a}/\mathbf{2}, \mathbf{a}/\mathbf{2})$$
$$\mathbf{a_2} = (\sqrt{\mathbf{3}}\mathbf{a}/\mathbf{2}, -\mathbf{a}/\mathbf{2})$$

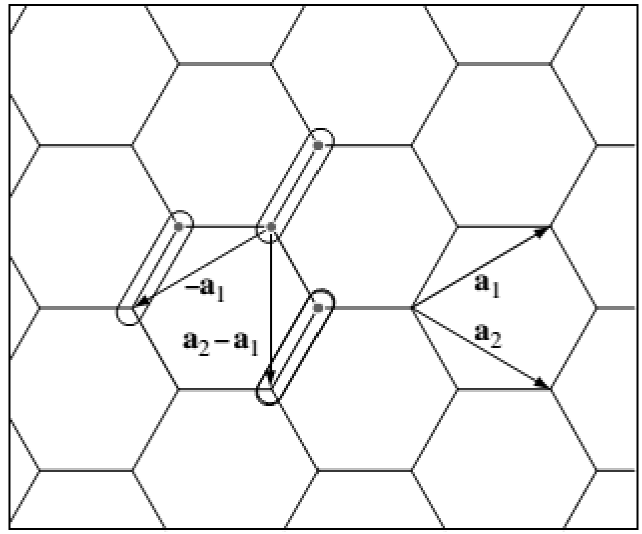

FIG. 1. A honeycomb crystal(Graphene).

Reciprocal lattice vectors:

$$\mathbf{G_1} = (\mathbf{2}\pi/\sqrt{\mathbf{3}}\mathbf{a}, \mathbf{2}\pi/\mathbf{a})$$
$$\mathbf{G_2} = (\mathbf{2}\pi/\sqrt{\mathbf{3}}\mathbf{a}, -\mathbf{2}\pi/\mathbf{a})$$

IV. FOURIER TRANSFORM, BASIS

$$|\psi_{\mathbf{Rn}}\rangle \equiv \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{k}.\mathbf{R}} |\psi_{\mathbf{kn}}$$

$$|\psi_{\mathbf{kn}}\rangle \equiv \frac{1}{\sqrt{N}} \sum_{\mathbf{R}} e^{i\mathbf{k}.\mathbf{R}} |\psi_{\mathbf{Rn}}$$

$$a^\dagger_\sigma(\mathbf{r}) = \sum_{\mathbf{i}} \psi^*_{\mathbf{R_i}} \mathbf{a}^\dagger_{\mathbf{i}\sigma} = \sum_{\mathbf{R}} \psi^*_{\mathbf{R}} \mathbf{a}^\dagger_{\mathbf{R}\sigma} \tag{2}$$

$$a^\dagger_{\mathbf{k}\sigma} = \frac{1}{\sqrt{N}} \sum_i e^{i\mathbf{k}.\mathbf{R_i}} a^\dagger_{i\sigma} \tag{3}$$

$$a^\dagger_{i\sigma} = \frac{1}{\sqrt{N}} \sum_i e^{-i\mathbf{k}.\mathbf{R_i}} a^\dagger_{\mathbf{k}\sigma} \tag{4}$$

Graphene:

$$H = \sum_{\mathbf{k}\sigma} \begin{bmatrix} a^\dagger_{1\mathbf{k}\sigma} & a^\dagger_{2\mathbf{k}\sigma} \end{bmatrix} \begin{bmatrix} 0 & -tf(\mathbf{k}) \\ -tf^*(\mathbf{k}) & 0 \end{bmatrix} \begin{bmatrix} a_{1\mathbf{k}\sigma} \\ a_{2\mathbf{k}\sigma} \end{bmatrix} \tag{5}$$

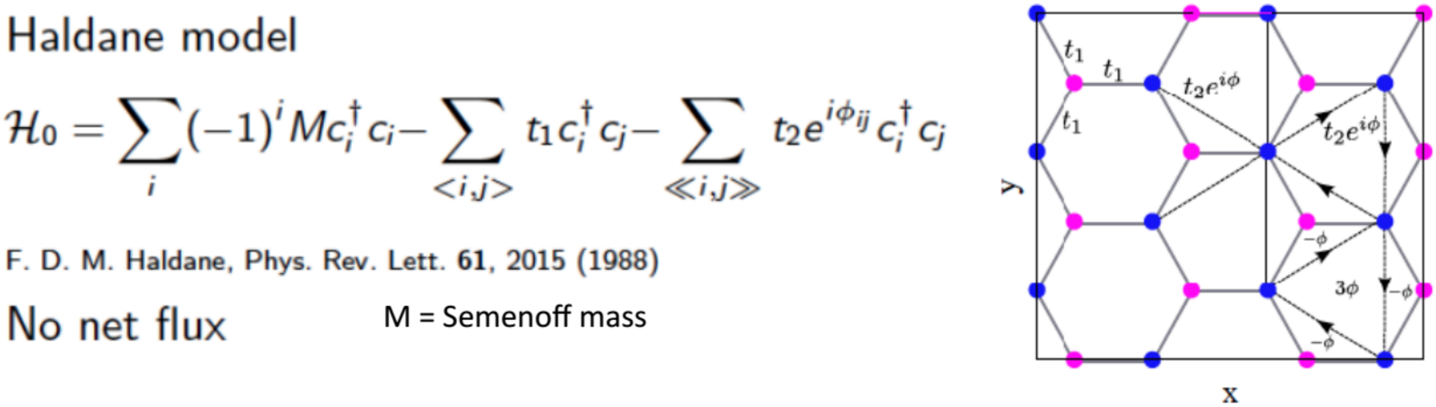

FIG. 2. Haldene Chern Insulator (Graphene).

where $f(\mathbf{k}) = \sum_{\mathbf{NN}} \mathbf{e^{ik.(R_j-R_i)}} = \mathbf{1} + \mathbf{e^{-ik_1a}} + \mathbf{e^{-i(k_2-k_1)a}}$

Haldene model:

$$H = \sum_{\mathbf{k}\sigma} \begin{bmatrix} a^\dagger_{1\mathbf{k}\sigma} & a^\dagger_{2\mathbf{k}\sigma} \end{bmatrix} \begin{bmatrix} -t^p g(\mathbf{k}) & -tf(\mathbf{k}) \\ -tf^*(\mathbf{k}) & -t^p g(\mathbf{k}) \end{bmatrix} \begin{bmatrix} a_{1\mathbf{k}\sigma} \\ a_{2\mathbf{k}\sigma} \end{bmatrix} \tag{6}$$

where $g(\mathbf{k}) = \sum_{\mathbf{NNN}} \mathbf{e^{ik.(R_j-R_i)}}$