QUANTUM PLAYBOOK TECH NOTE

URL

Quantum Dot Systems

Single–Orbital Quantum Dot (QD) Double Quantum Dot

Here, we consider a system of quantum dots that are described by the *Hubbard model*.

Q	Particle number operator
Hop	Hopping operator
FermionBasis	Fermion basis with certain features

Some useful functions when studying quantum dot systems.

First, make sure the package is loaded.

In[112]:=
```
<< Q3`
```

Choose a symbol to denote the dot operators.

In[113]:=
```
Let[Fermion, d]
```

It is also convenient to explicitly set the energy parameters to be real.

In[114]:=
```
Let[Real, ϵ, t, U]
```

Single-Orbital Quantum Dot (QD)

Single-particle (quadratic or non-interacting) part

Let us start from the single-particle (quadratic) part of the Hamiltonian. There are several equivalent ways:

The most obvious method is using the fermion operators:

In[115]:=
```
Dagger[d[Up]] ** d[Up]
```

Out[115]=
$$d_{\uparrow}^{\dagger} d_{\uparrow}$$

The above has a short cut Q[...] as following:

In[6]:=
```
Q[d[Up]]
```

Out[6]=
$$d_{\uparrow}^{\dagger} d_{\uparrow}$$

You need to sum over all spin (up and down):

```
In[7]:= Sum[Q[d[s]], {s, {Up, Down}}]
```

$$\text{Out[7]}= d_{\downarrow}^{\dagger} d_{\downarrow} + d_{\uparrow}^{\dagger} d_{\uparrow}$$

The above can be even simpler as the following two (equivalent) examples:

```
In[8]:= Q[d[{Up, Down}]]
        Q[d[All]]
```

$$\text{Out[8]}= d_{\downarrow}^{\dagger} d_{\downarrow} + d_{\uparrow}^{\dagger} d_{\uparrow}$$

$$\text{Out[9]}= d_{\downarrow}^{\dagger} d_{\downarrow} + d_{\uparrow}^{\dagger} d_{\uparrow}$$

So, the non-interacting part of the QD Hamiltonian is given by

```
In[116]:= H0 = ϵ * Q[d[All]]
```

$$\text{Out[116]}= \epsilon \left(d_{\downarrow}^{\dagger} d_{\downarrow} + d_{\uparrow}^{\dagger} d_{\uparrow} \right)$$

On-site interaction

Now, let us turn to the interaction (quartic) part:

```
In[117]:= Hint = U Q[d[Up]] ** Q[d[Down]]
```

$$\text{Out[117]}= U\, d_{\downarrow}^{\dagger} d_{\uparrow}^{\dagger} d_{\uparrow} d_{\downarrow}$$

Many-body eigenstates

Finally, the Hamiltonian for the quantum dot is given by

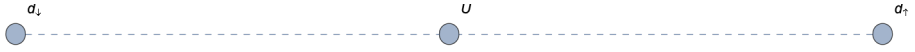
```
In[118]:= HH = H0 + Hint
```

$$\text{Out[118]}= \epsilon \left(d_{\downarrow}^{\dagger} d_{\downarrow} + d_{\uparrow}^{\dagger} d_{\uparrow} \right) + U\, d_{\downarrow}^{\dagger} d_{\uparrow}^{\dagger} d_{\uparrow} d_{\downarrow}$$

The above Hamiltonian may be described in graph as follows. Here, the vertex U with dashed lines denotes the interaction.

```
In[81]:= GraphForm[HH]
```

Out[81]=



We need to construct a basis for the fermionic Fock space. Recall that the Hamiltonian conserves both the charge (Q) and spin (S). Therefore, it is a good idea to organize the basis accordingly. Here, note that the sector $\{Q = 1,\ S = 1/2\}$ has only one state $\left|1_{d_{\uparrow}}\right\rangle$ but not $\left|1_{d_{\downarrow}}\right\rangle$. This is to avoid redundancy because both gives the same matrix elements.

```
In[34]:= bs = FermionBasis[d]
```

$$\text{Out[34]}= \left\langle \left| \{0, 0\} \to \left\{ \left| \_ \right\rangle \right\},\ \left\{1, \frac{1}{2}\right\} \to \left\{ \left| 1_{d_{\uparrow}} \right\rangle \right\},\ \{2, 0\} \to \left\{ - \left| 1_{d_{\downarrow}} 1_{d_{\uparrow}} \right\rangle \right\} \right| \right\rangle$$

Naturally, the Hamiltonian is block diagonal in this basis.

In[35]:=
```
big = MatrixIn[HH, bs, bs];
big = Values@KeyGroupBy[big, First, Values];
MatrixForm@Map[MatrixForm, big, {2}]
```

Out[37]//MatrixForm=

$$\begin{pmatrix} (0) & (0) & (0) \\ (0) & (\epsilon) & (0) \\ (0) & (0) & (U+2\epsilon) \end{pmatrix}$$

It is thus efficient to work on each diagonal block separately.

In[38]:=
```
mat = MatrixIn[HH, bs];
MatrixForm /@ mat
```

Out[39]=

$$\left\langle \left| \{0, 0\} \to (0), \left\{1, \frac{1}{2}\right\} \to (\epsilon), \{2, 0\} \to (U+2\epsilon) \right| \right\rangle$$

Double Quantum Dot

Let us now consider a double quantum dot (DQD). From the above example of single-orbital quantum dot, you now see that the following two statements are equivalent:

In[89]:=
```
Dagger[d[1, Up]] ** d[1, Up]
Q[d[1, Up]]
```

Out[89]=

$$d^{\dagger}_{1,\uparrow} d_{1,\uparrow}$$

Out[90]=

$$d^{\dagger}_{1,\uparrow} d_{1,\uparrow}$$

You should also be familiar with the following equivalent statements:

In[91]:=
```
Sum[Q[d[j, Up]], {j, 1, 2}]
Q[d[{1, 2}, Up]]
```

Out[91]=

$$d^{\dagger}_{1,\uparrow} d_{1,\uparrow} + d^{\dagger}_{2,\uparrow} d_{2,\uparrow}$$

Out[92]=

$$d^{\dagger}_{1,\uparrow} d_{1,\uparrow} + d^{\dagger}_{2,\uparrow} d_{2,\uparrow}$$

What about the sum over spin? The following two statements are equivalent:

In[93]:=
```
Q[d[1, {Up, Down}]]
Q[d[1, All]]
```

Out[93]=

$$d^{\dagger}_{1,\downarrow} d_{1,\downarrow} + d^{\dagger}_{1,\uparrow} d_{1,\uparrow}$$

Out[94]=

$$d^{\dagger}_{1,\downarrow} d_{1,\downarrow} + d^{\dagger}_{1,\uparrow} d_{1,\uparrow}$$

The single-particle part of the two *isolated* quantum dots is given by

In[95]:=
```
H0 = ϵ * Q[d[{1, 2}, All]]
```

Out[95]=

$$\epsilon \left(d^{\dagger}_{1,\downarrow} d_{1,\downarrow} + d^{\dagger}_{1,\uparrow} d_{1,\uparrow} + d^{\dagger}_{2,\downarrow} d_{2,\downarrow} + d^{\dagger}_{2,\uparrow} d_{2,\uparrow} \right)$$

Now, let us turn to the hopping between the two quantum dots. Again one straightforward method is as following:

In[96]:=
```
Sum[d[1, s]^Dagger ** d[2, s], {s, {Up, Down}}]
```
Out[96]=

$$d^{\dagger}_{1,\downarrow} d_{2,\downarrow} + d^{\dagger}_{1,\uparrow} d_{2,\uparrow}$$

The above has a short-cut as following:

In[97]:=
```
Hop[d[1, All], d[2, All]]
Hop[{d[1, All], d[2, All]}]
```
Out[97]=

$$d^{\dagger}_{1,\downarrow} d_{2,\downarrow} + d^{\dagger}_{1,\downarrow} d_{2,\uparrow} + d^{\dagger}_{1,\uparrow} d_{2,\downarrow} + d^{\dagger}_{1,\uparrow} d_{2,\uparrow}$$

Out[98]=

$$d^{\dagger}_{1,\downarrow} d_{2,\downarrow} + d^{\dagger}_{1,\uparrow} d_{2,\uparrow}$$

Do not forget to make it Hermitian. (There is one important reason why Hop[...] or FockHopping[...] does not include the hopping terms for both directions.)

In[99]:=
```
PlusDagger@Hop[{d[1, All], d[2, All]}]
```
Out[99]=

$$d^{\dagger}_{1,\downarrow} d_{2,\downarrow} + d^{\dagger}_{1,\uparrow} d_{2,\uparrow} + d^{\dagger}_{2,\downarrow} d_{1,\downarrow} + d^{\dagger}_{2,\uparrow} d_{1,\uparrow}$$

So, the hopping part is given by

In[100]:=
```
Ht = -PlusDagger@FockHopping[{d[1, All], d[2, All]}]
```
Out[100]=

$$-d^{\dagger}_{1,\downarrow} d_{2,\downarrow} - d^{\dagger}_{1,\uparrow} d_{2,\uparrow} - d^{\dagger}_{2,\downarrow} d_{1,\downarrow} - d^{\dagger}_{2,\uparrow} d_{1,\uparrow}$$

Then, the overall single-particle part is given by

In[101]:=
```
H1 = H0 + Ht
```
Out[101]=

$$-d^{\dagger}_{1,\downarrow} d_{2,\downarrow} - d^{\dagger}_{1,\uparrow} d_{2,\uparrow} - d^{\dagger}_{2,\downarrow} d_{1,\downarrow} - d^{\dagger}_{2,\uparrow} d_{1,\uparrow} + \epsilon \left(d^{\dagger}_{1,\downarrow} d_{1,\downarrow} + d^{\dagger}_{1,\uparrow} d_{1,\uparrow} + d^{\dagger}_{2,\downarrow} d_{2,\downarrow} + d^{\dagger}_{2,\uparrow} d_{2,\uparrow} \right)$$

On-site interactions

Here is the onsite interaction terms.

In[102]:=
```
Hint = U (Q[d[1, Up]] ** Q[d[1, Down]] + Q[d[2, Up]] ** Q[d[2, Down]])
```
Out[102]=

$$U \left(d^{\dagger}_{1,\downarrow} d^{\dagger}_{1,\uparrow} d_{1,\uparrow} d_{1,\downarrow} + d^{\dagger}_{2,\downarrow} d^{\dagger}_{2,\uparrow} d_{2,\uparrow} d_{2,\downarrow} \right)$$

Many-body eigenstates

Finally, the total Hamiltonian for the DQD is given by

In[103]:=
```
HH = H1 + Hint
```
Out[103]=

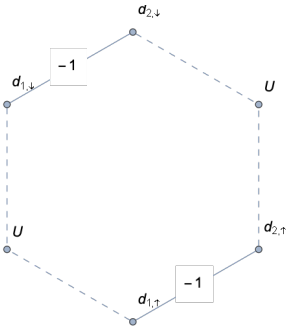
$$-d^{\dagger}_{1,\downarrow} d_{2,\downarrow} - d^{\dagger}_{1,\uparrow} d_{2,\uparrow} - d^{\dagger}_{2,\downarrow} d_{1,\downarrow} - d^{\dagger}_{2,\uparrow} d_{1,\uparrow} + \epsilon \left(d^{\dagger}_{1,\downarrow} d_{1,\downarrow} + d^{\dagger}_{1,\uparrow} d_{1,\uparrow} + d^{\dagger}_{2,\downarrow} d_{2,\downarrow} + d^{\dagger}_{2,\uparrow} d_{2,\uparrow} \right) + U \left(d^{\dagger}_{1,\downarrow} d^{\dagger}_{1,\uparrow} d_{1,\uparrow} d_{1,\downarrow} + d^{\dagger}_{2,\downarrow} d^{\dagger}_{2,\uparrow} d_{2,\uparrow} d_{2,\downarrow} \right)$$

The above Hamiltonian may be described in graph as follows. Here, the vertex U with dashed lines denotes the interaction and solid line indicates hopping.

In[105]:=

```
GraphForm[HH, ImageSize -> Small]
```

Out[105]=



Again, recall that the Hamiltonian conserves both the charge (Q) and spin (S). Therefore, it is a good idea to organize the basis accordingly. Here, note that in the sector $\{Q=1, S=1/2\}$, states $\left|1_{d_{1,\downarrow}}\right\rangle$ and $\left|1_{d_{2,\downarrow}}\right\rangle$ are missing. This is to avoid redundancy because both gives the same matrix elements.

In[72]:=

```
bs = FermionBasis[d@{1, 2}]
```

Out[72]=

$$\left\langle \left| \{0,\,0\} \to \left\{ \left|\_\right\rangle \right\},\ \left\{1,\,\frac{1}{2}\right\} \to \left\{ \left|1_{d_{2,\uparrow}}\right\rangle,\ \left|1_{d_{1,\uparrow}}\right\rangle \right\},\ \{2,\,0\} \to \left\{ -\left|1_{d_{1,\downarrow}}1_{d_{1,\uparrow}}\right\rangle,\ -\frac{\left|1_{d_{1,\downarrow}}1_{d_{2,\uparrow}}\right\rangle}{\sqrt{2}} + \frac{\left|1_{d_{1,\uparrow}}1_{d_{2,\downarrow}}\right\rangle}{\sqrt{2}},\ -\left|1_{d_{2,\downarrow}}1_{d_{2,\uparrow}}\right\rangle \right\},\right.$$
$$\left. \{2,\,1\} \to \left\{ \left|1_{d_{1,\uparrow}}1_{d_{2,\uparrow}}\right\rangle \right\},\ \left\{3,\,\frac{1}{2}\right\} \to \left\{ -\left|1_{d_{1,\downarrow}}1_{d_{1,\uparrow}}1_{d_{2,\uparrow}}\right\rangle,\ \left|1_{d_{1,\uparrow}}1_{d_{2,\downarrow}}1_{d_{2,\uparrow}}\right\rangle \right\},\ \{4,\,0\} \to \left\{ \left|1_{d_{1,\downarrow}}1_{d_{1,\uparrow}}1_{d_{2,\downarrow}}1_{d_{2,\uparrow}}\right\rangle \right\} \right| \right\rangle$$

Naturally, the Hamiltonian is block diagonal in this basis.

In[73]:=

```
big = MatrixIn[HH, bs, bs];
big = KeyGroupBy[big, First, Values];
MatrixForm@Values@Map[MatrixForm, big, {2}]
```

Out[75]//MatrixForm=

$$\begin{pmatrix} (0) & \begin{pmatrix} 0 & 0 \end{pmatrix} & \begin{pmatrix} 0 & 0 & 0 \end{pmatrix} & (0) & \begin{pmatrix} 0 & 0 \end{pmatrix} & (0) \\ \begin{pmatrix} 0 \\ 0 \end{pmatrix} & \begin{pmatrix} \epsilon & -1 \\ -1 & \epsilon \end{pmatrix} & \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} & \begin{pmatrix} 0 \\ 0 \end{pmatrix} & \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} & \begin{pmatrix} 0 \\ 0 \end{pmatrix} \\ \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} & \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} & \begin{pmatrix} U+2\epsilon & -\sqrt{2} & 0 \\ -\sqrt{2} & 2\epsilon & -\sqrt{2} \\ 0 & -\sqrt{2} & U+2\epsilon \end{pmatrix} & \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} & \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} & \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \\ (0) & \begin{pmatrix} 0 & 0 \end{pmatrix} & \begin{pmatrix} 0 & 0 & 0 \end{pmatrix} & (2\epsilon) & \begin{pmatrix} 0 & 0 \end{pmatrix} & (0) \\ \begin{pmatrix} 0 \\ 0 \end{pmatrix} & \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} & \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} & \begin{pmatrix} 0 \\ 0 \end{pmatrix} & \begin{pmatrix} U+3\epsilon & -1 \\ -1 & U+3\epsilon \end{pmatrix} & \begin{pmatrix} 0 \\ 0 \end{pmatrix} \\ (0) & \begin{pmatrix} 0 & 0 \end{pmatrix} & \begin{pmatrix} 0 & 0 & 0 \end{pmatrix} & (0) & \begin{pmatrix} 0 & 0 \end{pmatrix} & (2(U+2\epsilon)) \end{pmatrix}$$

Therefore, it is efficient to consider each block separately.

In[76]:=

```
mat = MatrixIn[HH, bs];
MatrixForm /@ mat
```

Out[77]=

$$\left\langle \left| \{0,\,0\} \to (0),\ \left\{1,\,\frac{1}{2}\right\} \to \begin{pmatrix} \epsilon & -1 \\ -1 & \epsilon \end{pmatrix},\ \{2,\,0\} \to \begin{pmatrix} U+2\epsilon & -\sqrt{2} & 0 \\ -\sqrt{2} & 2\epsilon & -\sqrt{2} \\ 0 & -\sqrt{2} & U+2\epsilon \end{pmatrix},\right.\right.$$
$$\left.\left. \{2,\,1\} \to (2\epsilon),\ \left\{3,\,\frac{1}{2}\right\} \to \begin{pmatrix} U+3\epsilon & -1 \\ -1 & U+3\epsilon \end{pmatrix},\ \{4,\,0\} \to (2(U+2\epsilon)) \right| \right\rangle$$

Related Guides

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