Anderson Molecule

1 Exact diagonalization of the Anderson Molecule

The Hamiltonian

$$\mathcal{H} = -t\sum_{\sigma}\left(c^{\dagger}_{1\sigma}c_{2\sigma} + c^{\dagger}_{2\sigma}c_{1\sigma}\right) + U\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} + \epsilon_s\sum_{\sigma}\hat{n}_{2\sigma} + \epsilon_d\sum_{\sigma}\hat{n}_{1\sigma} \tag{1}$$

I have two lattice sites, indexed by 1 and 2, occupied by electrons. μ is the chemical potential, $c^{\dagger}_{i\sigma}$ and $c_{i\sigma}$ are the fermionic creation and annihilation operators at the $\mathrm{i^{th}}$ site, with spin-index σ. σ can take values $\uparrow$ and $\downarrow$, denoting spin-up and spin-down states respectively. $\hat{n}_{i\sigma} = c^{\dagger}_{i\sigma}c_{i\sigma}$ is the number operator for the i^{th} site and at spin-index σ; it counts the number of fermions with the designated quantum numbers. $\hat{N} = \sum_{i\sigma}\hat{n}_{i\sigma}$ is the total number operator; it counts the total number of fermions at all sites and spin-indices. t is the hopping strength; the more the t, the more are the electrons likely to hop between sites. U is the on-site repulsion cost; it represents the increase in energy when two electrons occupy the same site. The model has on-site repulsion only for the first site. The sites have energies of ϵ_s and ϵ_s respectively.

1.1 Symmetries of the problem

The following operators commute with the Hamiltonian.

1. **Total number operator**: $\left[\mathcal{H}, \hat{N}\right] = 0$.

2. **Magnetization operator**: $\left[\mathcal{H}, \hat{S}^z_{tot}\right] = 0$.

3. **Total Spin Operator**: Total spin angular momentum operator,

$$\hat{S}^2_{tot} = \hat{(}S^x_{tot})^2 + \hat{(}S^y_{tot})^2 + \hat{(}S^z_{tot})^2 = S^+_{tot}S^-_{tot} - \hbar S^z_{tot} + (S^z_{tot})^2 \tag{2}$$

Since all the terms in the Hamiltonian are spin-preserving (all events conserve the number of particles having a definite spin σ), total angular momentum will be conserved. It's obvious that the number operator term do so. The hopping term does so as well; $c^{\dagger}_{i\sigma}c_{j\sigma}$ destroys a particle of spin σ and creates a particle of the same spin; the total angular momentum remain conserved in the process, although the number of particles at a particular site is not conserved. Thus, $\left[\hat{S}^2_{tot}, \mathcal{H}\right] = 0$.

1.2 N = 1

- $S^z_{tot} = -1$: $\left|\downarrow, 0\right\rangle, \left|0, \downarrow\right\rangle$
- $S^z_{tot} = +1$: $\left|\uparrow, 0\right\rangle, \left|0, \uparrow\right\rangle$

1.2.1 $S^z_{tot} = -1$

Let us first see the action of the Hamiltonian on the eigenfunctions with $S^z_{tot} = -1$.

$$\begin{aligned}\mathcal{H}\left|\downarrow, 0\right\rangle &= \epsilon_d\left|\downarrow, 0\right\rangle - t\left|0, \downarrow\right\rangle \\ \mathcal{H}\left|0, \downarrow\right\rangle &= \epsilon_s\left|0, \downarrow\right\rangle - t\left|\downarrow, 0\right\rangle\end{aligned} \tag{3}$$

We get the following matrix for this tiny subspace of the Hamiltonian:

$$\begin{array}{c c} & \begin{array}{cc} \left|\downarrow, 0\right\rangle & \left|0, \downarrow\right\rangle \end{array} \\ \begin{array}{c} \left|\downarrow, 0\right\rangle \\ \\ \left|0, \downarrow\right\rangle \end{array} & \begin{pmatrix} \epsilon_d & -t \\ \\ -t & \epsilon_s \end{pmatrix} \end{array} \tag{4}$$

Eigenvalues: $\frac{1}{2}\left[\epsilon_d + \epsilon_s \pm \sqrt{(\epsilon_d - \epsilon_s)^2 + 4t^2}\right]$. For $\epsilon_s = \epsilon_d + \frac{U}{2}$ and $\Delta = \sqrt{U^2 + 16t^2}$, eigenvalues, $\lambda_{\pm} = \epsilon_d + \frac{1}{4}(U \pm \Delta)$.
The eigenvectors are $\frac{1}{N_{\pm}}\left(t\left|\downarrow, 0\right\rangle - \frac{1}{4}(U \pm \Delta)\left|0, \downarrow\right\rangle\right)$, where $N^2_{\pm} = t^2 + (\frac{U \pm \Delta}{4})^2$

1.2.2 $S^z_{tot} = +1$

$$\begin{aligned} \mathcal{H}\left|\uparrow,0\right\rangle &= \epsilon_d \left|\uparrow,0\right\rangle - t\left|0,\uparrow\right\rangle \\ \mathcal{H}\left|0,\uparrow\right\rangle &= \epsilon_s \left|0,\uparrow\right\rangle - t\left|\uparrow,0\right\rangle \end{aligned} \tag{5}$$

Clearly, this gives the same matrix as the spin-down states. So, the eigenvalues will be exactly the same, and the eigenvectors will be correspondingly modified in the new basis.
eigenvectors : $\frac{1}{N_\pm}\left(t\left|\uparrow,0\right\rangle + (\epsilon_d - \lambda_\pm)\left|0,\uparrow\right\rangle\right)$

1.3 N=3

- $S^z_{tot} = -1$: $\left|\uparrow\downarrow,\downarrow\right\rangle, \left|\downarrow,\uparrow\downarrow\right\rangle$
- $S^z_{tot} = +1$: $\left|\uparrow\downarrow,\uparrow\right\rangle, \left|\uparrow,\uparrow\downarrow\right\rangle$

1.3.1 $S^z_{tot} = -1$

$$\begin{aligned} \mathcal{H}\left|\uparrow\downarrow,\downarrow\right\rangle &= -t\left|\downarrow,\uparrow\downarrow\right\rangle + (2\epsilon_d + \epsilon_s + U)\left|\uparrow\downarrow,\downarrow\right\rangle \\ \mathcal{H}\left|\downarrow,\uparrow\downarrow\right\rangle &= -t\left|\uparrow\downarrow,\downarrow\right\rangle + (2\epsilon_s + \epsilon_d)\left|\downarrow,\uparrow\downarrow\right\rangle \end{aligned} \tag{6}$$

$$\begin{array}{cc} & \begin{array}{cc} \left|\uparrow\downarrow,\downarrow\right\rangle & \left|\downarrow,\uparrow\downarrow\right\rangle \end{array} \\ \begin{array}{c} \left|\uparrow\downarrow,\downarrow\right\rangle \\ \\ \left|\downarrow,\uparrow\downarrow\right\rangle \end{array} & \begin{pmatrix} 2\epsilon_d + \epsilon_s + U & -t \\ & \\ -t & 2\epsilon_s + \epsilon_d \end{pmatrix} \end{array} \tag{7}$$

Again setting $\epsilon_s = \epsilon_d + \frac{U}{2}$, eigenvalues: $3\epsilon_d + \frac{5}{4}U \pm \frac{1}{4}\Delta$.
Corresponding eigenvectors $\frac{1}{N_\pm}(t\left|\uparrow\downarrow,\downarrow\right\rangle - \frac{1}{4}(U \pm \Delta)\left|\downarrow,\uparrow\downarrow\right\rangle)$

1.3.2 $S^z_{tot} = +1$

$$\begin{aligned} \mathcal{H}\left|\uparrow\downarrow,\uparrow\right\rangle &= -t\left|\uparrow,\uparrow\downarrow\right\rangle + (2\epsilon_d + \epsilon_s + U)\left|\uparrow\downarrow,\uparrow\right\rangle \\ \mathcal{H}\left|\uparrow,\uparrow\downarrow\right\rangle &= -t\left|\uparrow\downarrow,\uparrow\right\rangle + (2\epsilon_s + \epsilon_d)\left|\uparrow,\uparrow\downarrow\right\rangle \end{aligned} \tag{8}$$

Again the same matrix. Hence the eigenvalues are same. Eigenvectors are $\frac{1}{N_\pm}(t\left|\uparrow\downarrow,\uparrow\right\rangle - \frac{1}{4}(U \pm \Delta)\left|\uparrow,\uparrow\downarrow\right\rangle)$

1.4 N=2

This is the eigenvalue that has the largest subspace.

- $S^z_{tot} = -1$: $\left|\downarrow,\downarrow\right\rangle$
- $S^z_{tot} = +1$: $\left|\uparrow,\uparrow\right\rangle$
- $S^z_{tot} = 0$: $\left|\uparrow,\downarrow\right\rangle, \left|\downarrow,\uparrow\right\rangle, \left|0,\uparrow\downarrow\right\rangle, \left|\uparrow\downarrow,0\right\rangle$

1.4.1 $S^z_{tot} = \pm 1$

These two subspaces have a single state each, so theya are obviously eigenstates. Since they both have identical spins on both sites, the hopping term is 0, and the U-term is also zero because of single occupation. As a result, they both have zero eigenvalue

$$\mathcal{H}\left|\downarrow,\downarrow\right\rangle = \mathcal{H}\left|\uparrow,\uparrow\right\rangle = \epsilon_s + \epsilon_d \tag{9}$$

1.4.2 $S^z_{tot} = 0$

This subspace has four eigenvectors,

$$|\uparrow,\downarrow\rangle\,, \qquad |\downarrow,\uparrow\rangle\,, \qquad |0,\uparrow\downarrow\rangle\,, \qquad |\uparrow\downarrow,0\rangle \tag{10}$$

so it is easier to first find eigenstates of S^2_{tot}. Since these are states with zero S^z, S^2_{tot} for these states is just S^+S^-

$$\begin{aligned} S^+S^-|\uparrow,\downarrow\rangle &= S^+S^-|\downarrow,\uparrow\rangle = |\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle \\ S^+S^-|\uparrow\downarrow,0\rangle &= S^+S^-|0,\uparrow\downarrow\rangle = 0 \end{aligned} \tag{11}$$

The eigenstates are

$$\frac{|\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle}{\sqrt{2}}(S^2_{tot}=1), \qquad \left\{\frac{|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle}{\sqrt{2}}, |\uparrow\downarrow,0\rangle\,, |0,\uparrow\downarrow\rangle\right\}(S^2_{tot}=0) \tag{12}$$

$S^2_{tot} = 1$ immediately delivers an eigenstate:

$$\mathcal{H}\frac{|\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle}{\sqrt{2}} = (\epsilon_d + \epsilon_s)\left(\frac{|\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle}{\sqrt{2}}\right) \tag{13}$$

Next I diagonalize the subspace $S^2_{tot} = 0$.

$$\begin{aligned} \mathcal{H}\frac{|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle}{\sqrt{2}} &= (\epsilon_d + \epsilon_s)\left(\frac{|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle}{\sqrt{2}}\right) + \sqrt{2}t(|\uparrow\downarrow,0\rangle - |0,\uparrow\downarrow\rangle) \\ \mathcal{H}|\uparrow\downarrow,0\rangle &= (2\epsilon_d + U)|\uparrow\downarrow,0\rangle + \sqrt{2}t\frac{|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle}{\sqrt{2}} \\ \mathcal{H}|0,\uparrow\downarrow\rangle &= (2\epsilon_d + U)|0,\uparrow\downarrow\rangle - \sqrt{2}t\frac{|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle}{\sqrt{2}} \end{aligned} \tag{14}$$

We get the following matrix

$$\begin{pmatrix} 2\epsilon_d + \frac{U}{2} & \sqrt{2}t & -\sqrt{2}t \\ \sqrt{2}t & 2\epsilon_d + U & 0 \\ -\sqrt{2}t & 0 & 2\epsilon_d + U \end{pmatrix} \tag{15}$$

The eigenvectors are

- $|\uparrow\downarrow,0\rangle - |0,\uparrow\downarrow\rangle : 2\epsilon_d + U$
- $\frac{U-\Delta}{4\sqrt{2}t}\frac{|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle}{\sqrt{2}} - |\uparrow\downarrow,0\rangle + |0,\uparrow\downarrow\rangle : 2\epsilon_d + \frac{3}{4}U + \frac{1}{2}\Delta(\frac{U}{2},t)$
- $\frac{U+\Delta}{4\sqrt{2}t}\frac{|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle}{\sqrt{2}} - |\uparrow\downarrow,0\rangle + |0,\uparrow\downarrow\rangle : 2\epsilon_d + \frac{3}{4}U - \frac{1}{2}\Delta(\frac{U}{2},t)$

1.5 The total spectrum

The final spectrum is already obtained. One final thing to do is to just add the respective values of $-\mu N$ to the eigenvalues.

$\hat{N}$	S^z_{tot}	E	$\lvert\Phi\rangle$
0	-	0	$\lvert 0,0\rangle$
1	-1	$\epsilon_d + \frac{1}{4}(U \pm \Delta)$	$\frac{1}{N_\pm}\left(t\lvert\downarrow,0\rangle - \frac{1}{4}(U\pm\Delta)\lvert 0,\downarrow\rangle\right)$
	1	$\epsilon_d + \frac{1}{4}(U \pm \Delta)$	$\frac{1}{N_\pm}\left(t\lvert\downarrow,0\rangle - \frac{1}{4}(U\pm\Delta)\lvert 0,\downarrow\rangle\right)$
2	-1	$2\epsilon_d + \frac{U}{2}$	$\lvert\downarrow,\downarrow\rangle$
	1	$2\epsilon_d + \frac{U}{2}$	$\lvert\uparrow,\uparrow\rangle$
	0	$2\epsilon_d + \frac{U}{2}$	$\frac{\lvert\uparrow,\downarrow\rangle+\lvert\downarrow,\uparrow\rangle}{\sqrt{2}}$
		$2\epsilon_d + U$	$\frac{\lvert\uparrow\downarrow,0\rangle+\lvert 0,\uparrow\downarrow\rangle}{\sqrt{2}}$
		$2\epsilon_d + \frac{3}{4}U \pm \frac{1}{2}\Delta(\frac{U}{2},t)$	$\frac{U\mp\Delta}{4\sqrt{2}t}\frac{\lvert\uparrow,\downarrow\rangle-\lvert\downarrow,\uparrow\rangle}{\sqrt{2}} - \lvert\uparrow\downarrow,0\rangle + \lvert 0,\uparrow\downarrow\rangle$
3	-1	$3\epsilon_d + \frac{5}{4}U \pm \frac{1}{4}\Delta$	$\frac{1}{N_\pm}(t\lvert\uparrow\downarrow,\downarrow\rangle - \frac{1}{4}(U\pm\Delta)\lvert\downarrow,\uparrow\downarrow\rangle)$
	1	$3\epsilon_d + \frac{5}{4}U \pm \frac{1}{4}\Delta$	$\frac{1}{N_\pm}(t\lvert\uparrow\downarrow,\downarrow\rangle - \frac{1}{4}(U\pm\Delta)\lvert\downarrow,\uparrow\downarrow\rangle)$
4	0	$2(\epsilon_s + \epsilon_d) + U$	$\lvert\uparrow\downarrow,\uparrow\downarrow\rangle$