Hubbard dimer : exact hamiltonian solutions

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1 Introduction

Conventions :

$$|\uparrow\downarrow \quad \uparrow\downarrow\rangle = c^\dagger_{2\downarrow} c^\dagger_{2\uparrow} c^\dagger_{1\downarrow} c^\dagger_{1\uparrow} |0 \quad 0\rangle$$

$$c^\dagger_i \left|\ldots, n_i, \ldots\right\rangle_a = (1 - n_i) \cdot (-1)^{\sum_{j>i} n_j} \left|\ldots, n_i + 1, \ldots\right\rangle_a$$

$$c_i \left|\ldots, n_i, \ldots\right\rangle_a = n_i \cdot (-1)^{\sum_{j>i} n_j} \left|\ldots, n_i - 1, \ldots\right\rangle_a$$

$$\hat{n}_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$$

$$\hat{n}_{i\sigma} \left|\ldots, n_{i\sigma}, \ldots\right\rangle_a = n_{i\sigma} \left|\ldots, n_{i\sigma}, \ldots\right\rangle_a$$

Hamiltonian :

$$H = -t \sum_{\substack{i,j=1,2 \\ i \neq j}} \sum_\sigma c^\dagger_{i\sigma} c_{j\sigma} + \frac{U}{2} \sum_{i=1,2} \sum_{\sigma\sigma'} c^\dagger_{i\sigma} c^\dagger_{i\sigma'} c_{i\sigma'} c_{i\sigma} + \epsilon_0 \sum_{\sigma, i=1,2} n_{i\sigma}$$

Useful relations :

$$\left\{c_{i\sigma}, c^\dagger_{j\sigma'}\right\} = \delta_{\sigma\sigma'} \delta_{ij} \quad \{c_{i\sigma}, c_{j\sigma'}\} = 0 \quad \left\{c^\dagger_{i\sigma}, c^\dagger_{j\sigma'}\right\} = 0$$

$$< \alpha | c_i | \beta > = < \beta | c^\dagger_i | \alpha >$$

2 General case : $U_1 \neq U_2$ and $\epsilon_1 \neq \epsilon_2$

2.1 Hamiltonian solutions

2.1.1 one electron solution

$$H = \begin{pmatrix} \epsilon_1 & 0 & -t & 0 \\ 0 & \epsilon_1 & 0 & -t \\ -t & 0 & \epsilon_2 & 0 \\ 0 & -t & 0 & \epsilon_2 \end{pmatrix}$$

E_i	$\vert\uparrow 0\rangle$	$\vert\downarrow 0\rangle$	$\vert 0\uparrow\rangle$	$\vert 0\downarrow\rangle$
$(\epsilon_1+\epsilon_2)/2-d$	0	$-(\epsilon_1-\epsilon_2-2d)/e$	0	$2t/e$
$(\epsilon_1+\epsilon_2)/2-d$	$-(\epsilon_1-\epsilon_2-2d)/e$	0	$2t/e$	0
$(\epsilon_1+\epsilon_2)/2+d$	0	$-(\epsilon_1-\epsilon_2+2d)/f$	0	$2t/f$
$(\epsilon_1+\epsilon_2)/2+d$	$-(\epsilon_1-\epsilon_2+2d)/f$	0	$2t/f$	0

with $d = \sqrt{(\epsilon_1-\epsilon_2)^2+4t^2}/2$, $e = \sqrt{(\epsilon_1-\epsilon_2-2d)^2+4t^2}$, and $f = \sqrt{(\epsilon_1-\epsilon_2+2d)^2+4t^2}$.

2.1.2 two electrons solution

$$H = \begin{pmatrix} \epsilon_1+\epsilon_2 & 0 & 0 & 0 & -t & -t \\ 0 & \epsilon_1+\epsilon_2 & 0 & 0 & t & t \\ 0 & 0 & \epsilon_1+\epsilon_2 & 0 & 0 & 0 \\ 0 & 0 & 0 & \epsilon_1+\epsilon_2 & 0 & 0 \\ -t & t & 0 & 0 & 2\epsilon_1+U_1 & 0 \\ -t & t & 0 & 0 & 0 & 2\epsilon_2+U_2 \end{pmatrix}$$

$$a = (18t^2+3U_1U_2-9(\epsilon_1-\epsilon_2)(\epsilon_1-\epsilon_2+U_1-U_2))(U_1+U_2)-2(U_1^3+U_2^3)$$
$$b = -3(\epsilon_1-\epsilon_2)^2-3(U_1-U_2)(\epsilon_1-\epsilon_2)-U_1^2-U_2^2+U_1U_2-12t^2$$
$$d = \left(a+\sqrt{4b^3+a^2}\right)^{\frac{1}{3}}$$
$$p = -b/9$$
$$q = -a/45$$

$$K_0 = \frac{U_1+U_2}{3} - \frac{(1+i\sqrt{3})b}{3\times 2^{\frac{2}{3}}d} + \frac{(1-i\sqrt{3})d}{6\times 2^{\frac{1}{3}}} = \frac{U_1+U_2}{3} + 2\sqrt{p}\cos\left(\arccos\left(\frac{q}{p^{\frac{3}{2}}}\right)/3\right)$$
$$K_1 = \frac{U_1+U_2}{3} - \frac{(1-i\sqrt{3})b}{3\times 2^{\frac{2}{3}}d} + \frac{(1+i\sqrt{3})d}{6\times 2^{\frac{1}{3}}} = \frac{U_1+U_2}{3} + 2\sqrt{p}\cos\left(\left(\arccos\left(\frac{q}{p^{\frac{3}{2}}}\right)-2\pi\right)/3\right)$$
$$K_2 = \frac{U_1+U_2}{3} + \frac{2^{\frac{1}{3}}b}{3d} - \frac{d}{3\times 2^{\frac{1}{3}}} = \frac{U_1+U_2}{3} + 2\sqrt{p}\cos\left(\left(\arccos\left(\frac{q}{p^{\frac{3}{2}}}\right)-4\pi\right)/3\right)$$

Despite K_i have imaginary parts, especially with D which is an imaginary number, all these quantites are real when evaluated numerically !

E_i	$\vert\uparrow\ \ \downarrow\rangle$	$\vert\downarrow\ \ \uparrow\rangle$	$\vert\uparrow\ \ \uparrow\rangle$	$\vert\downarrow\ \ \downarrow\rangle$	$\vert\uparrow\downarrow 0\rangle$	$\vert 0\uparrow\downarrow\rangle$
$\epsilon_1+\epsilon_2+K_0$	$-\frac{1}{C_0}\frac{t(U_1+U_2-2K_0)}{K_0(\epsilon_1-\epsilon_2+U_1-K_0)}$	$\frac{1}{C_0}\frac{t(U_1+U_2-2K_0)}{K_0(\epsilon_1-\epsilon_2+U_1-K_0)}$	0	0	$\frac{1}{C_0}\frac{\epsilon_2-\epsilon_1+U_2-K_0}{\epsilon_1-\epsilon_2+U_1-K_0}$	$\frac{1}{C_0}$
$\epsilon_1+\epsilon_2+K_1$	$-\frac{1}{C_1}\frac{t(U_1+U_2-2K_1)}{K_1(\epsilon_1-\epsilon_2+U_1-K_1)}$	$\frac{1}{C_1}\frac{t(U_1+U_2-2K_1)}{K_1(\epsilon_1-\epsilon_2+U_1-K_1)}$	0	0	$\frac{1}{C_1}\frac{\epsilon_2-\epsilon_1+U_2-K_1}{\epsilon_1-\epsilon_2+U_1-K_1}$	$\frac{1}{C_1}$
$\epsilon_1+\epsilon_2+K_2$	$-\frac{1}{C_2}\frac{t(U_1+U_2-2K_2)}{K_2(\epsilon_1-\epsilon_2+U_1-K_2)}$	$\frac{1}{C_2}\frac{t(U_1+U_2-2K_2)}{K_2(\epsilon_1-\epsilon_2+U_1-K_2)}$	0	0	$\frac{1}{C_2}\frac{\epsilon_2-\epsilon_1+U_2-K_2}{\epsilon_1-\epsilon_2+U_1-K_2}$	$\frac{1}{C_2}$
$\epsilon_1+\epsilon_2$	0	0	0	1	0	0
$\epsilon_1+\epsilon_2$	0	0	1	0	0	0
$\epsilon_1+\epsilon_2$	$1/\sqrt{2}$	$1/\sqrt{2}$	0	0	0	0

By normalizing the vectors :

$$C_i = \sqrt{\left|-\frac{t(U_1+U_2-2K_i)}{K_i(\epsilon_1-\epsilon_2+U_1-K_i)}\right|^2 + \left|\frac{t(U_1+U_2-2K_i)}{K_i(\epsilon_1-\epsilon_2+U_1-K_i)}\right|^2 + \left|\frac{\epsilon_2-\epsilon_1+U_2-K_i}{\epsilon_1-\epsilon_2+U_1-K_i}\right|^2 + 1}$$

Numerically, we have these solution converging to the basic case solution !

2.1.3 three electrons solution

$$H = \begin{pmatrix} \epsilon_1+2\epsilon_2+U_2 & 0 & -t & 0 \\ 0 & \epsilon_1+2\epsilon_2+U_2 & 0 & -t \\ -t & 0 & 2\epsilon_1+\epsilon_2+U_1 & 0 \\ 0 & -t & 0 & 2\epsilon_1+\epsilon_2+U_1 \end{pmatrix}$$

E_i	$\vert\uparrow\uparrow\downarrow\rangle$	$\vert\downarrow\uparrow\downarrow\rangle$	$\vert\uparrow\downarrow\uparrow\rangle$	$\vert\uparrow\downarrow\downarrow\rangle$
$\frac{1}{2}(3\epsilon_1+3\epsilon_2+U_1+U_2-g)$	0	$\frac{m_+}{\sqrt{1+m_+^2}}$	0	$\frac{1}{\sqrt{1+m_+^2}}$
$\frac{1}{2}(3\epsilon_1+3\epsilon_2+U_1+U_2-g)$	$\frac{m_+}{\sqrt{1+m_+^2}}$	0	$\frac{1}{\sqrt{1+m_+^2}}$	0
$\frac{1}{2}(3\epsilon_1+3\epsilon_2+U_1+U_2+g)$	0	$\frac{m_-}{\sqrt{1+m_-^2}}$	0	$\frac{1}{\sqrt{1+m_-^2}}$
$\frac{1}{2}(3\epsilon_1+3\epsilon_2+U_1+U_2+g)$	$\frac{m_-}{\sqrt{1+m_-^2}}$	0	$\frac{1}{\sqrt{1+m_-^2}}$	0

with $g=\sqrt{((\epsilon_1-\epsilon_2)+(U_1-U_2))^2+4t^2}$, $m_+ = \frac{\epsilon_1-\epsilon_2+U_1-U_2+g}{2t}$, $m_- = \frac{\epsilon_1-\epsilon_2+U_1-U_2-g}{2t}$

2.1.4 other solutions

$$H|0\quad 0\rangle = 0|0\quad 0\rangle$$

$$H|\uparrow\downarrow\quad\uparrow\downarrow\rangle = (2\epsilon_1+2\epsilon_2+U_1+U_2)|\uparrow\downarrow\quad\uparrow\downarrow\rangle$$

3 Basic case : $U_1 = U_2 = U$ and $\epsilon_1 = \epsilon_2 = \epsilon_0$

3.1 Hamiltonian solutions

3.1.1 one electron solution

$$H = \begin{pmatrix} \epsilon_0 & 0 & -t & 0 \\ 0 & \epsilon_0 & 0 & -t \\ -t & 0 & \epsilon_0 & 0 \\ 0 & -t & 0 & \epsilon_0 \end{pmatrix}$$

E_i	$\lvert\uparrow 0\rangle$	$\lvert\downarrow 0\rangle$	$\lvert 0\uparrow\rangle$	$\lvert 0\downarrow\rangle$
$\epsilon_0 - t$	0	$1/\sqrt{2}$	0	$1/\sqrt{2}$
$\epsilon_0 - t$	$1/\sqrt{2}$	0	$1/\sqrt{2}$	0
$\epsilon_0 + t$	0	$1/\sqrt{2}$	0	$-1/\sqrt{2}$
$\epsilon_0 + t$	$1/\sqrt{2}$	0	$-1/\sqrt{2}$	0

3.1.2 two electrons solution

$$H = \begin{pmatrix} 2\epsilon_0 & 0 & 0 & 0 & -t & -t \\ 0 & 2\epsilon_0 & 0 & 0 & t & t \\ 0 & 0 & 2\epsilon_0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2\epsilon_0 & 0 & 0 \\ -t & t & 0 & 0 & 2\epsilon_0 + U & 0 \\ -t & t & 0 & 0 & 0 & 2\epsilon_0 + U \end{pmatrix}$$

E_i	$\lvert\uparrow\downarrow\rangle$	$\lvert\downarrow\uparrow\rangle$	$\lvert\uparrow\uparrow\rangle$	$\lvert\downarrow\downarrow\rangle$	$\lvert\uparrow\downarrow 0\rangle$	$\lvert 0\uparrow\downarrow\rangle$
$2\epsilon_0 + (U-c)/2$	$\frac{4t}{a(c-U)}$	$-\frac{4t}{a(c-U)}$	0	0	1/a	1/a
$2\epsilon_0 + (U+c)/2$	$-\frac{4t}{b(c+U)}$	$\frac{4t}{b(c+U)}$	0	0	1/b	1/b
$2\epsilon_0 + U$	0	0	0	0	$-1/\sqrt{2}$	$1/\sqrt{2}$
$2\epsilon_0$	0	0	0	1	0	0
$2\epsilon_0$	0	0	1	0	0	0
$2\epsilon_0$	$1/\sqrt{2}$	$1/\sqrt{2}$	0	0	0	0

With $a = \frac{\sqrt{2}}{(c-U)}\sqrt{16t^2 + (c-U)^2}$, $b = \frac{\sqrt{2}}{(c+U)}\sqrt{16t^2 + (c+U)^2}$, $c = \sqrt{16t^2 + U^2}$.

3.1.3 three electrons solution

$$H = \begin{pmatrix} 3\epsilon_0 + \mathrm{U} & 0 & -t & 0 \\ 0 & 3\epsilon_0 + \mathrm{U} & 0 & -t \\ -t & 0 & 3\epsilon_0 + \mathrm{U} & 0 \\ 0 & -t & 0 & 3\epsilon_0 + \mathrm{U} \end{pmatrix}$$

E_i	$\vert\uparrow\uparrow\downarrow\rangle$	$\vert\downarrow\uparrow\downarrow\rangle$	$\vert\uparrow\downarrow\uparrow\rangle$	$\vert\uparrow\downarrow\downarrow\rangle$
$3\epsilon_0 + \mathrm{U} - \mathrm{t}$	0	$1/\sqrt{2}$	0	$1/\sqrt{2}$
$3\epsilon_0 + \mathrm{U} - \mathrm{t}$	$1/\sqrt{2}$	0	$1/\sqrt{2}$	0
$3\epsilon_0 + \mathrm{U} + \mathrm{t}$	0	$-1/\sqrt{2}$	0	$1/\sqrt{2}$
$3\epsilon_0 + \mathrm{U} + \mathrm{t}$	$-1/\sqrt{2}$	0	$1/\sqrt{2}$	0