

EKT

Julien Prodhon

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$$V_{ij}^\nu = \sum_m (E_0 - E_m^{N-1}) A_{m,ij\sigma}$$

$$\epsilon_\nu = \frac{\sum_m \sum_i \sum_j C_{i\nu}^* C_{j\nu} (E_0 - E_m^{N-1}) A_{m,ij\sigma}^{N=2}}{\sum_m \sum_i \sum_j C_{i\nu}^* C_{j\nu} A_{m,ij\sigma}^{N=2}}$$

$$\epsilon_\nu = \frac{\sum_i \sum_j C_{i\nu}^* C_{j\nu} V_{ij}^\nu}{\sum_i \sum_j C_{i\nu}^* C_{j\nu} \gamma_{ij\sigma}^{N=2}}$$

if ϕ is in the initial basis and ψ is in the basis of the density matrix eigenvectors B_p , we have :

$$\begin{pmatrix} \psi_{1\uparrow} \\ \psi_{2\uparrow} \\ \psi_{1\downarrow} \\ \psi_{2\downarrow} \end{pmatrix} = \begin{pmatrix} a_{1\uparrow 1\uparrow} & a_{1\uparrow 2\uparrow} & 0 & 0 \\ a_{2\uparrow 1\uparrow} & a_{2\uparrow 2\uparrow} & 0 & 0 \\ 0 & 0 & a_{1\downarrow 1\downarrow} & a_{1\downarrow 2\downarrow} \\ 0 & 0 & a_{2\downarrow 1\downarrow} & a_{2\downarrow 2\downarrow} \end{pmatrix} \begin{pmatrix} \phi_{1\uparrow} \\ \phi_{2\uparrow} \\ \phi_{1\downarrow} \\ \phi_{2\downarrow} \end{pmatrix} = \begin{pmatrix} a_{11\uparrow} & a_{12\uparrow} & 0 & 0 \\ a_{21\uparrow} & a_{22\uparrow} & 0 & 0 \\ 0 & 0 & a_{11\downarrow} & a_{12\downarrow} \\ 0 & 0 & a_{21\downarrow} & a_{22\downarrow} \end{pmatrix} \begin{pmatrix} \phi_{1\uparrow} \\ \phi_{2\uparrow} \\ \phi_{1\downarrow} \\ \phi_{2\downarrow} \end{pmatrix}$$

$$\Lambda_{ij}^R = \frac{1}{\sqrt{n_i n_j}} \left[n_i h_{ji} + \sum_{klm} V_{jmk} \Gamma_{klmi}^{(2)} \right]$$

We now describe i, j by $d_i \sigma_i, d_j \sigma_j$ where d corresponds to the number of the site (1 or 2) and σ the spin (up or down). We can also write

$$a_{ij} = a_{d_i \sigma_i d_j \sigma_j} = \delta_{\sigma_i \sigma_j} a_{d_i d_j \sigma}$$

Hence, we have :

With :

$$\phi_i = \sum_{d_p} \sum_{\sigma_p} a_{ip}$$

we have :

$$h_{ij}^{B_p} = \sum_{d_p} \sum_{\sigma_p} \sum_{d_q} \sum_{\sigma_q} a_{ip} a_{jq} h_{pq}$$

$$V_{jmk}^{B_p} = \sum_{d_p} \sum_{\sigma_p} \sum_{d_q} \sum_{\sigma_q} \sum_{d_r} \sum_{\sigma_r} \sum_{d_s} \sum_{\sigma_s} a_{jp} a_{mq} a_{kr} a_{ls} U_{pqrs}$$

Since :

$$\text{if } d_p = d_q = d_r = d_s = d : U_{pqrs} = U_d \text{ else } : U_{pqrs} = 0$$

$$V_{jmk}^{B_p} = \sum_d \sum_{\sigma_p} \sum_{\sigma_q} \sum_{\sigma_r} \sum_{\sigma_s} a_{dj \sigma_j} a_{dp \sigma_p} a_{dm \sigma_m} a_{dq \sigma_q} a_{dk \sigma_k} a_{dr \sigma_r} a_{dl \sigma_l} a_{ds \sigma_s} U_d$$

$$V_{jmk}^{B_p} = \sum_d a_{ddj \sigma_j} a_{ddm \sigma_m} a_{ddk \sigma_k} a_{ddl \sigma_l} U_d = a_{1dj \sigma_j} a_{1dm \sigma_m} a_{1dk \sigma_k} a_{1dl \sigma_l} U_1 + a_{2dj \sigma_j} a_{2dm \sigma_m} a_{2dk \sigma_k} a_{2dl \sigma_l} U_2$$

Γ	$c_{1\uparrow}c_{1\uparrow}$	$c_{1\uparrow}c_{1\downarrow}$	$c_{1\uparrow}c_{2\uparrow}$	$c_{1\uparrow}c_{2\downarrow}$	$c_{1\downarrow}c_{1\uparrow}$	$c_{1\downarrow}c_{1\downarrow}$	$c_{1\downarrow}c_{2\uparrow}$	$c_{1\downarrow}c_{2\downarrow}$	$c_{2\uparrow}c_{1\uparrow}$	$c_{2\uparrow}c_{1\downarrow}$	$c_{2\uparrow}c_{2\uparrow}$	$c_{2\uparrow}c_{2\downarrow}$	$c_{2\downarrow}c_{1\uparrow}$	$c_{2\downarrow}c_{1\downarrow}$	$c_{2\downarrow}c_{2\uparrow}$
$c_{1\uparrow}^\dagger c_{1\uparrow}^\dagger$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger$	0	$-\alpha_3^2$	0	$-\alpha_1\alpha_3$	α_3^2	0	$-\alpha_2\alpha_3$	0	0	$\alpha_2\alpha_3$	0	$-\alpha_3\alpha_4$	$\alpha_1\alpha_3$	0	$\alpha_3\alpha_4$
$c_{1\uparrow}^\dagger c_{2\uparrow}^\dagger$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$c_{1\uparrow}^\dagger c_{2\downarrow}^\dagger$	0	$-\alpha_1\alpha_3$	0	$-\alpha_1^2$	$\alpha_1\alpha_3$	0	$-\alpha_1\alpha_2$	0	0	$\alpha_1\alpha_2$	0	$-\alpha_1\alpha_4$	α_1^2	0	$\alpha_1\alpha_4$
$c_{1\downarrow}^\dagger c_{1\uparrow}^\dagger$	0	α_3^2	0	$\alpha_1\alpha_3$	$-\alpha_3^2$	0	$\alpha_2\alpha_3$	0	0	$-\alpha_2\alpha_3$	0	$\alpha_3\alpha_4$	$-\alpha_1\alpha_3$	0	$-\alpha_3\alpha_4$
$c_{1\downarrow}^\dagger c_{1\downarrow}^\dagger$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$c_{1\downarrow}^\dagger c_{2\uparrow}^\dagger$	0	$-\alpha_2\alpha_3$	0	$-\alpha_1\alpha_2$	$\alpha_2\alpha_3$	0	$-\alpha_2^2$	0	0	α_2^2	0	$-\alpha_2\alpha_4$	$\alpha_1\alpha_2$	0	$\alpha_2\alpha_4$
$c_{1\downarrow}^\dagger c_{2\downarrow}^\dagger$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$c_{2\uparrow}^\dagger c_{1\uparrow}^\dagger$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$c_{2\uparrow}^\dagger c_{1\downarrow}^\dagger$	0	$\alpha_2\alpha_3$	0	$\alpha_1\alpha_2$	$-\alpha_2\alpha_3$	0	α_2^2	0	0	$-\alpha_2^2$	0	$\alpha_2\alpha_4$	$-\alpha_1\alpha_2$	0	$-\alpha_2\alpha_4$
$c_{2\uparrow}^\dagger c_{2\uparrow}^\dagger$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$c_{2\uparrow}^\dagger c_{2\downarrow}^\dagger$	0	$-\alpha_3\alpha_4$	0	$-\alpha_1\alpha_4$	$\alpha_3\alpha_4$	0	$-\alpha_2\alpha_4$	0	0	$\alpha_2\alpha_4$	0	$-\alpha_4^2$	$\alpha_1\alpha_4$	0	α_4^2
$c_{2\downarrow}^\dagger c_{1\uparrow}^\dagger$	0	$\alpha_1\alpha_3$	0	α_1^2	$-\alpha_1\alpha_3$	0	$\alpha_1\alpha_2$	0	0	$-\alpha_1\alpha_2$	0	$\alpha_1\alpha_4$	$-\alpha_1^2$	0	$-\alpha_1\alpha_4$
$c_{2\downarrow}^\dagger c_{1\downarrow}^\dagger$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$c_{2\downarrow}^\dagger c_{2\uparrow}^\dagger$	0	$\alpha_3\alpha_4$	0	$\alpha_1\alpha_4$	$-\alpha_3\alpha_4$	0	$\alpha_2\alpha_4$	0	0	$-\alpha_2\alpha_4$	0	α_4^2	$-\alpha_1\alpha_4$	0	$-\alpha_4^2$
$c_{2\downarrow}^\dagger c_{2\downarrow}^\dagger$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0