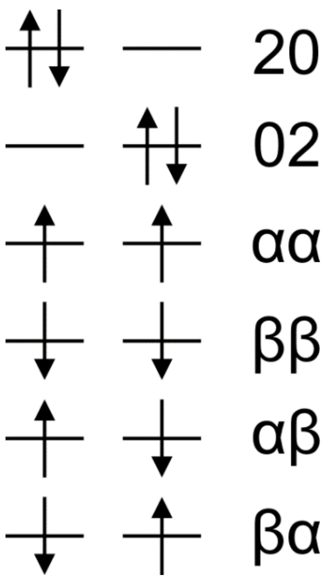
Static correlations: 2c2e model



S	S_z	χ
1	1	αα
1	-1	ββ
1	0	αβ-βα
0	0	αβ+βα
0	0	20
0	0	02

the only states representable by HF (αα, ββ)

no single Slater determinant (αβ-βα, αβ+βα)

spin contamination

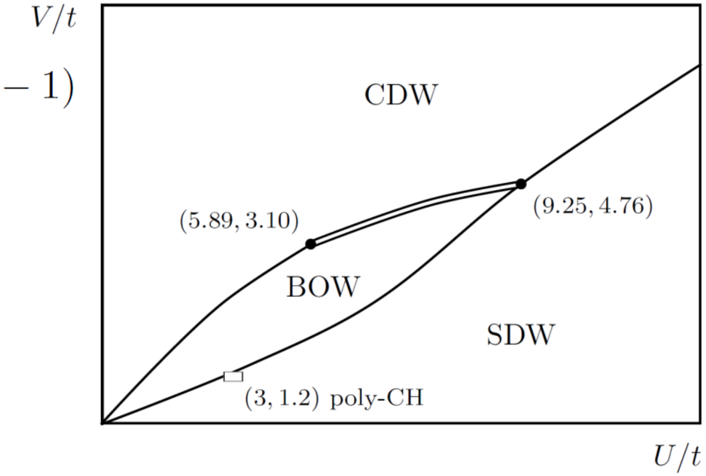
static correlations

$$\beta\alpha = \left| \begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix} \right\rangle \equiv \left| \begin{smallmatrix} 2 \\ 1 \end{smallmatrix} \right\rangle = \frac{1}{\sqrt{2}} \begin{vmatrix} \varphi_2(x_1)\chi_\uparrow(\sigma_1) & \varphi_1(x_1)\chi_\downarrow(\sigma_1) \\ \varphi_2(x_2)\chi_\uparrow(\sigma_2) & \varphi_1(x_2)\chi_\downarrow(\sigma_2) \end{vmatrix}$$

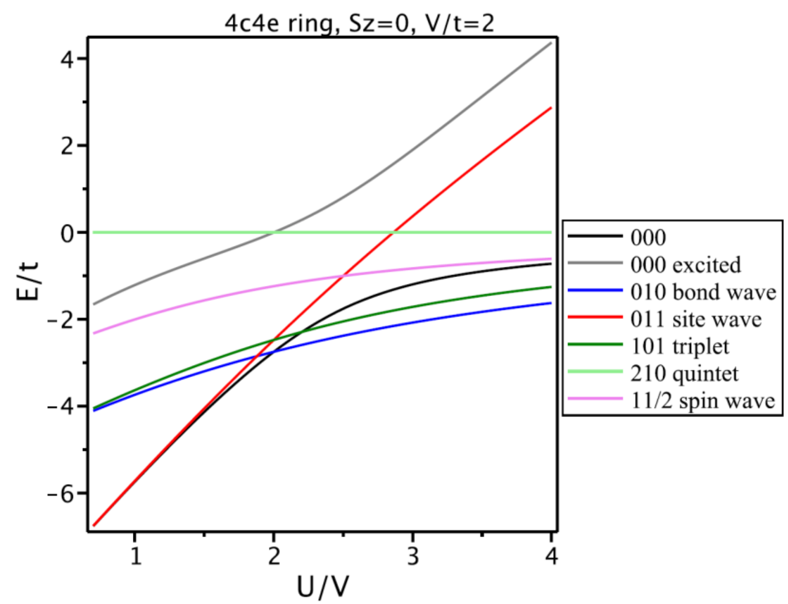
Static correlations: 4c4e model
(the simplest one featuring 1D Extended Hubbard model)

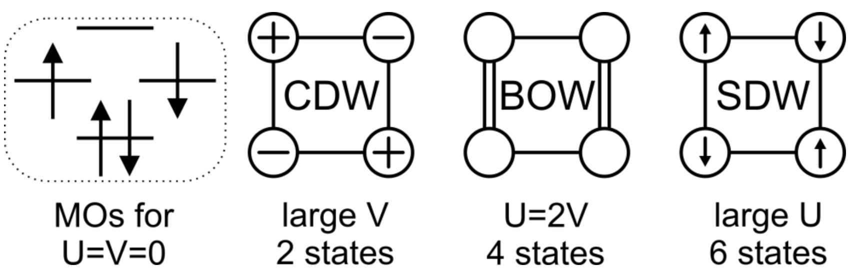
$$\hat{H} = \sum_i \varepsilon_i \hat{n}_i + \sum_{i<j} t_{ij} \hat{T}_{ij} + \sum_i U_i \hat{n}_i^{\uparrow} \hat{n}_i^{\downarrow} + \sum_{i<j} V_{ij} (\hat{n}_i - 1)(\hat{n}_j - 1)$$

$$\hat{T}_{ij} = \sum_{\sigma} \left(c_{i\sigma}^{+} c_{j\sigma} + c_{i\sigma} c_{j\sigma}^{+} \right)$$

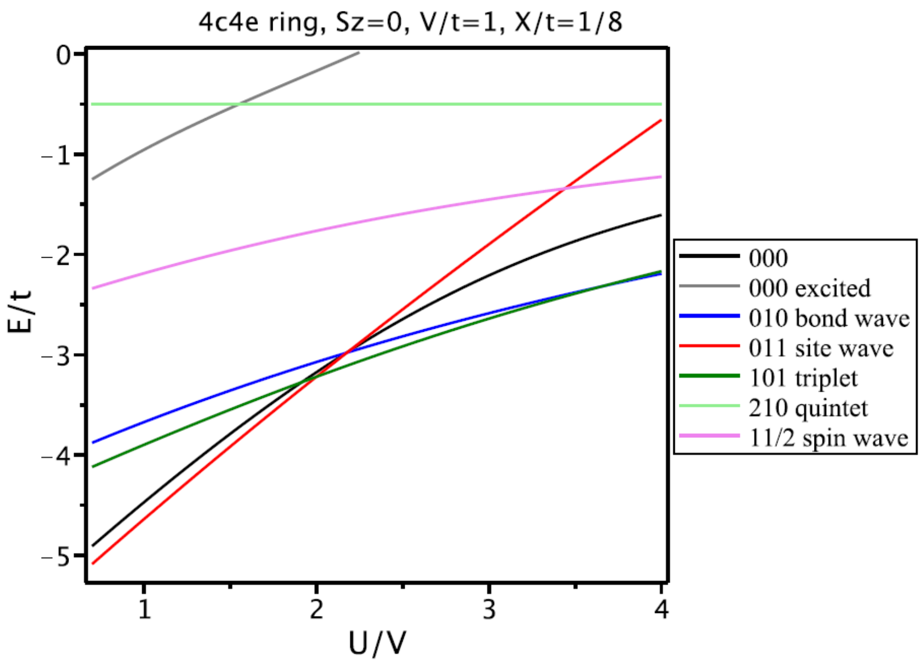


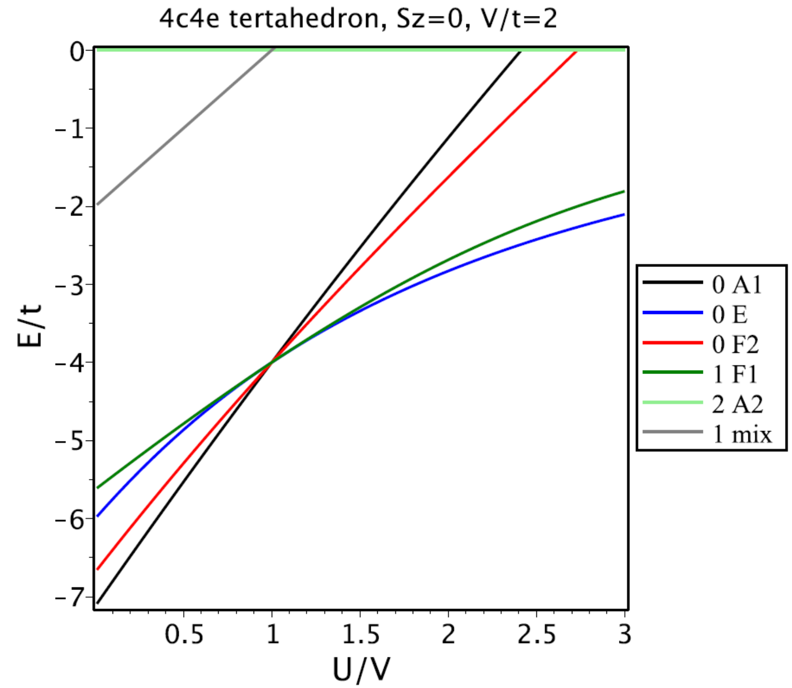
- Three kinds of electron density waves
- Quantum phase transition at U=2V
- Ground state degeneracy
- Levels crowding at large U
- Meaningless noninteracting MOs
- Two Slater determinants for variational function





Static correlations: 4c4e model
(square vs tetrahedron)





Example: Full CI analytically for 4-site model

Symmetries: particle number, spin, spin projection, translation, inversion, particle-hole

256	total configuration space
36	subspace Q=0, S_z=0
4	largest irreducible representation after all symmetries are taken into account

S	T	inversion	particle-hole
0	$-\frac{1}{2}$	*undefined*	$(E^2-2EU+EV+U^2-UV-4)(E^2-3EU+EV+2U^2-2UV-4)$
0	$\frac{1}{2}$	*undefined*	$(E^2-2EU+EV+U^2-UV-4)(E^2-3EU+EV+2U^2-2UV-4)$
1	$-\frac{1}{2}$	*undefined*	$(E^2-EU+EV-4)(E^2-2EU+EV+U^2-UV-4)$
1	$\frac{1}{2}$	*undefined*	$(E^2-EU+EV-4)(E^2-2EU+EV+U^2-UV-4)$
0	0	0	$(E-U)(E^4-5E^3U+5E^3V+8E^2U^2-16E^2UV+4E^2V^2-4EU^3+12EU^2V-8EUV^2-16E^2+40EU-32EV-16U^2+32UV)$
0	0	1	$E+V-U$
0	1	0	$E^3-3E^2U+E^2V+2EU^2-2EUV-16E+24U$
0	1	1	$E^3-4E^2U+5E^2V+5EU^2-11EUV+4EV^2-2U^3+6U^2V-4UV^2-16E+24U-32V$
1	0	0	$E+V-U$
1	0	1	$E^3-2E^2U+E^2V+EU^2-EUV-16E+8U$
1	1	0	$(E-U)(E+V-U)$
1	1	1	$E+V-U$
2	1	0	E

Electronic correlations: NO occupations

Strong correlations: Extended Hubbard model

Population analysis: ground state, hole, exciton; $U/V = 2/1$ vs $16/4$