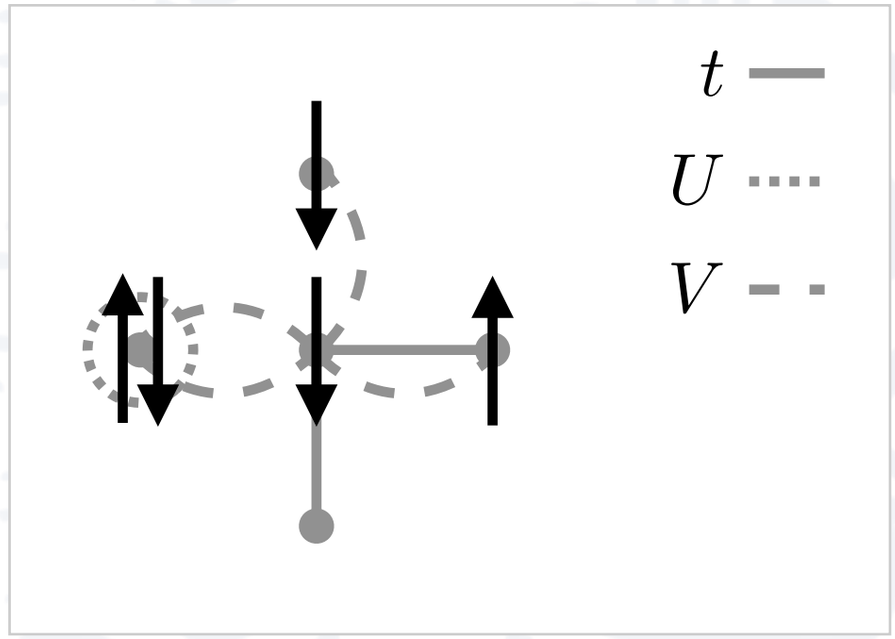
The Extended Hubbard Model

An Illustrated Primer

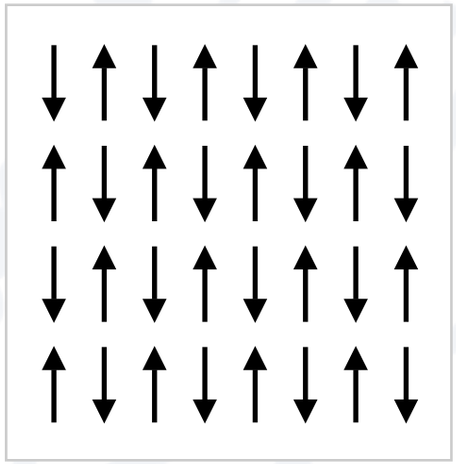
The Extended Hubbard Hamiltonian

$$H = -\sum_{i \neq j,\sigma} t_{i,j} c^{\dagger}_{i,\sigma} c_{j,\sigma} + \sum_{i} U_i n_{i,\uparrow} n_{i,\downarrow}$$

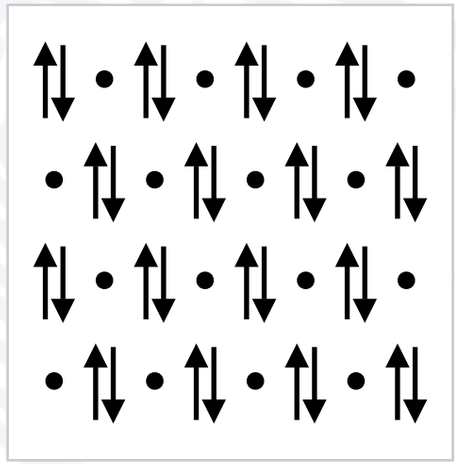
$$+ \frac{1}{2} \sum_{i \neq j,\sigma} V^{\uparrow\uparrow}_{i,j} n_{i,\sigma} n_{j,\sigma} + \frac{1}{2} \sum_{i \neq j,\sigma} V^{\uparrow\downarrow}_{i,j} n_{i,\sigma} n_{j,-\sigma}$$



Spin & Charge Density Wave Phases

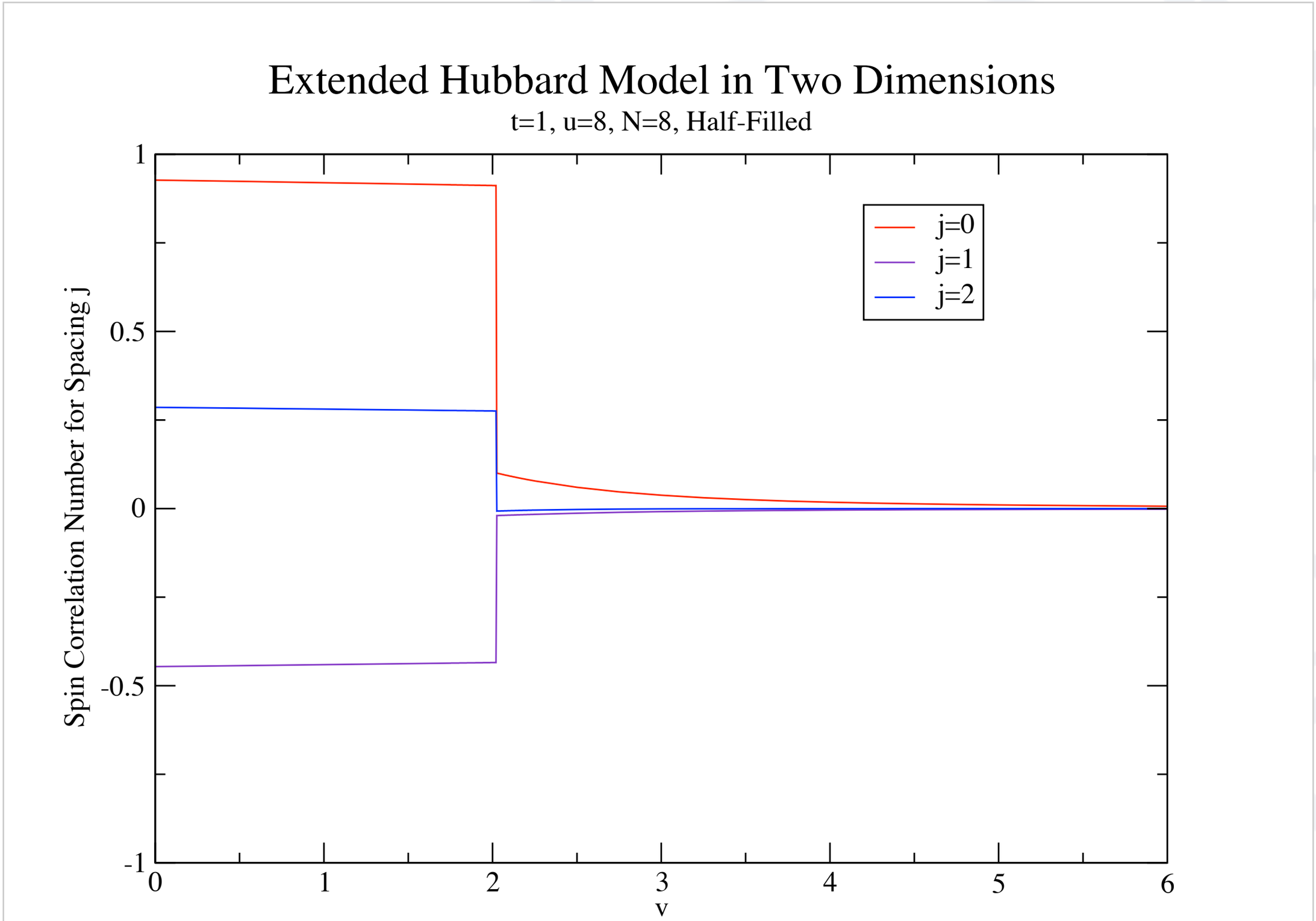


Spin Density Wave (SDW)
$U \gg 4V$

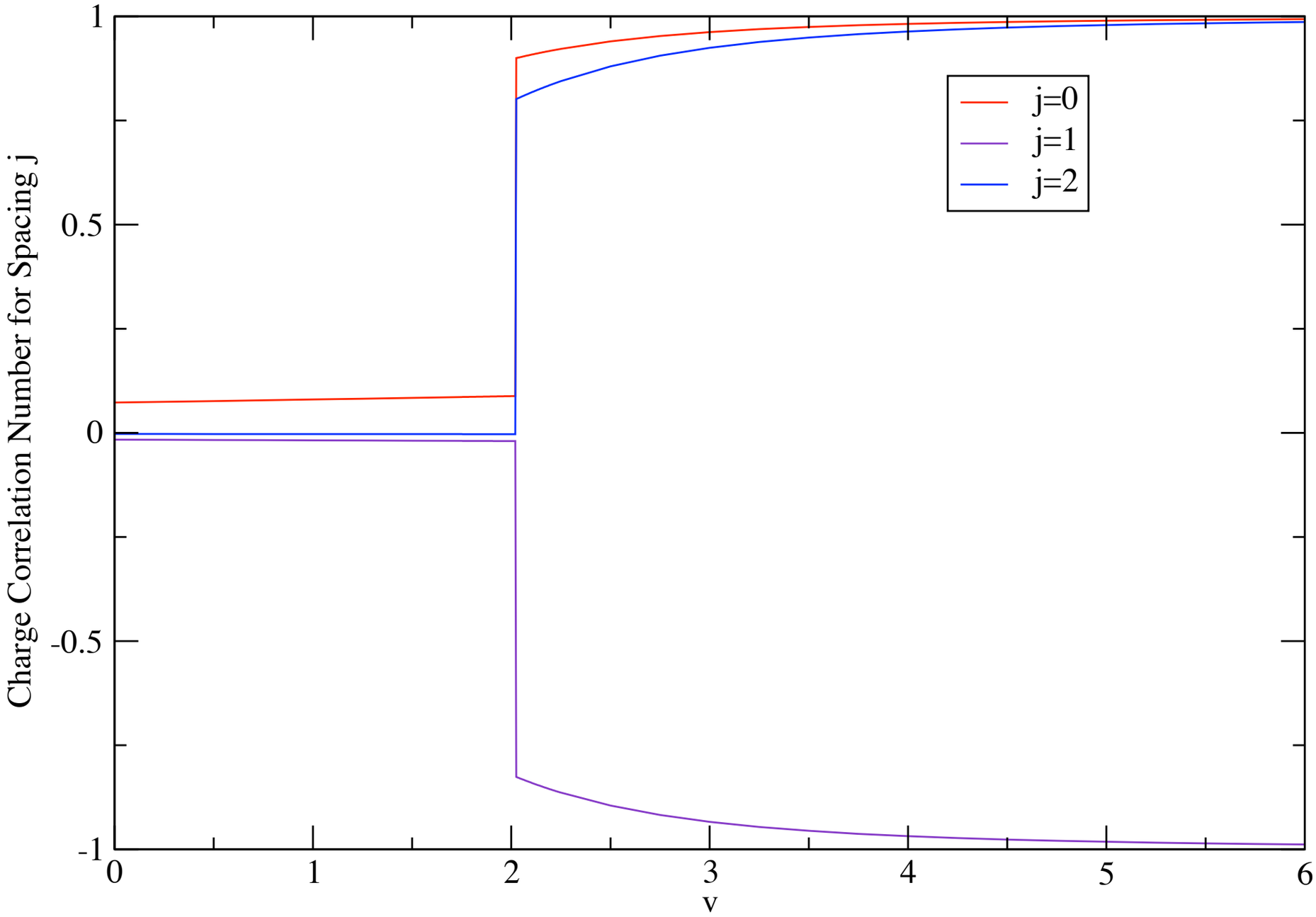


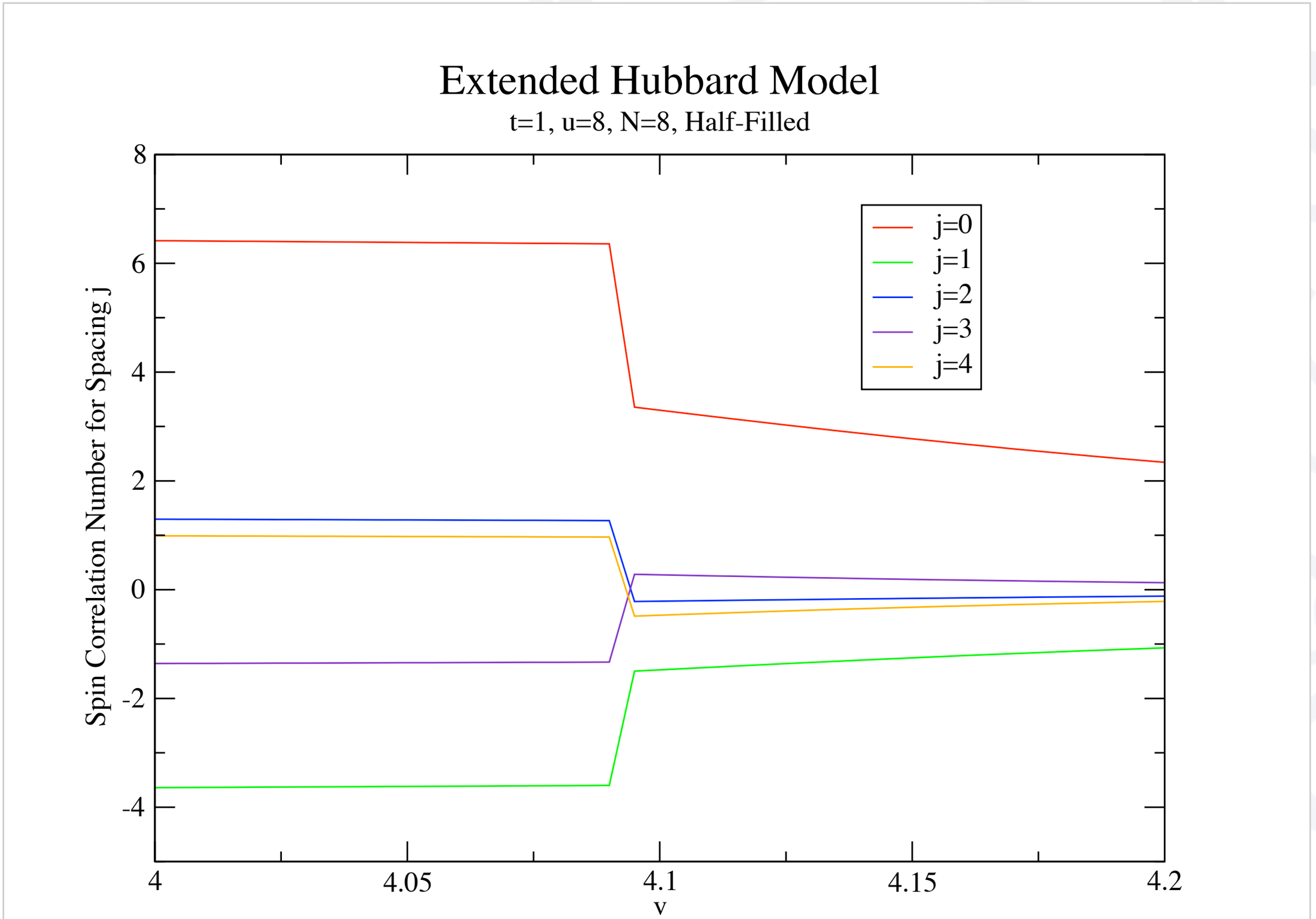
Charge Density Wave (CDW)
$U \ll 4V$

Spin Density Wave Example

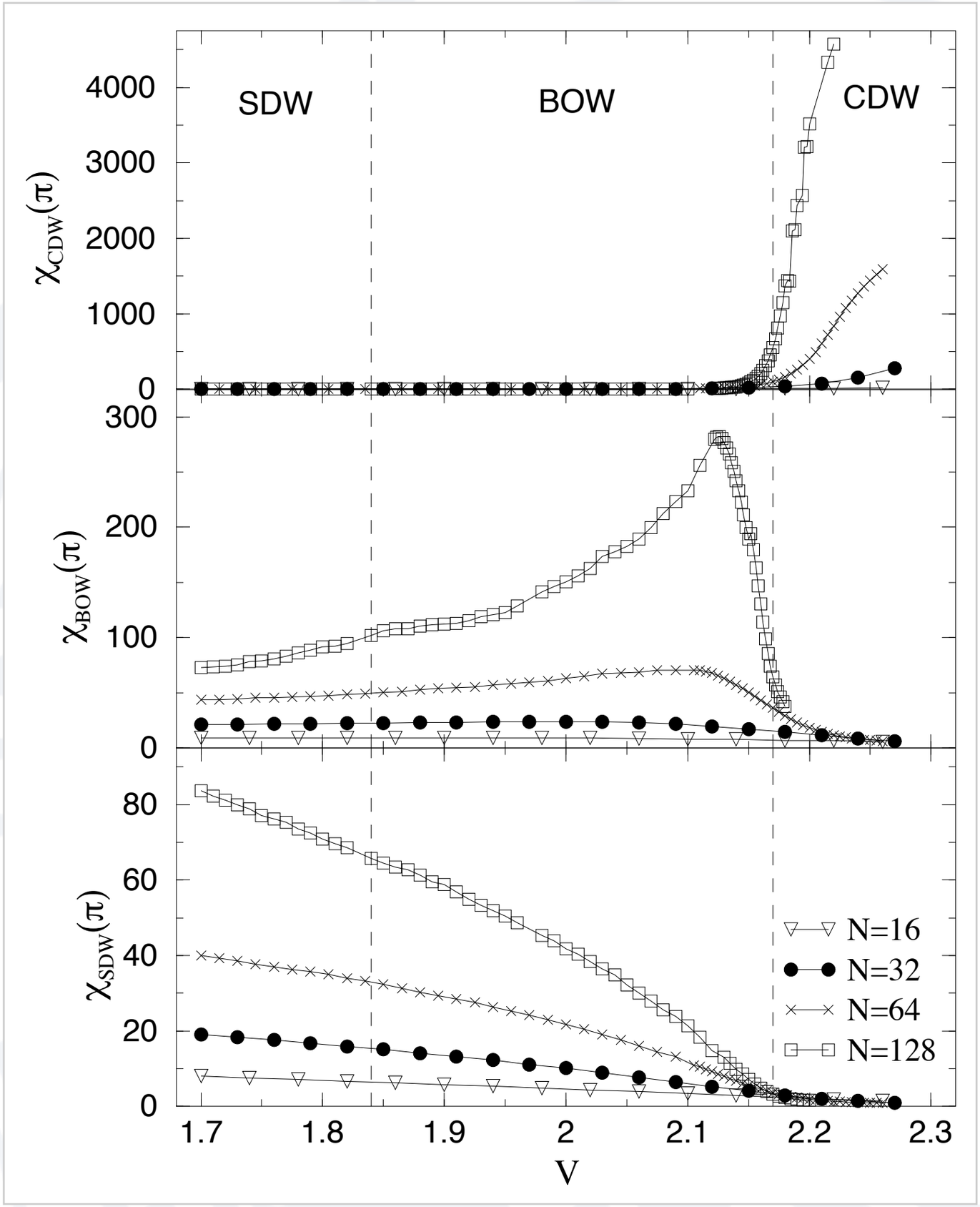


Charge Density Wave Example



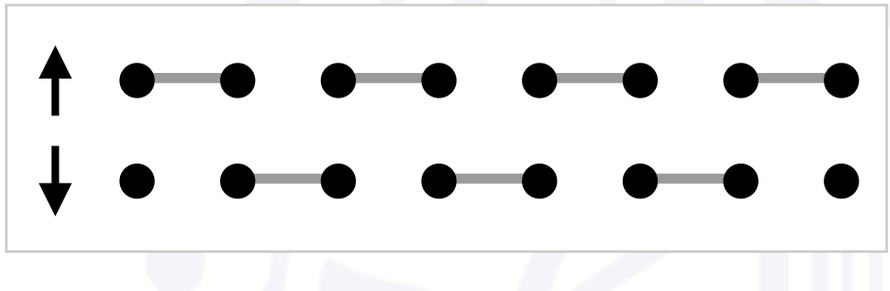

Extended Hubbard Model
t=1, u=8, N=8, Half-Filled
Spin Correlation Number for Spacing j
v
8
6
4
2
0
-2
-4
4
4.05
4.1
4.15
4.2
j=0
j=1
j=2
j=3
j=4

1D Phase Diagram

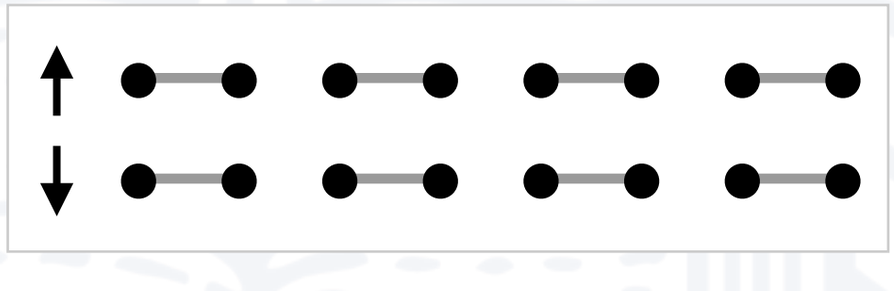


P. Sengupta, A. Sandvik, and D. Campbell, arXiv:cond-mat/0102141 (2002)

Bond Ordered Wave Phases

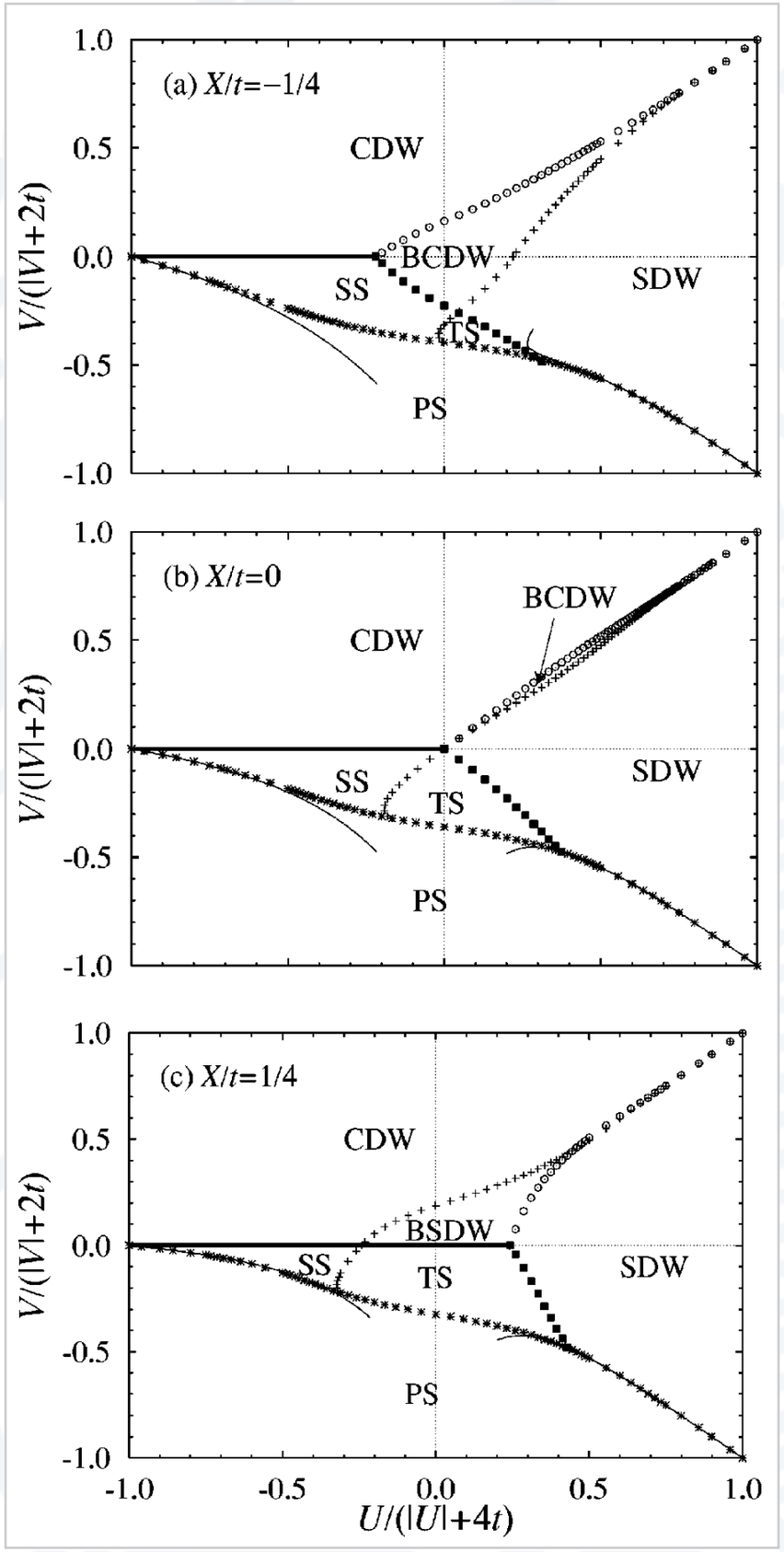


Bond Spin Density Wave (BSDW)



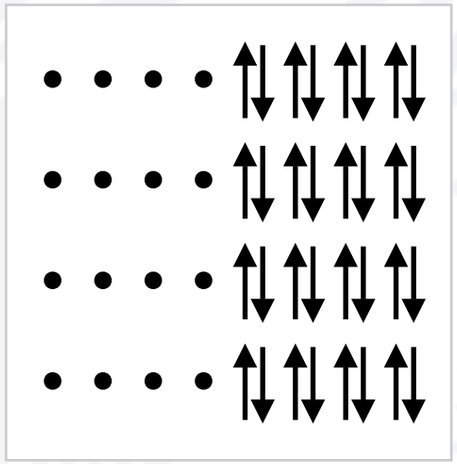
Bond Charge Density Wave (BCDW)
or
Bond Ordered Wave (BOW)

1D Phase Diagram Expanded



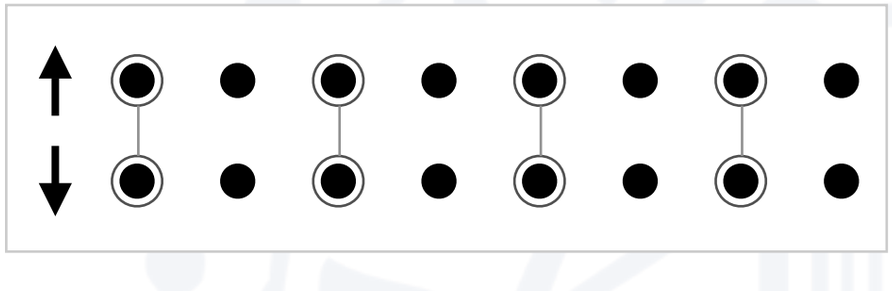
M. Nakamura, Phys. Rev. B 61, 377 (2000)

Negative U & V Behavior

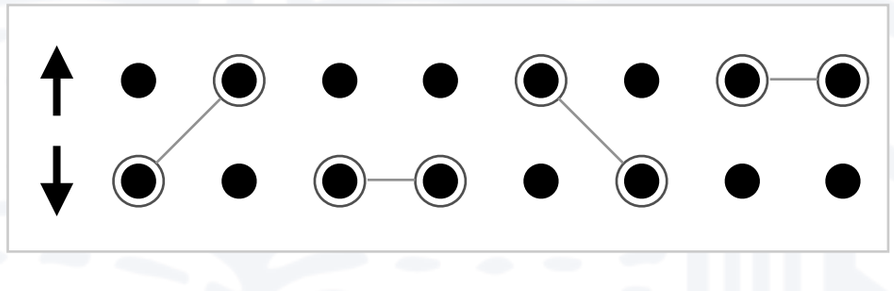


Phase-Separated State (PS)

Superconducting Phases



Singlet Superconducting Phase (SS)
or
Intra-site Cooper Pair



Triplet Superconducting Phase (TS)
or
Inter-site Cooper Pair

Summary of Expected Phases

$$SDW < n_{i,\uparrow} - n_{i,\downarrow} >$$
$$CDW < n_{i,\uparrow} + n_{i,\downarrow} - 1 >$$
$$BOW < c^{\dagger}_{i+j,\sigma} c_{i,\sigma} >$$
$$SS < c^{\dagger}_{i+j,\uparrow} c^{\dagger}_{i+j,\downarrow} c_{i,\uparrow} c_{i,\downarrow} >$$
$$TS < c^{\dagger}_{i+j,\sigma} c^{\dagger}_{i+j+1,\pm\sigma} c_{i,\sigma} c_{i+1,\pm\sigma} >$$

Exact Results for a Dimer

$$E_1 = 0; \quad |E_1\rangle = |0\rangle,$$

$$\begin{aligned}
E_2 &= -t; \quad |E_2\rangle = \tfrac{1}{\sqrt{2}}(|11\rangle + |13\rangle),\\
E_3 &= t; \quad |E_3\rangle = \tfrac{1}{\sqrt{2}}(|11\rangle - |13\rangle),\\
E_4 &= -t; \quad |E_4\rangle = \tfrac{1}{\sqrt{2}}(|12\rangle + |14\rangle),\\
E_5 &= t; \quad |E_5\rangle = \tfrac{1}{\sqrt{2}}(|12\rangle - |14\rangle),
\end{aligned}$$

$$\begin{aligned}
E_6 &= J^{(2)}; && |E_6\rangle = \tfrac{1}{\sqrt{2}}(|23\rangle + |24\rangle),\\
E_7 &= U; && |E_7\rangle = \tfrac{1}{\sqrt{2}}(|21\rangle - |26\rangle),\\
E_8 &= C + \tfrac{U+J^{(2)}}{2}; && |E_8\rangle = a_1(|21\rangle + |26\rangle) - a_2(|23\rangle - |24\rangle),\\
E_9 &= -C + \tfrac{U+J^{(2)}}{2}; && |E_9\rangle = a_2(|21\rangle + |26\rangle) + a_1(|23\rangle - |24\rangle),\\
E_{10} &= J^{(1)}; && |E_{10}\rangle = |22\rangle,\\
E_{11} &= J^{(1)}; && |E_{11}\rangle = |25\rangle,
\end{aligned}$$

$$\begin{aligned}
E_{12} &= t + U + J^{(1)} + J^{(2)}; && |E_{12}\rangle = \tfrac{1}{\sqrt{2}}(|31\rangle + |33\rangle),\\
E_{13} &= -t + U + J^{(1)} + J^{(2)}; && |E_{13}\rangle = \tfrac{1}{\sqrt{2}}(|31\rangle - |33\rangle),\\
E_{14} &= t + U + J^{(1)} + J^{(2)}; && |E_{14}\rangle = \tfrac{1}{\sqrt{2}}(|32\rangle + |34\rangle),\\
E_{15} &= -t + U + J^{(1)} + J^{(2)}; && |E_{15}\rangle = \tfrac{1}{\sqrt{2}}(|32\rangle - |34\rangle),
\end{aligned}$$

$$E_{16} = 2(U + J^{(1)} + J^{(2)}); \quad |E_{16}\rangle = |4\rangle$$

$$\begin{aligned}
|0\rangle &= |0,0;0,0\rangle, && |21\rangle = |1,1;0,0\rangle, && |31\rangle = |0,1;1,1\rangle,\\
& && |22\rangle = |1,0;1,0\rangle, && |32\rangle = |1,0;1,1\rangle,\\
|11\rangle &= |1,0;0,0\rangle, && |23\rangle = |1,0;0,1\rangle, && |33\rangle = |1,1;0,1\rangle,\\
|12\rangle &= |0,1;0,0\rangle, && |24\rangle = |0,1;1,0\rangle, && |34\rangle = |1,1;1,0\rangle,\\
|13\rangle &= |0,0;1,0\rangle, && |25\rangle = |0,1;0,1\rangle, &&\\
|14\rangle &= |0,0;0,1\rangle, && |26\rangle = |0,0;1,1\rangle, && |4\rangle = |1,1;1,1\rangle.
\end{aligned}$$

B. Grabiec, S. Krawiec, M. Matlak, and Z. Szafrana, arXiv:cond-mat/0511329 (2005)

Exact Results for a Dimer

$$H_D^{(3)} = E_6 P_6 = -J^{(2)}[{S_1}^z \cdot {S_2}^z - \frac{n_1^a n_2^a}{4}] + \frac{J^{(2)}}{2}\left({S_1}^+ \cdot {S_2}^- + {S_1}^- \cdot {S_2}^+\right) \quad (17)$$

$$\begin{aligned} H_D^{(4)} &= E_7 P_7 = \frac{U}{4}[n_1^b(1 - n_2^a - \frac{n_2^b}{2}) + n_2^b(1 - n_1^a - \frac{n_1^b}{2})] \\ &\quad -\frac{U}{2}[b_{1,\uparrow}^+ a_{1,\downarrow}^+ a_{2,\downarrow} b_{2,\uparrow} + b_{2,\uparrow}^+ a_{2,\downarrow}^+ a_{1,\downarrow} b_{1,\uparrow}], \end{aligned} \quad (18)$$

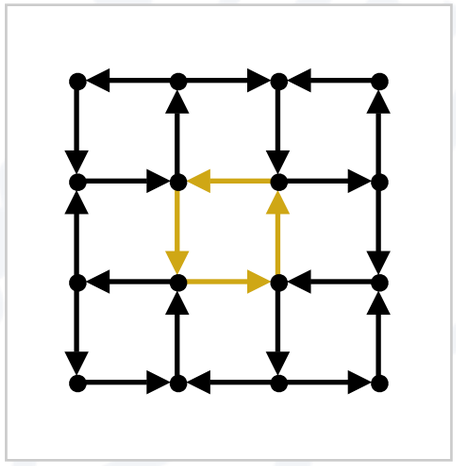
$$\begin{aligned} H_D^{(5)} &= E_8 P_8 = \left\{-\frac{J^{(2)}}{2} + [\frac{J^{(2)}(U - J^{(2)})}{4C} - \frac{2t^2}{C}]\right\}[\overrightarrow{S_1} \cdot \overrightarrow{S_2} - \frac{n_1^a n_2^a}{4}] \\ &\quad + \frac{1}{4}[U + C + \frac{(U^2 - (J^{(2)})^2)}{4C}][b_{1,\uparrow}^+ a_{1,\downarrow}^+ a_{2,\downarrow} b_{2,\uparrow} + b_{2,\uparrow}^+ a_{2,\downarrow}^+ a_{1,\downarrow} b_{1,\uparrow}] \\ &\quad + \left\{\frac{U}{8} + \frac{1}{8}[C + \frac{(U^2 - (J^{(2)})^2)}{4C}]\right\}[n_1^b(1 - n_2^a - \frac{n_2^b}{2}) + n_2^b(1 - n_1^a - \frac{n_1^b}{2})] \\ &\quad + \left\{-\frac{t}{2} - \frac{t(U + J^{(2)})}{4C}\right\}\sum_\sigma \sum_{i=1}^{2}[a_{i,\sigma}^+ b_{\bar{i},\sigma} + b_{i,\sigma}^+ a_{\bar{i},\sigma}], \end{aligned} \quad (19)$$

$$\begin{aligned} H_D^{(6)} &= E_9 P_9 = \left\{-\frac{J^{(2)}}{2} - [\frac{J^{(2)}(U - J^{(2)})}{4C} - \frac{2t^2}{C}]\right\}[\overrightarrow{S_1} \cdot \overrightarrow{S_2} - \frac{n_1^a n_2^a}{4}] \\ &\quad + \frac{1}{4}[U - C - \frac{(U^2 - (J^{(2)})^2)}{4C}][b_{1,\uparrow}^+ a_{1,\downarrow}^+ a_{2,\downarrow} b_{2,\uparrow} + b_{2,\uparrow}^+ a_{2,\downarrow}^+ a_{1,\downarrow} b_{1,\uparrow}] \\ &\quad + \left\{\frac{U}{8} - \frac{1}{8}[C + \frac{(U^2 - (J^{(2)})^2)}{4C}]\right\}[n_1^b(1 - n_2^a - \frac{n_2^b}{2}) + n_2^b(1 - n_1^a - \frac{n_1^b}{2})] \\ &\quad + \left\{-\frac{t}{2} + \frac{t(U + J^{(2)})}{4C}\right\}\sum_\sigma \sum_{i=1}^{2}[a_{i,\sigma}^+ b_{\bar{i},\sigma} + b_{i,\sigma}^+ a_{\bar{i},\sigma}], \end{aligned} \quad (20)$$

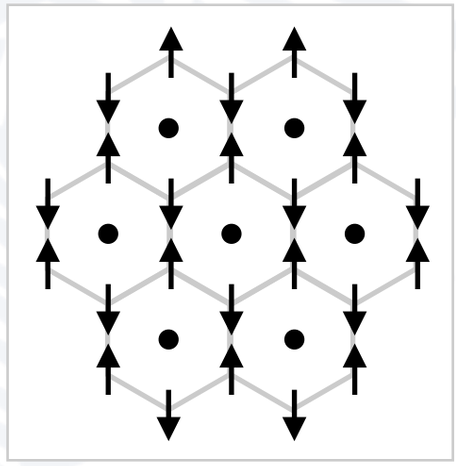
$$H_D^{(7)} = E_{10} P_{10} + E_{11} P_{11} = 2J^{(1)}[{S_1}^z \cdot {S_2}^z + \frac{n_1^a n_2^a}{4}] \quad (21)$$

B. Grabiec, S. Krawiec, M. Matlak, and Z. Szafrana, arXiv:cond-mat/0511329 (2005)

What We Hope to See



Flux Ordered Wave
(Andrew)



Spin Density Wave
(Chris)

References

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