A theoretical description of the interplay of collective fluctuations in strongly correlated systems

Erik Linnér

Erik Linnér, A. I. Lichtenstein, S. Biermann and E. A. Stepanov, arXiv:2210.05540 (2022)
Erik Linnér, C. Dutreix, S. Biermann and E. A. Stepanov, arXiv:2301.10755 (2023)

GDR MEETICC Conférence plénière 2023 - 31st of May 2023

Interplaying collective fluctuations

- A hallmark of materials with strong electronic Coulomb correlations :
  Rich phase diagrams exhibiting various kinds of ordering phenomena

- **WANTED:** Efficient approaches to describe interplaying collective fluctuations

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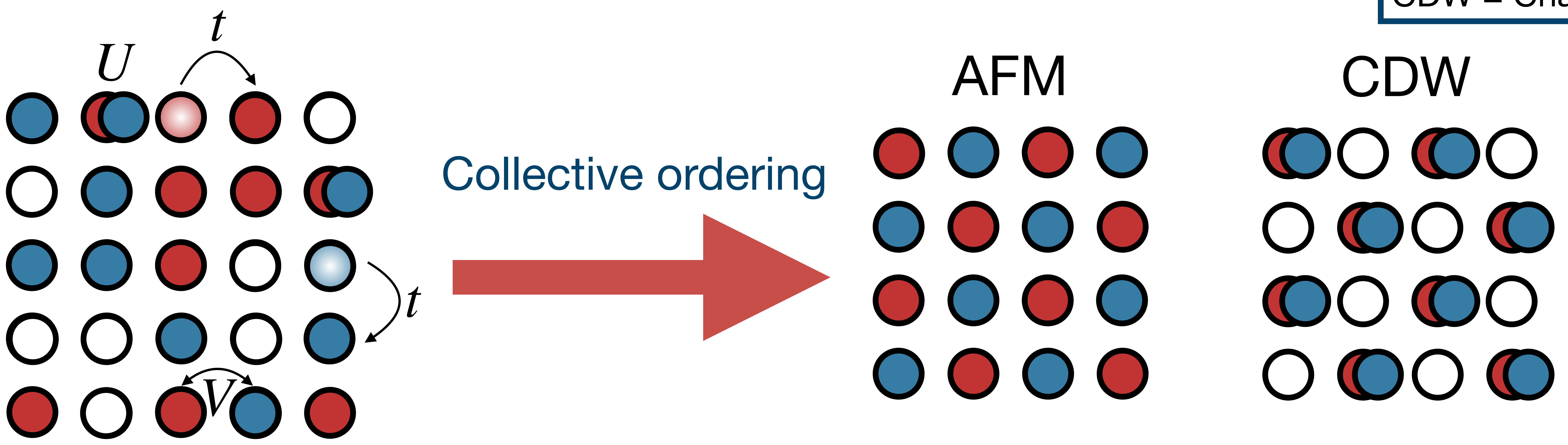
- Model for interplaying collective fluctuations in a fermionic system:
  Extended Hubbard model

- Competing local on-site U and nearest neighbour non-local V

$$\hat{H} = -t \sum_{\langle i,j \rangle,\sigma} \hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + U \sum_{i} \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} + \frac{1}{2}V \sum_{\langle i,j \rangle,\sigma\sigma'} \hat{n}_{i\sigma}\hat{n}_{j\sigma'} \qquad \hat{n}_{i\sigma} = \hat{c}^{\dagger}_{i\sigma}\hat{c}_{i\sigma}$$

t = hopping, U = local on-site interaction, V = non-local nearest-neighbour interaction

AFM = Antiferromagnetism
CDW = Charge density wave



Previous work (non-exhaustive)

Extended Hubbard model :

Earliest considerations

J. Hubbard, Proc. R. Soc. Long. A **276**, 238-257 (1963)
R. A. Bari, Phys. Rev. B **3**, 2662-2670 (1971)
V. J. Emery, Phys. Rev. B **14**, 2989-2994 (1976)
J. Sólyom, Adv. Phys. **28**, 201-303 (1979)

Experimentally relevant work :

J. M. Tranquada, et. al. Nature **375**, 561 (1995)
J. Hoffman, et. al. Science **295**, 466 (2002)
C. Howald, Proc. Natl. Acad. Sci. USA **100**, 9705 (2003)
Y. Wang, et. al. Phys. Rev. Lett. **127**, 197003 (2021)
X. Wang, et. al. Nat Commun **13**, 6824 (2022)
Q. Li, et. al. Nature **609**, 479 (2022)

Wanted :

Efficient approach to describe interplaying collective fluctuations with:

- No explicit symmetry breaking
- Direct treatment of interplaying fluctuations
- Numerically low-cost approach

Competing instabilities in the model two-dimensional model :

- Repulsive interactions :

  B. Fourcade and G. Spronken, Phys. Rev. B **29**, 5096-5102 (1984)
  A. M. Oleś, R. Micnas, S. Robaszkiewicz, and K. A. Chao, Phys. Lett. A **102**, 323-326 (1984)
  J. E. Hirsch, Phys. Rev. Lett. **53**, 2327-2330 (1984)
  Y. Zhang and J. Callaway, Phys. Rev. B **42**, 465-474 (1990)
  J. Callaway, et. al. , Phys. Rev. B **42**, 465-474 (1990)
  M. Aichhorn, H. G. Evertz, W. von der Linden, and M. Potthoff, Phys. Rev. B **70**, 235107 (2004)
  B. Davoudi, and A.-M. S. Tremblay, Phys. Rev. B **74**, 035113 (2006)
  B. Davoudi, and A.-M. S. Tremblay, Phys. Rev. B **76**, 085115 (2007)
  T. Ayral, P. Werner, and S. Biermann, Phys. Rev. Lett. **109**, 226401 (2012)
  T. Ayral, S. Biermann, and P. Werner, Phys. Rev. B **87**, 125149 (2013)
  H. Terletska, T. Chen, and E. Gull, Phys. Rev. B **95**, 115149 (2017)
  J. Paki, H. Terletska, S. Iskakov, and E. Gull, Phys. Rev. B **99**, 245146 (2019)
  P. Pudleiner, A. Kauch, K. Held, and G. Li, Phys. Rev. B **100**, 075108 (2019)

- Attractive interactions :

  V. J. Emery, Phys. Rev. B **14**, 2989-2994 (1976)
  S. Robaszkiewicz, R. Micnas, K. A. Chao, Phys. Rev. B **23**, 1447-1458 (1981)
  R. T. Scaletter, et. al., Phys. Rev. Lett. **62**, 1407-1410 (1989)
  C. N. Yang, Phys. Rev. Lett. **63**, 2144-2147 (1989)
  A. A. Aligia, Phys. Rev. B 61, 7028-7032 (2000)
  B. Davoudi, and A.-M. S. Tremblay, Phys. Rev. B **76**, 085115 (2007)
  E. G. C. P. Van Loon, and M. I. Katsnelson, J. Phys.: Conf. Ser. 1136, 012006 (2018)
  M. Yao, D. Wang, and Q.-H. Wang, Phys. Rev. B **106**, 195121 (2022)

Multi-Channel Fluctuating Field theory

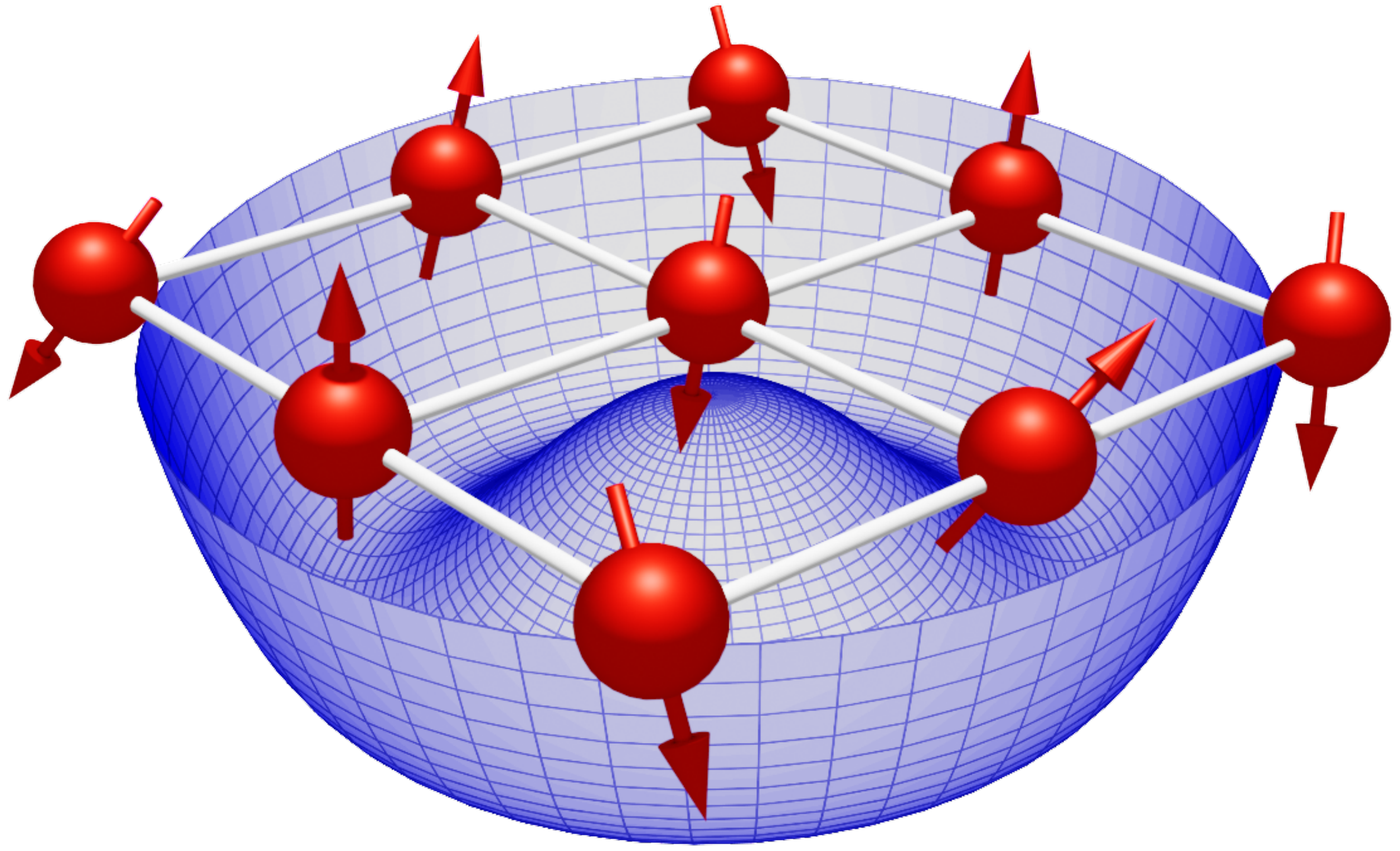
Action of a correlated quantum lattice system
Unfeasible to solve exactly

Variational optimisation →

Trial action incorporating leading collective fluctuations
Exactly solvable

- **Fluctuating (local) field (FF) : Variational construction of a trial system allowing for a cheap non-perturbative treatment of the spin channel**
  A. N. Rubtsov, PRE 97, 052120 (2018)
  A. N. Rubtsov, E. A. Stepanov, and A. I. Lichtenstein, PRB 102, 224423 (2020)

- **Here: Development of a multi-channel generalisation of the FF approach in order to study interplaying collective fluctuations**
  EL, A. I. Lichtenstein, S. Biermann and E. A. Stepanov, arXiv:2210.05540 (2022)



A. N. Rubtsov, et. al., PRB 102 224423 (2020)

Variational optimisation

Action construction of the extended Hubbard model:

$$\mathcal{S} = -\frac{1}{\beta N}\sum_{\mathbf{k},\nu,\sigma} c^*_{\mathbf{k}\nu\sigma}\mathcal{G}^{-1}_{\mathbf{k}\nu}c_{\mathbf{k}\nu\sigma} + \frac{U}{\beta N}\sum_{\mathbf{q},\omega} n_{\mathbf{q}\omega\uparrow}n_{-\mathbf{q},-\omega\downarrow} + \frac{1}{2\beta N}\sum_{\mathbf{q},\omega,\sigma\sigma'} V_{\mathbf{q}}n_{\mathbf{q}\omega\sigma}n_{-\mathbf{q},-\omega\sigma'}$$

Inverse temperature β Number of sites N Inverse bare Green's function $\mathcal{G}^{-1}_{\mathbf{k}\nu} = i\nu + \mu - \epsilon_{\mathbf{k}}$

Bare dispersion $\epsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y)$ Chemical potential μ Non-local interaction $V_{\mathbf{q}} = 2V(\cos q_x + \cos q_y)$

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Multi-channel fluctuating field trial action:

$$\mathcal{S}^* = -\frac{1}{\beta N}\sum_{\mathbf{k},\nu,\sigma} c^*_{\mathbf{k}\nu\sigma}\mathcal{G}^{-1}_{\mathbf{k}\nu}c_{\mathbf{k}\nu\sigma} + \sum_{\mathbf{Q},\varsigma}\left[\phi^{\varsigma}_{\mathbf{Q}}n^{\varsigma}_{-\mathbf{Q}} - \frac{1}{2}\frac{\beta N}{J^{\varsigma}_{\mathbf{Q}}}\phi^{\varsigma}_{\mathbf{Q}}\phi^{\varsigma}_{-\mathbf{Q}}\right]$$

CDW = Charge density wave
AFM = Antiferromagnetism
s-SC = *s*-wave superconductivity
PS = Phase separation

Collective CDW/AFM/s-SC fluctuations are incorporated with $\varsigma = c/s/s-SC$ [c = charge, s = spin, $s-SC$ = s-wave SC] for a given ordering vector $\mathbf{Q}$ [e.g. $\mathbf{M} = (\pi,\pi)$ for CDW, AFM and s-SC, and $\mathbf{\Gamma} = (0,0)$ for PS]

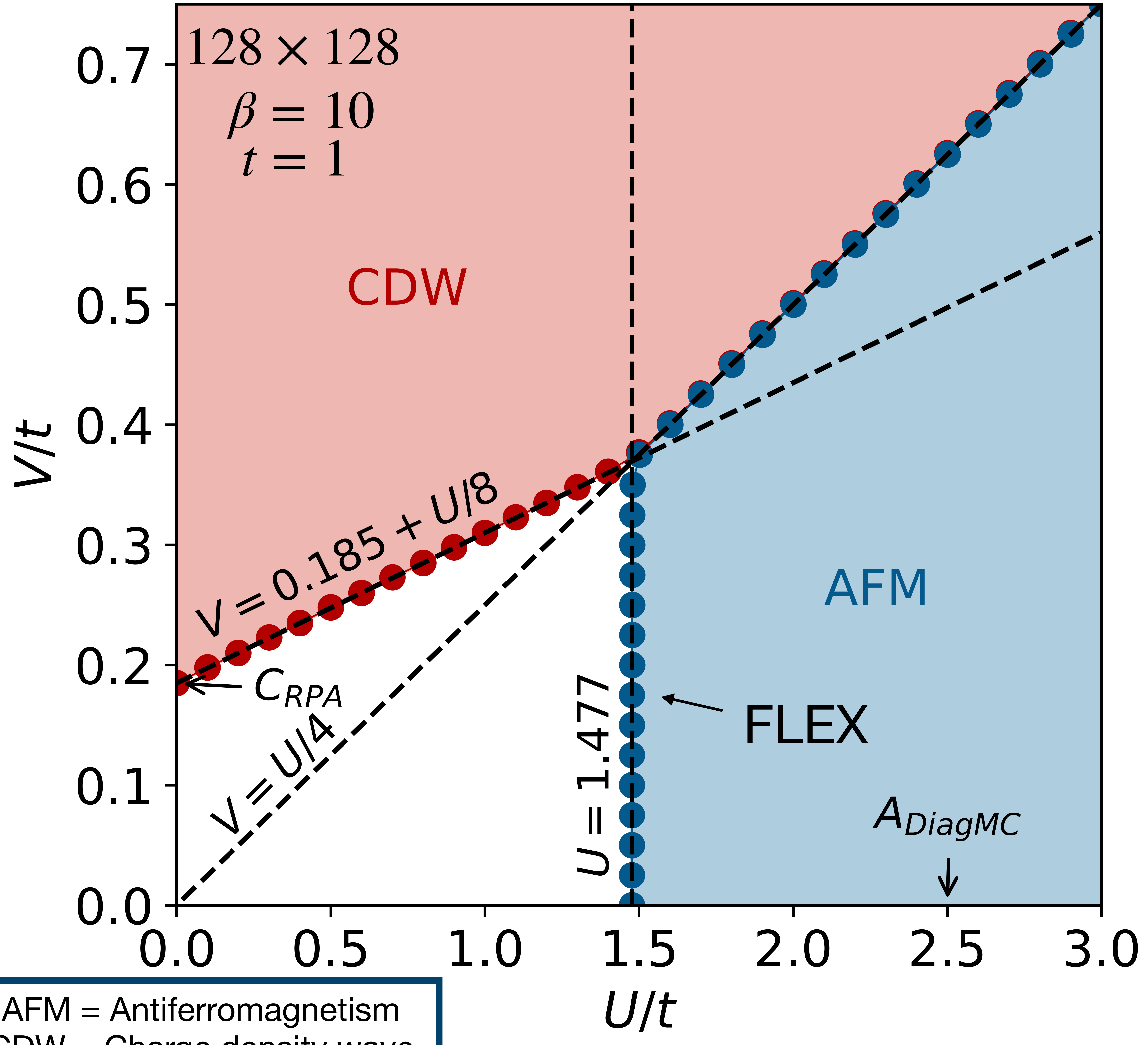
- Stiffness parameters $J^{\varsigma}_{\mathbf{Q}}$ are determined by a variational principle: $J^c_{\mathbf{M}} = U/2 - 4V$, $J^s_{\mathbf{M}} = -U/2$, $J^{s-SC}_{\mathbf{M}} = U/2$, $J^c_{\mathbf{\Gamma}} = U/2 - 4V$
- Simplified action allows for a numerically exact treatment without any explicit symmetry breaking
- Collective fluctuations are studied through a free energy construction, allowing to distinguish stable and metastable states

Phase diagram of the extended Hubbard model
with repulsive local U interaction
and repulsive nearest-neighbour V interaction

Repulsive $U - V$ phase diagram

Local interaction : U
Nearest-neighbour interaction : V

arXiv:2210.05540 (2022)



AFM = Antiferromagnetism
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A_{DiagMC} taken from F. Simkovic, et. al., PRL 124, 017003 (2020)

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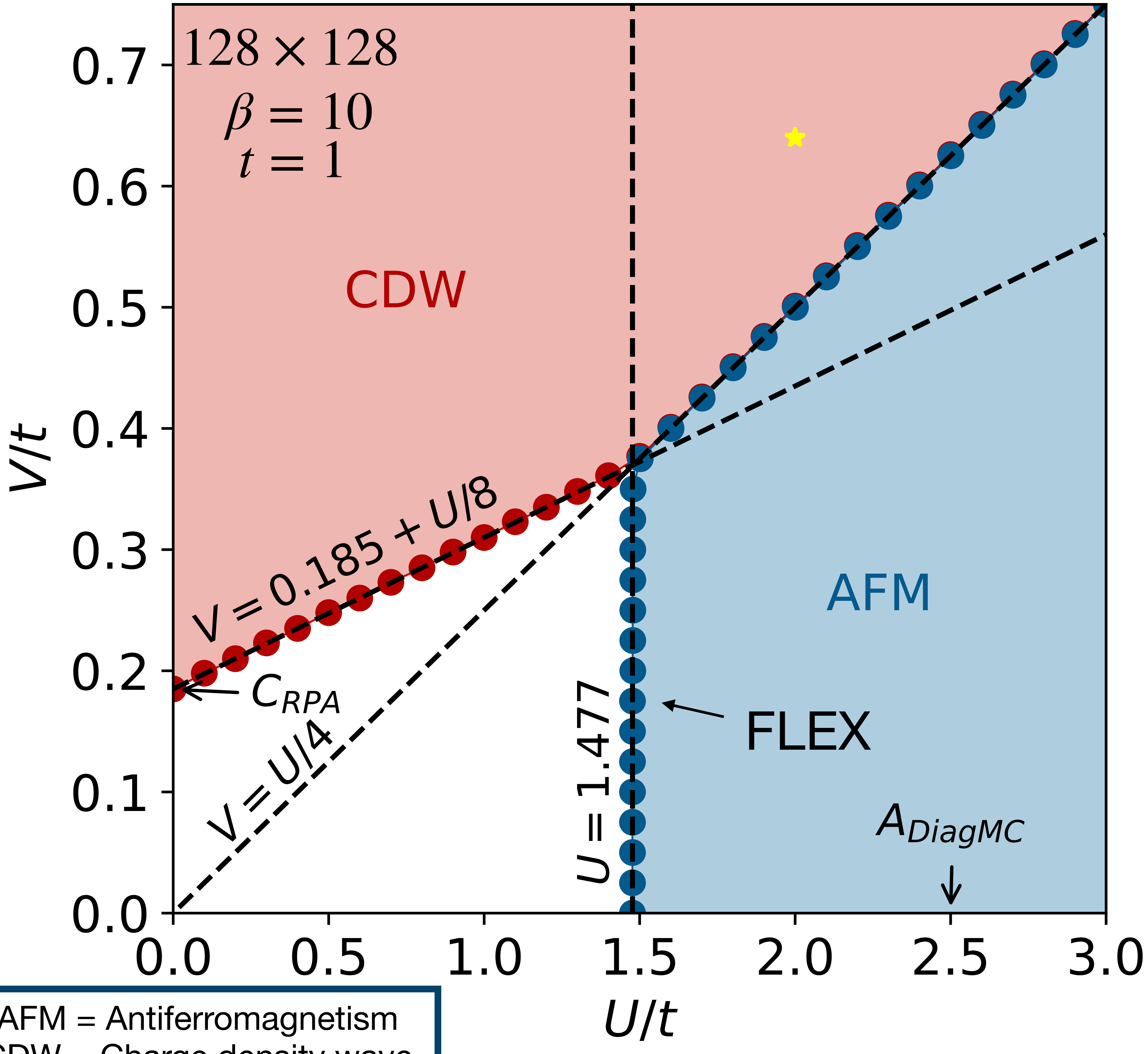

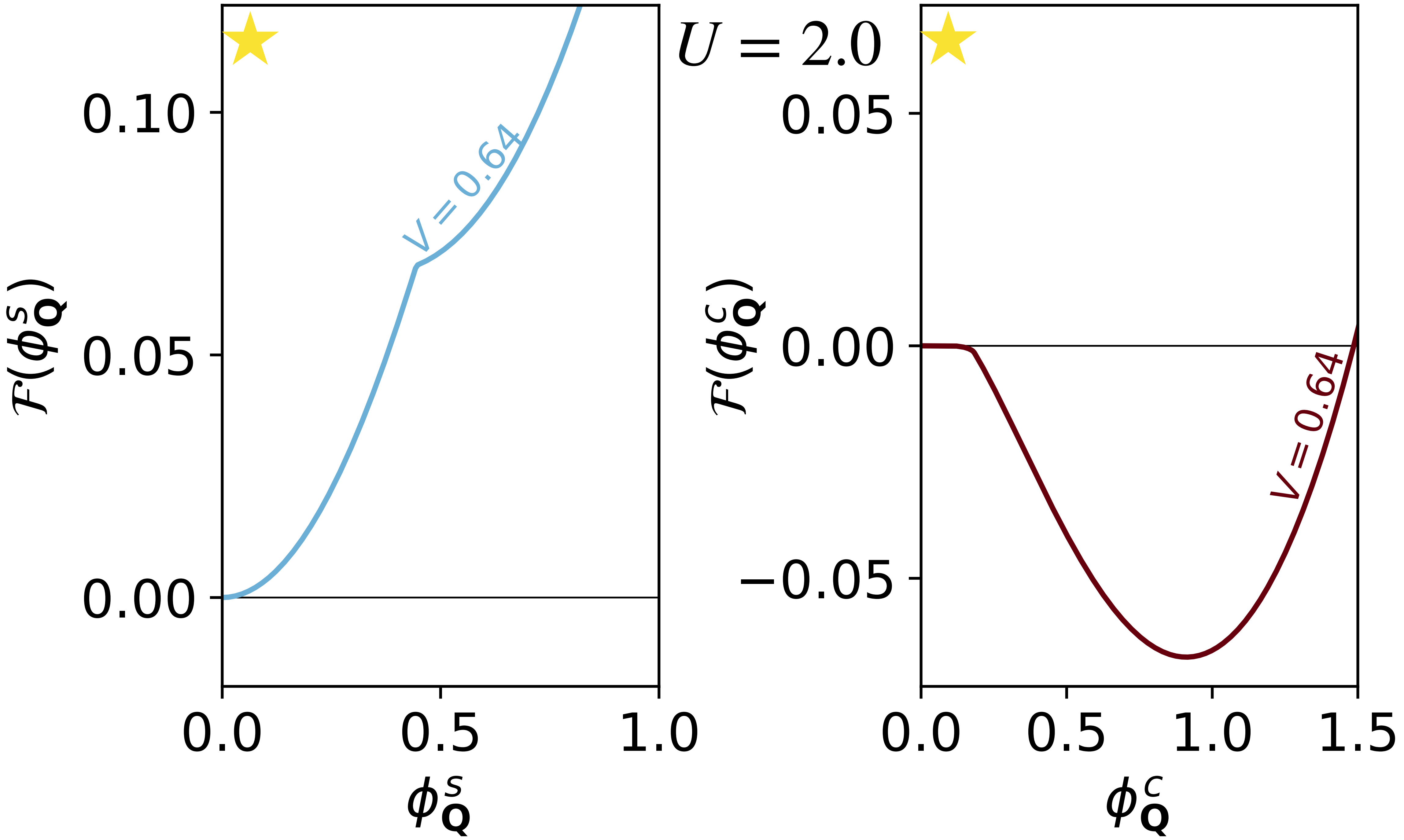

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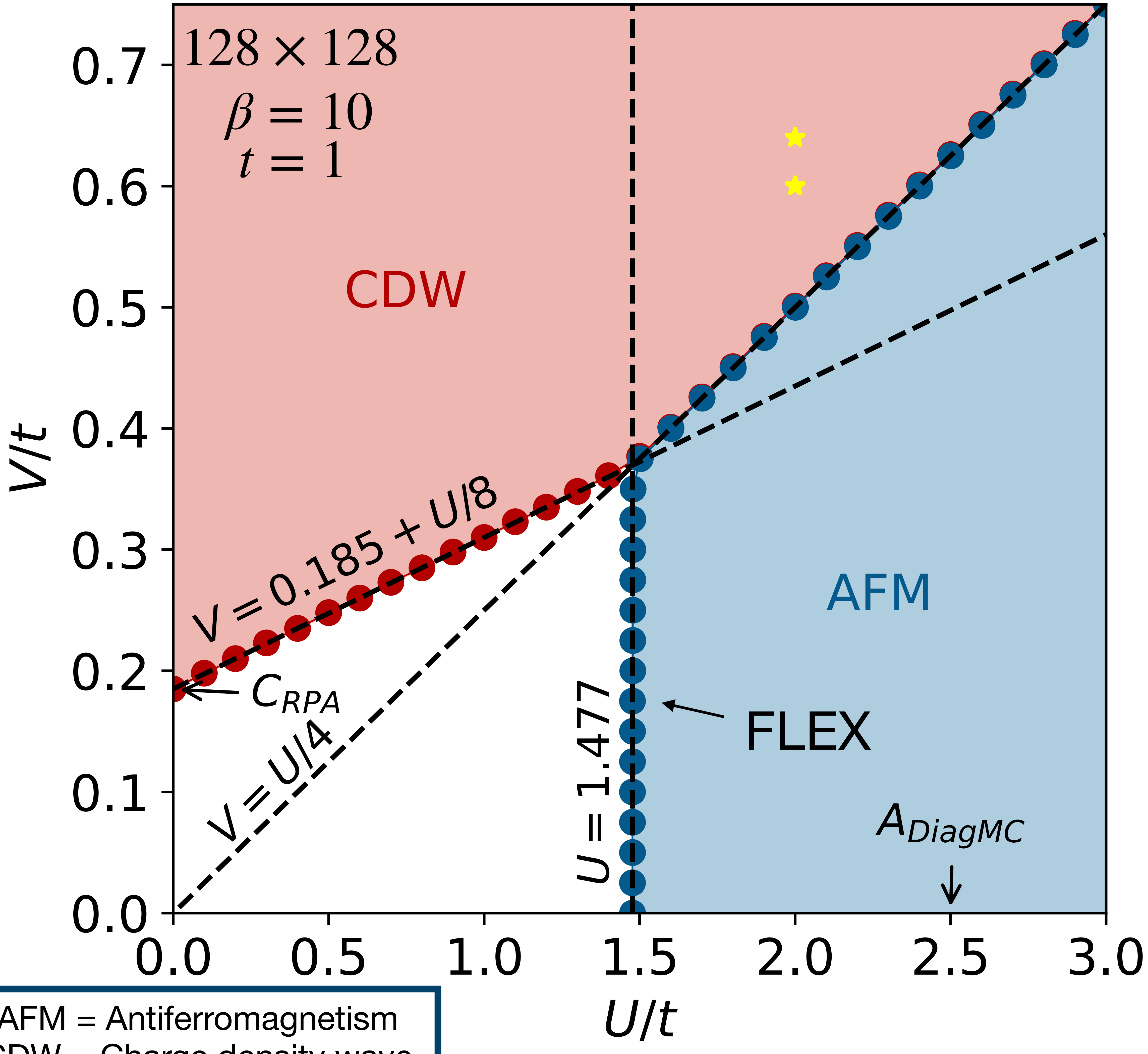

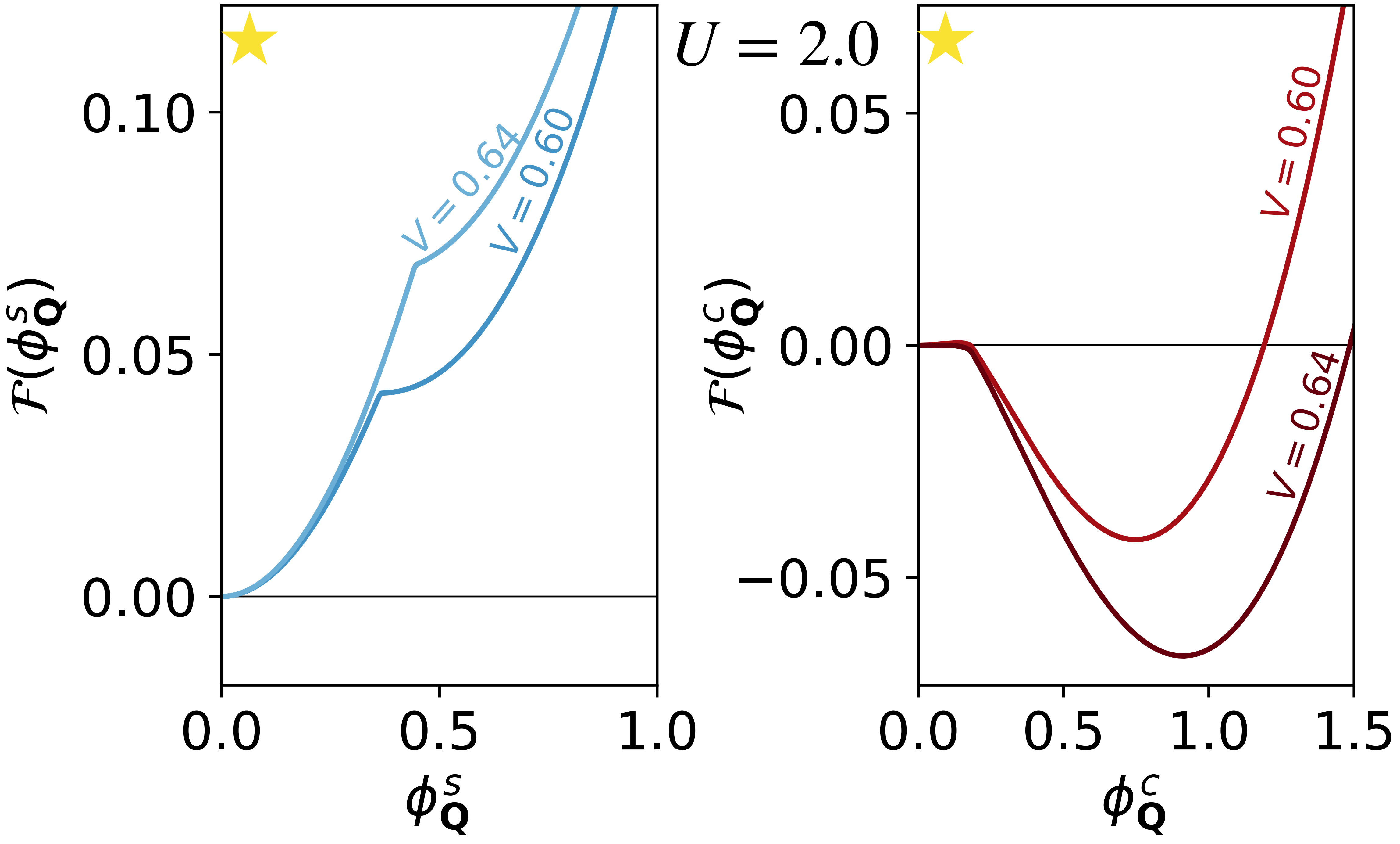

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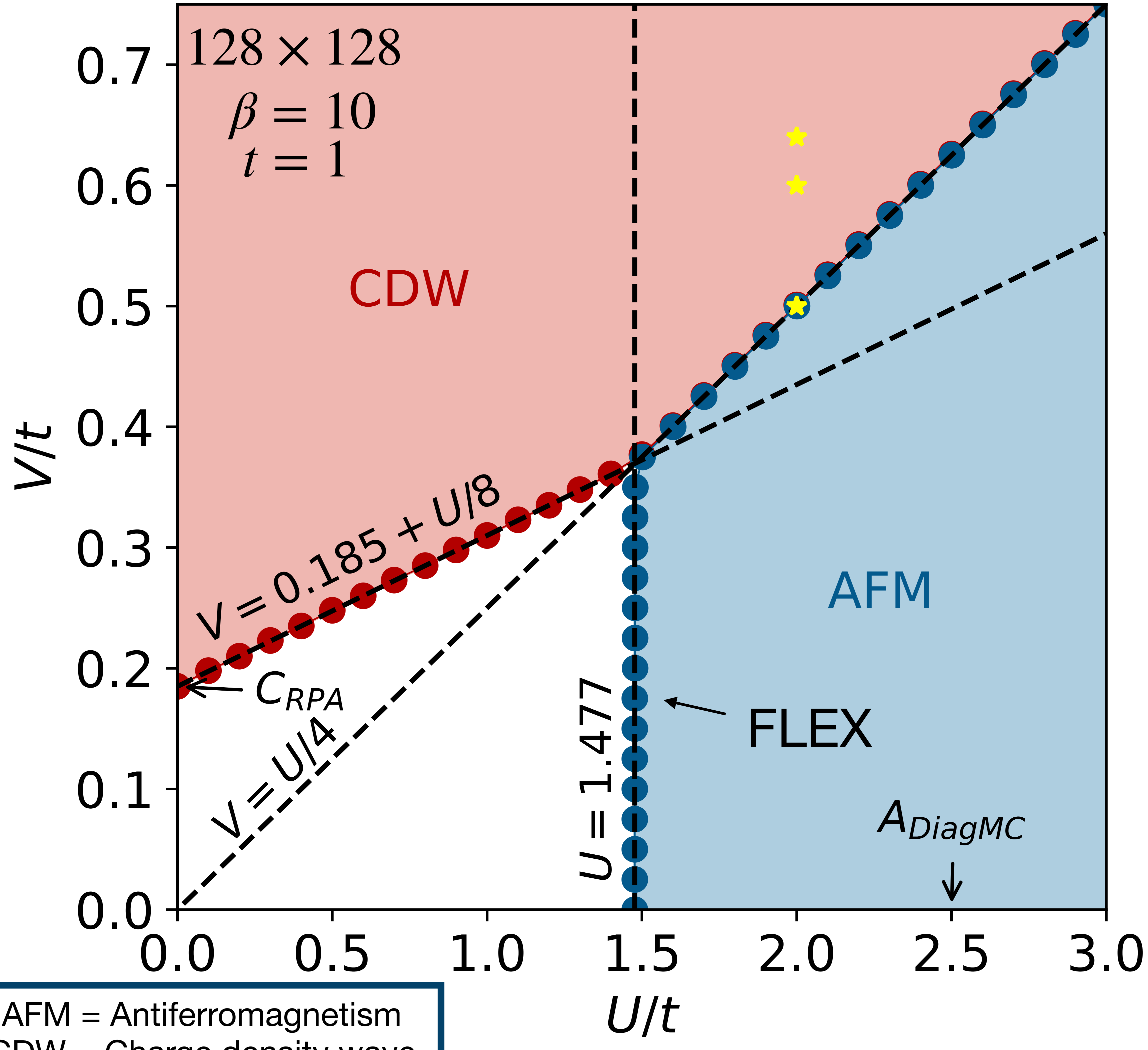

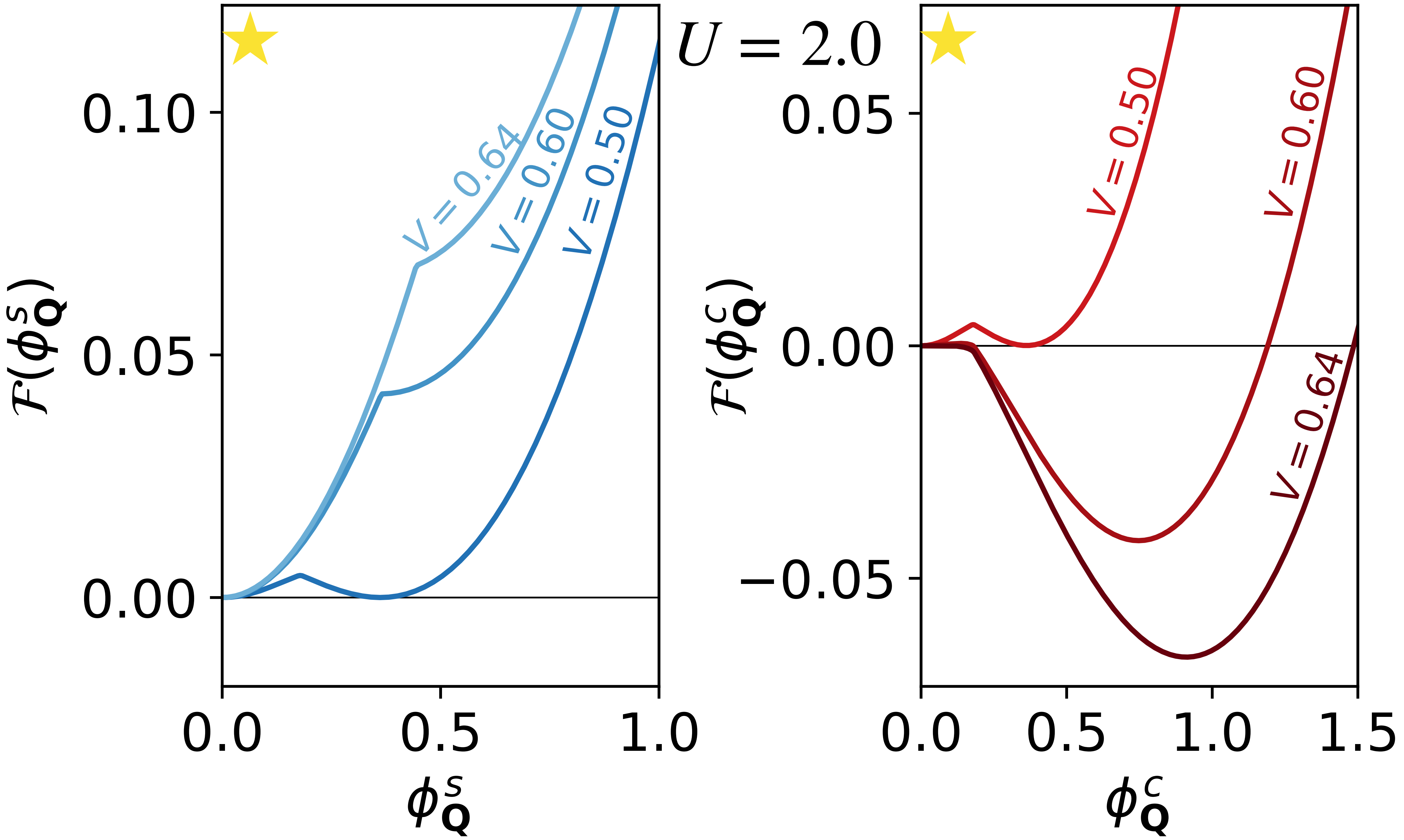

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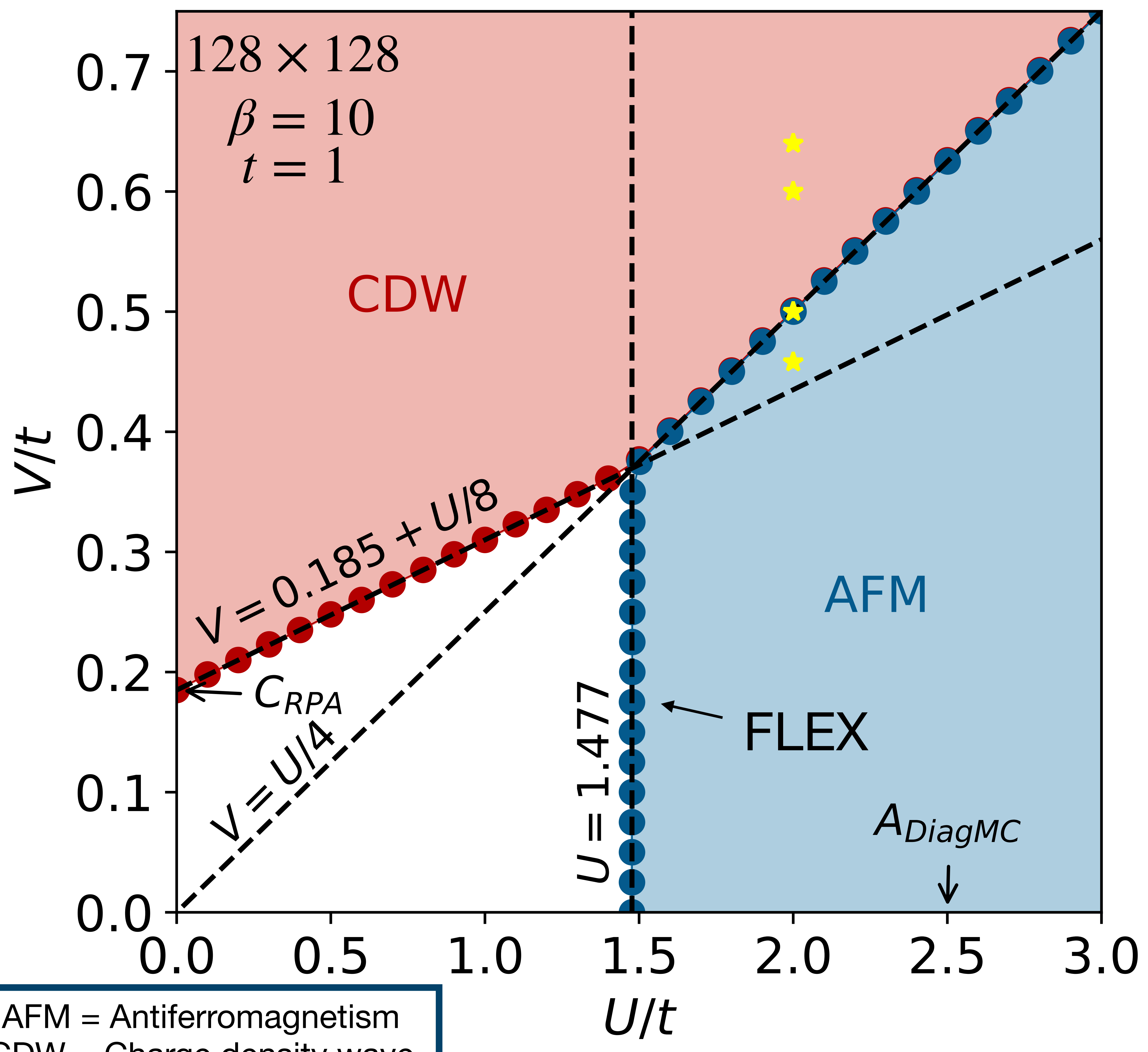

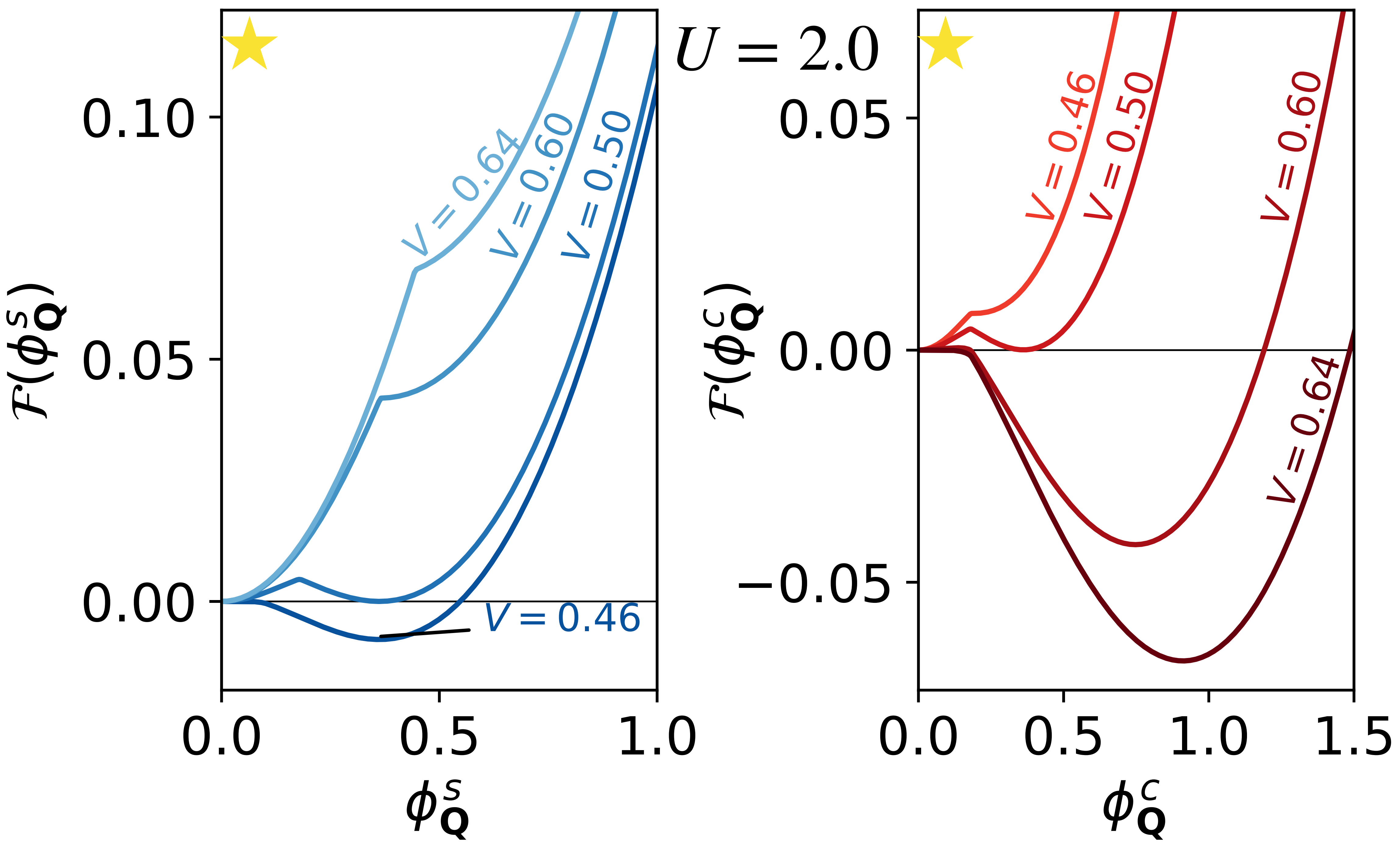

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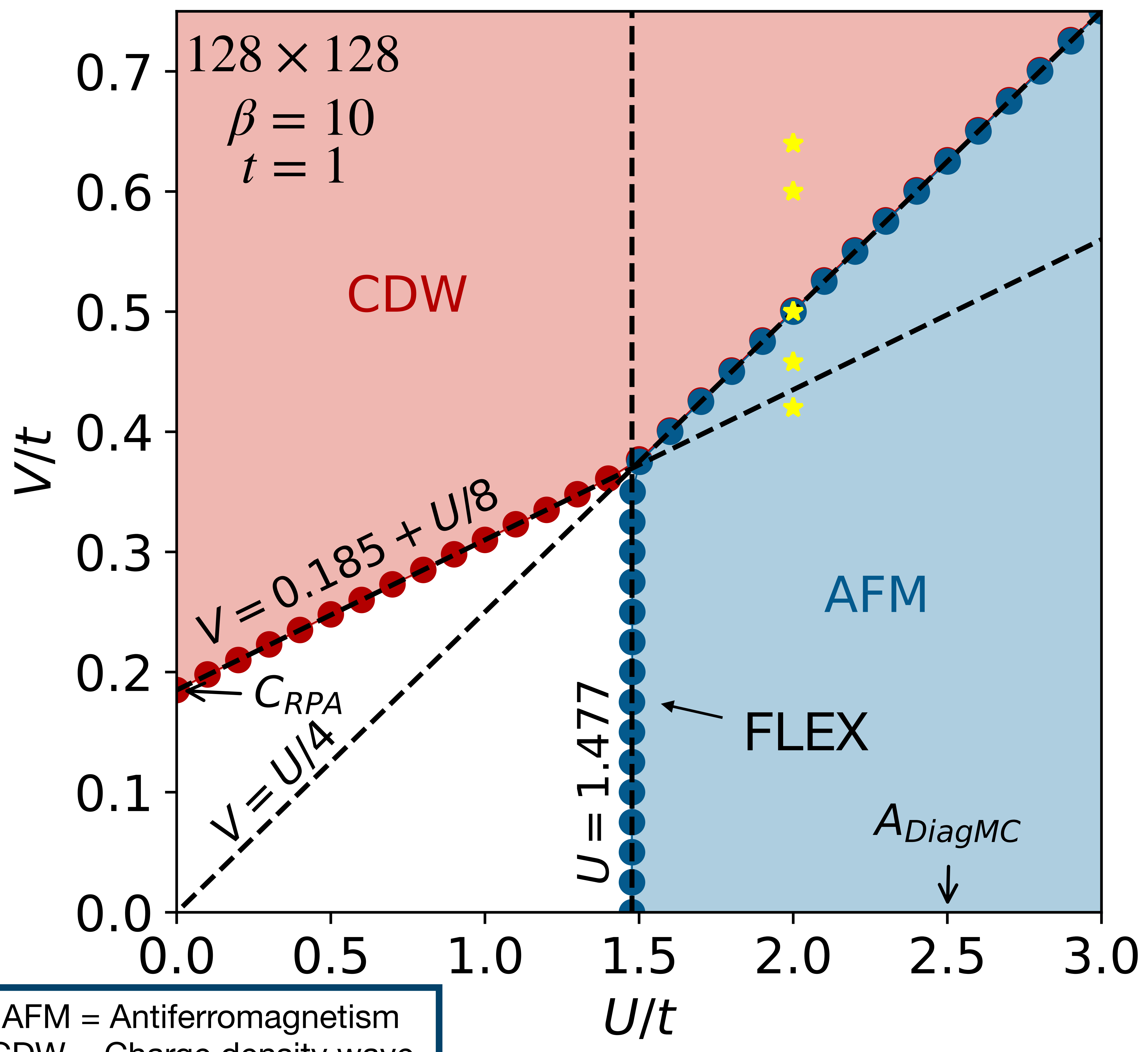

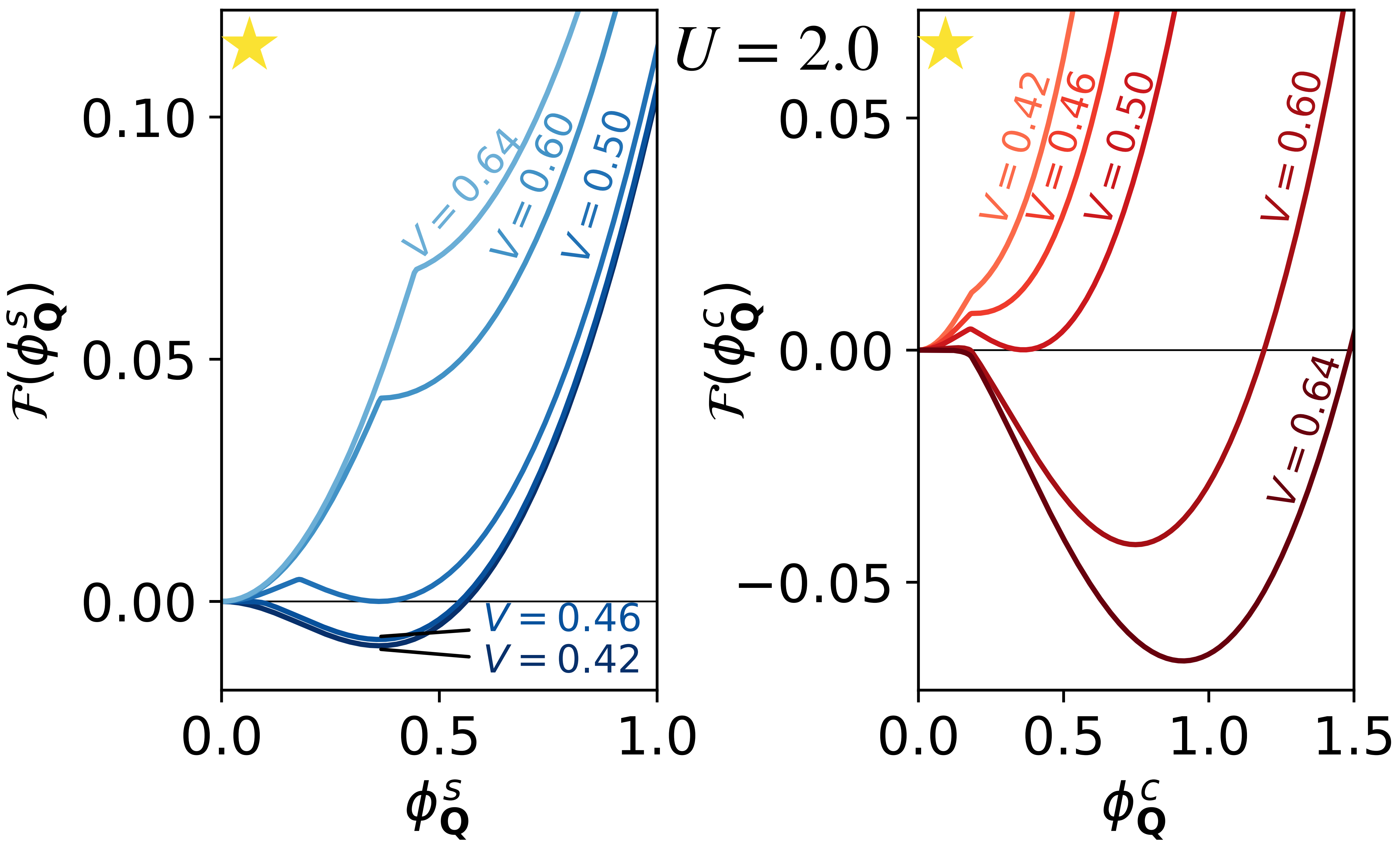

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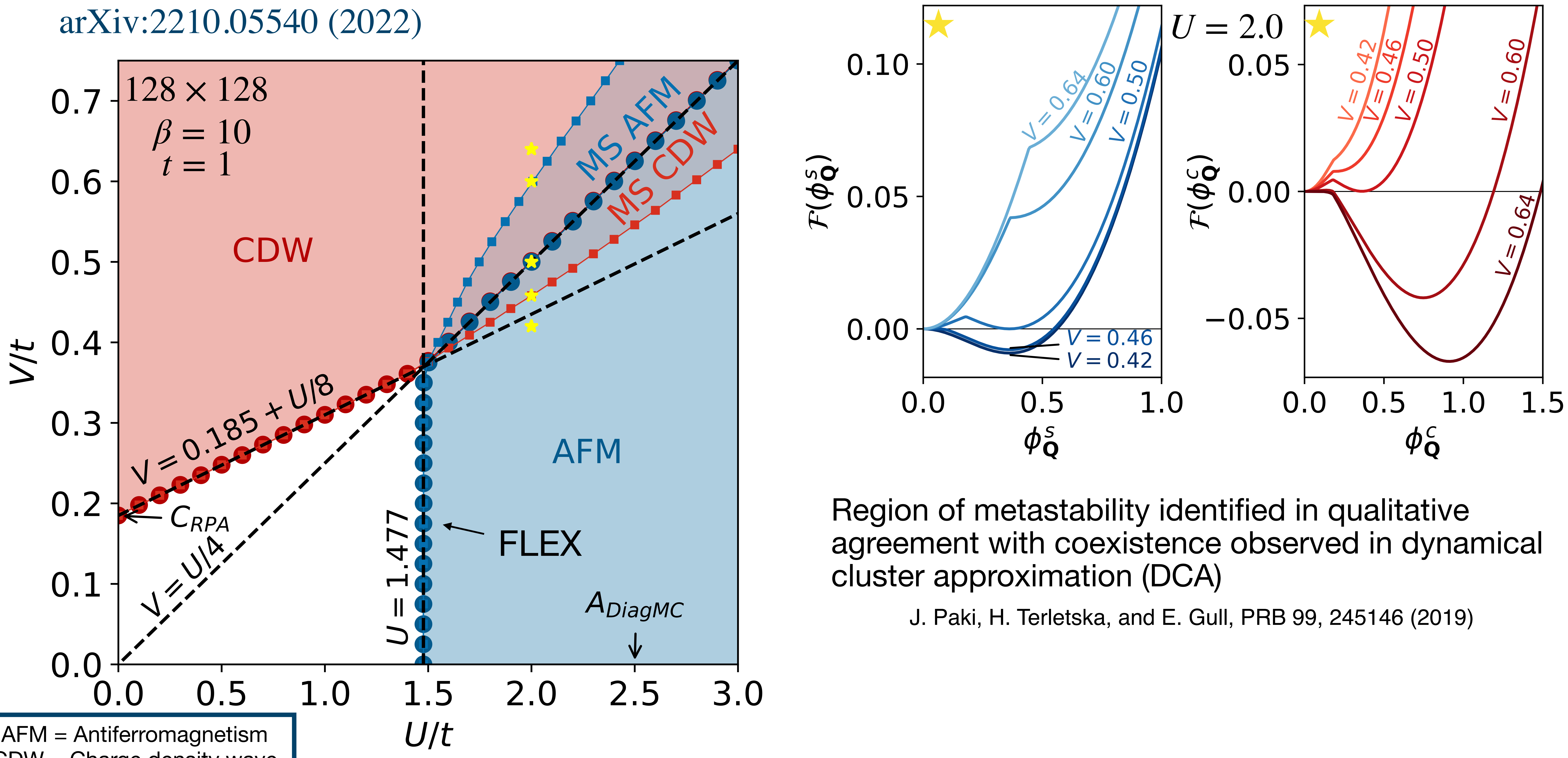

Region of metastability identified in qualitative agreement with coexistence observed in dynamical cluster approximation (DCA)

J. Paki, H. Terletska, and E. Gull, PRB 99, 245146 (2019)

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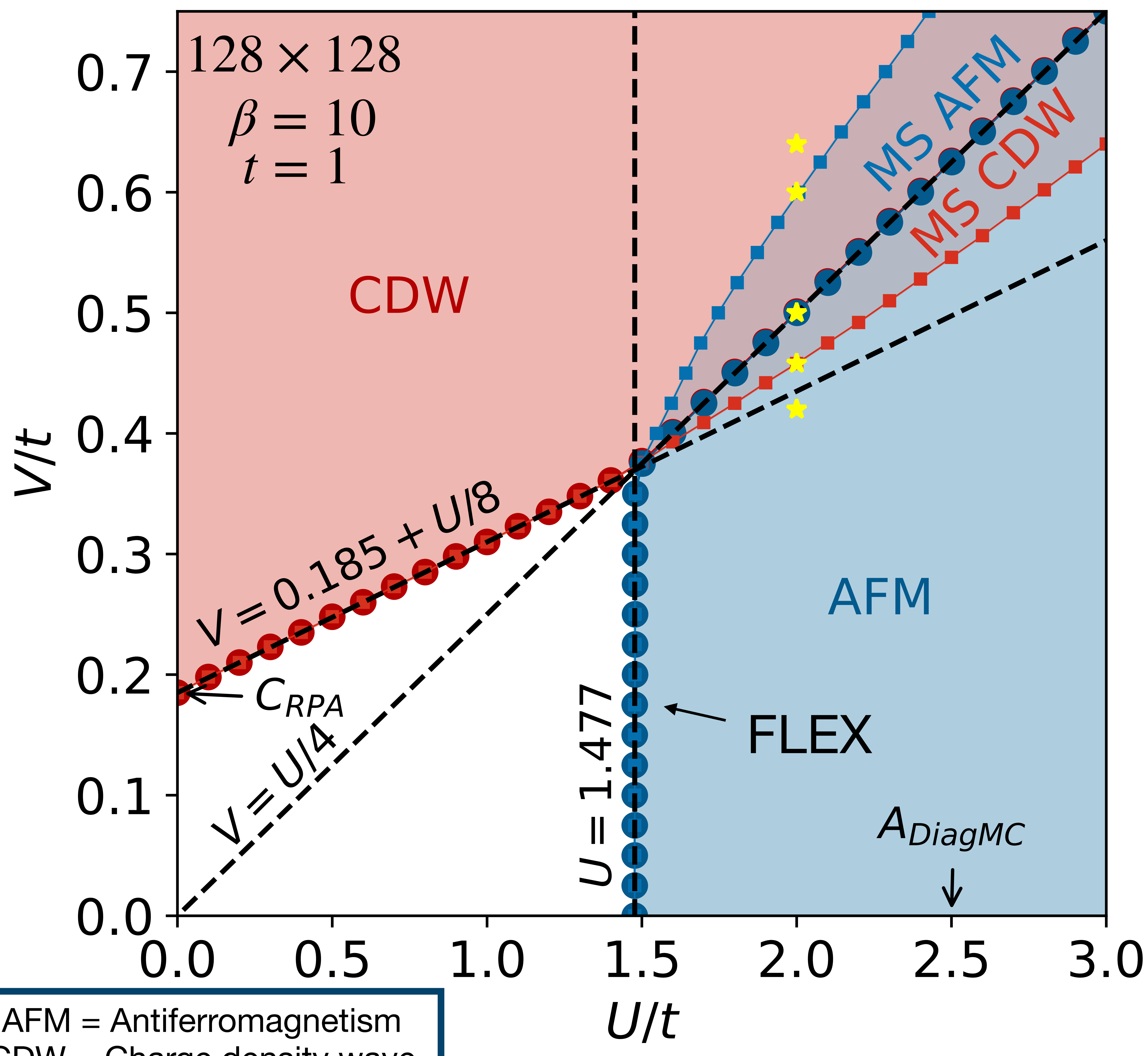

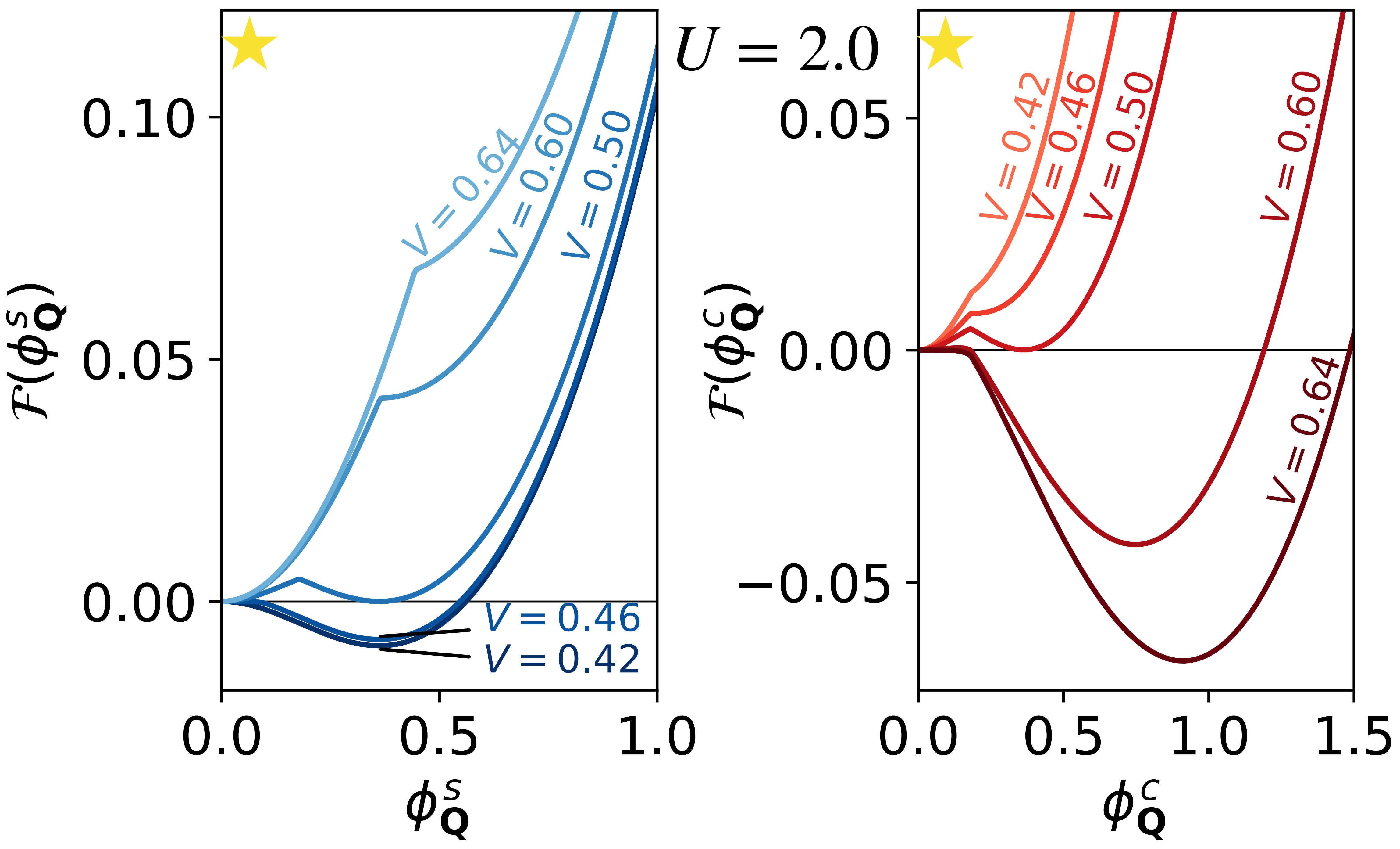

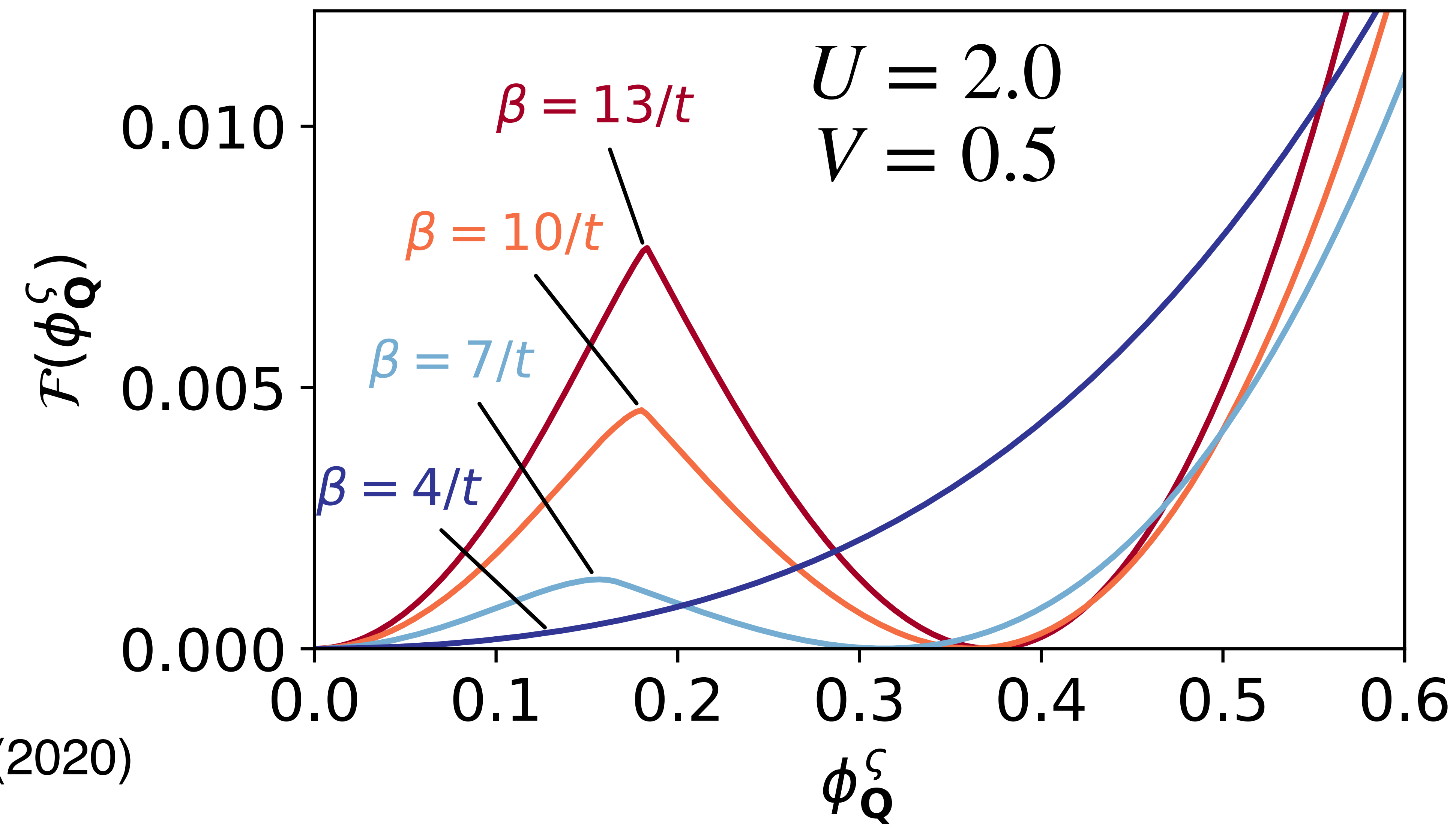

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Phase diagram of the extended Hubbard model
with attractive local U interaction
and repulsive/attractive next-nearest neighbour V interaction

$U < 0$ phase diagram

arXiv:2301.10755 (2023)

Local interaction : U
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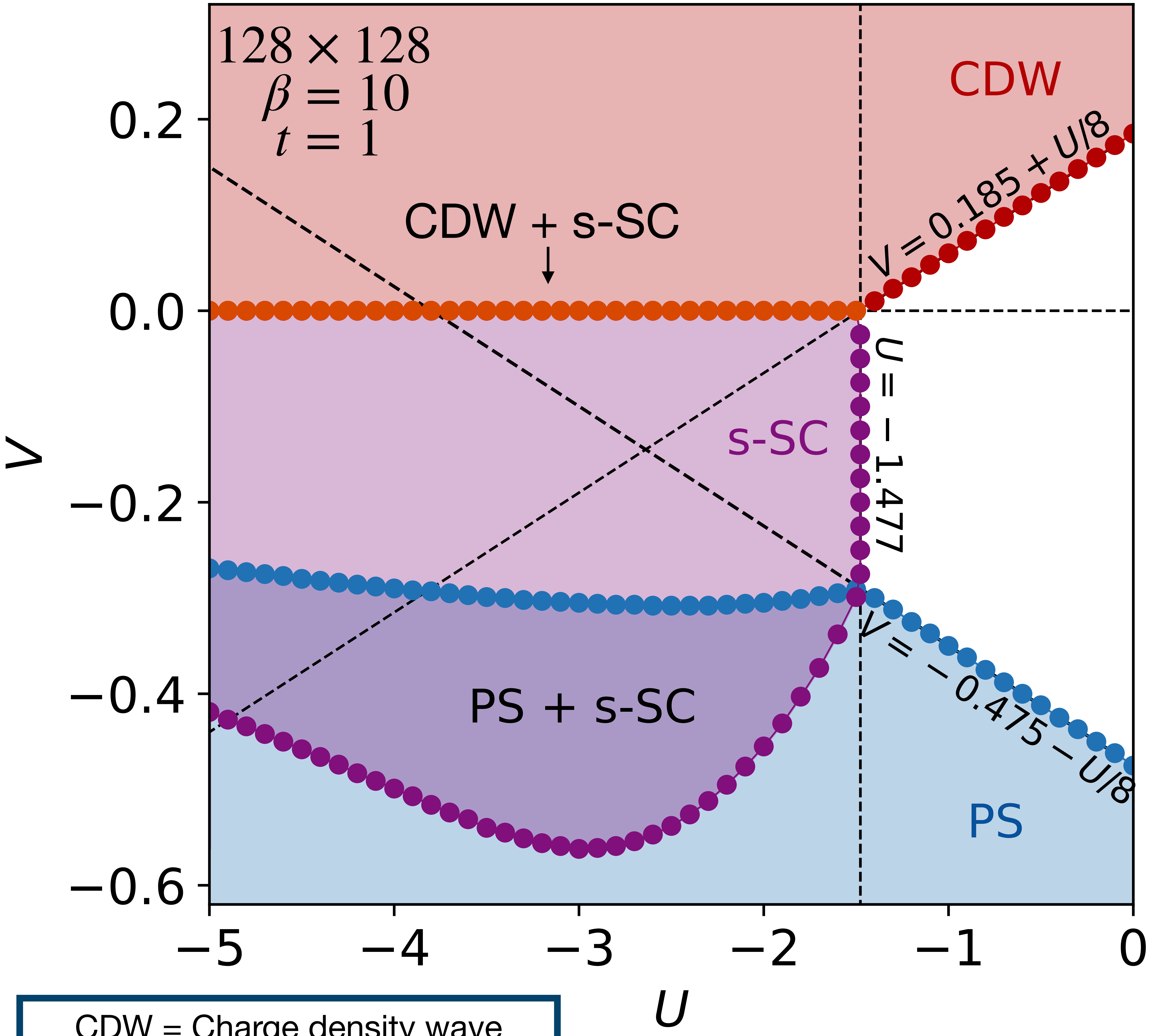

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$U < 0$ phase diagram

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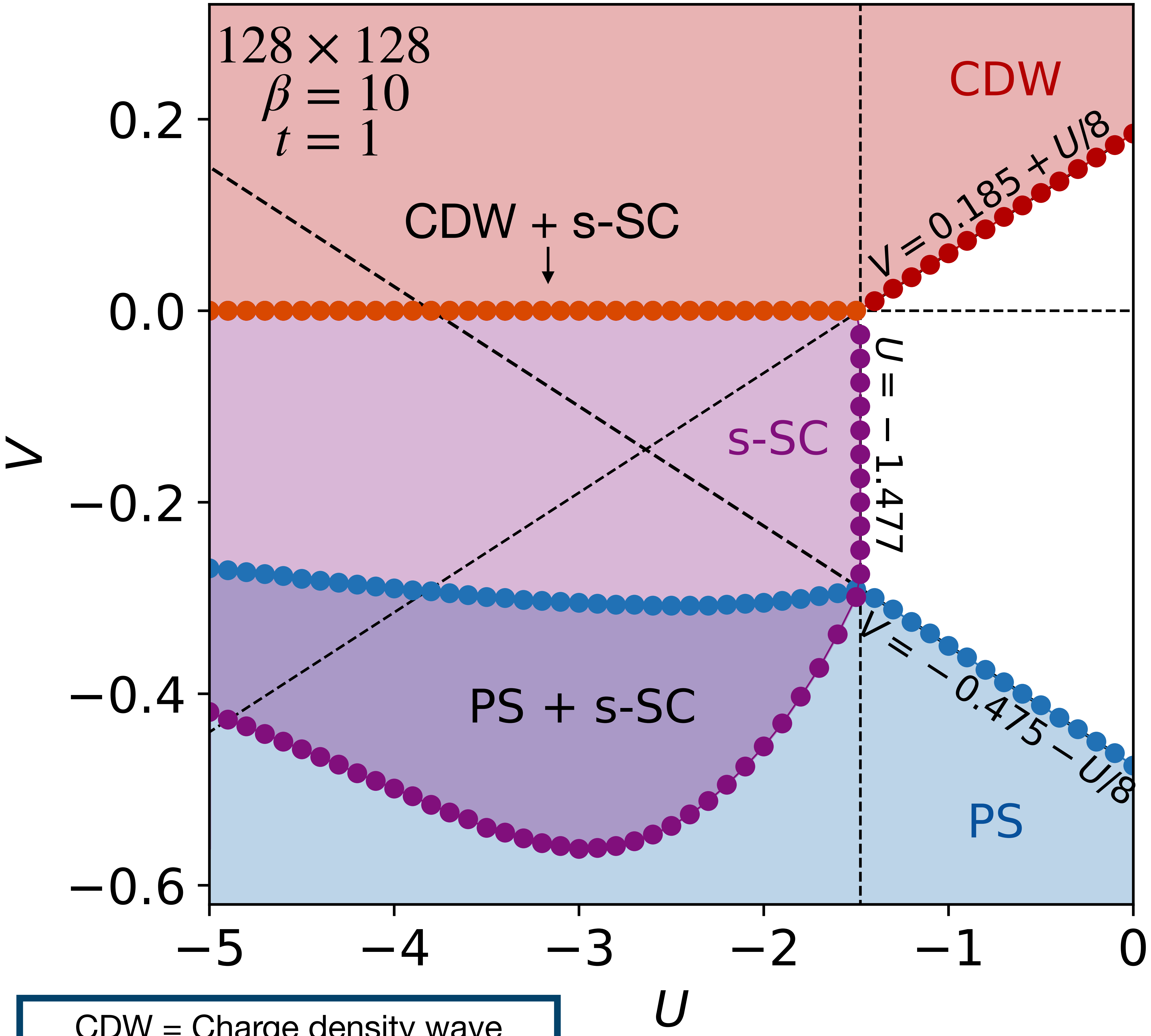

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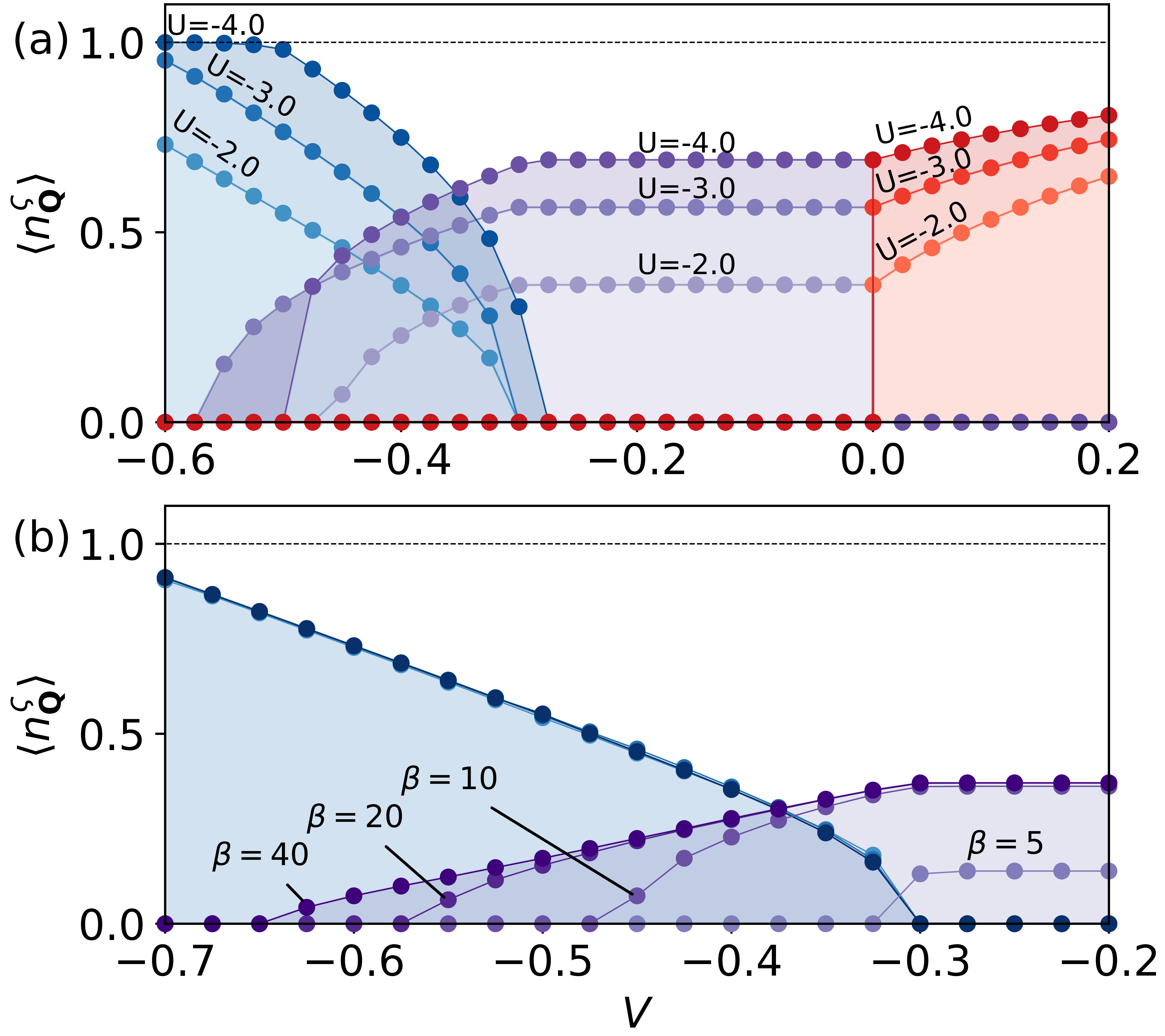
Normalised order parameters (at saddle point)



Coexistence phase incorporating collective PS and *s*-SC fluctuations discovered!

$U < 0$ phase diagram

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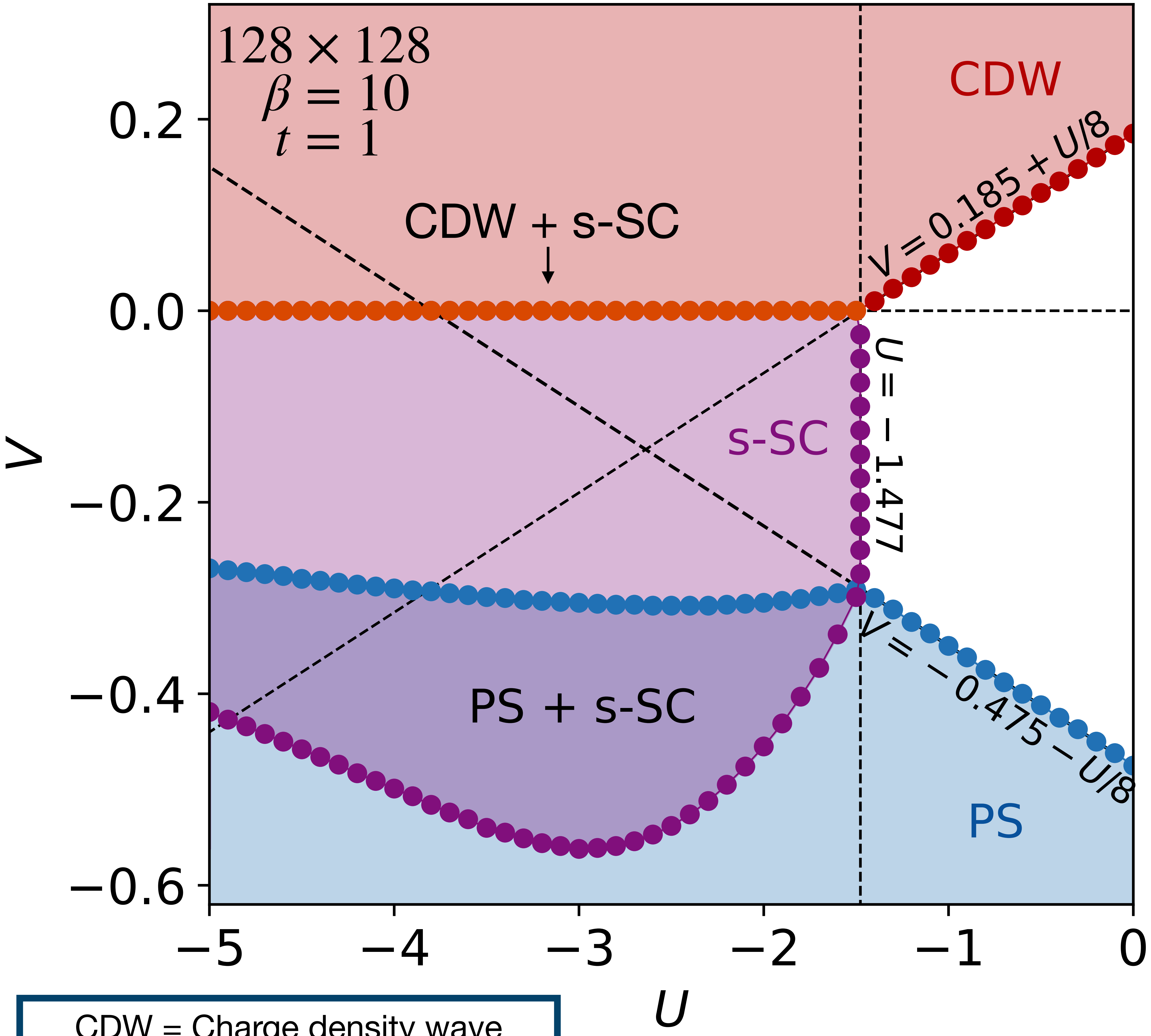

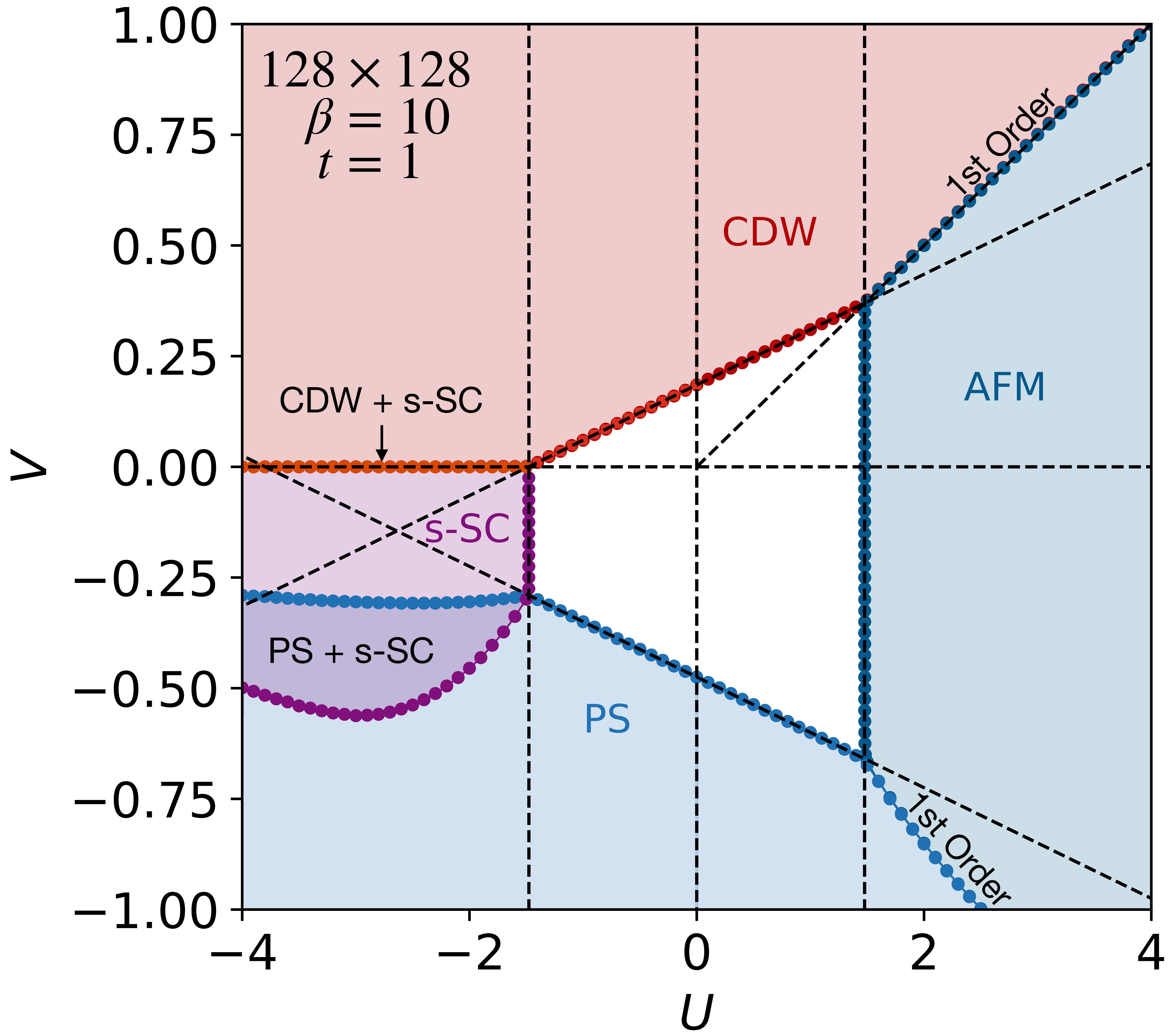

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Summary

Multi-channel fluctuating field theory :

- Novel approach allowing us to study interplaying collective fluctuations in large systems with low computational cost can be implemented for general correlated quantum lattice systems
- Identification of a novel phase with coexisting *s*-wave superconductivity and phase separation fluctuations

Thank you for your attention!

Contact: **erik.linner@polytechnique.edu**

For more information:

Erik Linnér, A. I. Lichtenstein, S. Biermann and E. A. Stepanov, arXiv:2210.05540 (2022)

Erik Linnér, C. Dutreix, S. Biermann and E. A. Stepanov, arXiv:2301.10755 (2023)

Free energy construction

Multi-channel fluctuating field trial action:

$$\mathcal{S}^* = -\frac{1}{\beta N}\sum_{\mathbf{k},\nu,\sigma} c^*_{\mathbf{k}\nu\sigma}\mathcal{G}^{-1}_{\mathbf{k}\nu}c_{\mathbf{k}\nu\sigma} + \sum_{\mathbf{Q},\varsigma}\left[\phi^{\varsigma}_{\mathbf{Q}}n^{\varsigma}_{-\mathbf{Q}} - \frac{1}{2}\frac{\beta N}{J^{\varsigma}_{\mathbf{Q}}}\phi^{\varsigma}_{\mathbf{Q}}\phi^{\varsigma}_{-\mathbf{Q}}\right], \quad n^{\varsigma}_{\mathbf{Q}} = \frac{1}{\beta N}\sum_{\mathbf{k},\nu,\sigma\sigma'} c^*_{\mathbf{k}+\mathbf{Q},\nu\sigma}\sigma^{\varsigma}_{\sigma\sigma'}c_{\mathbf{k}\nu\sigma'}$$

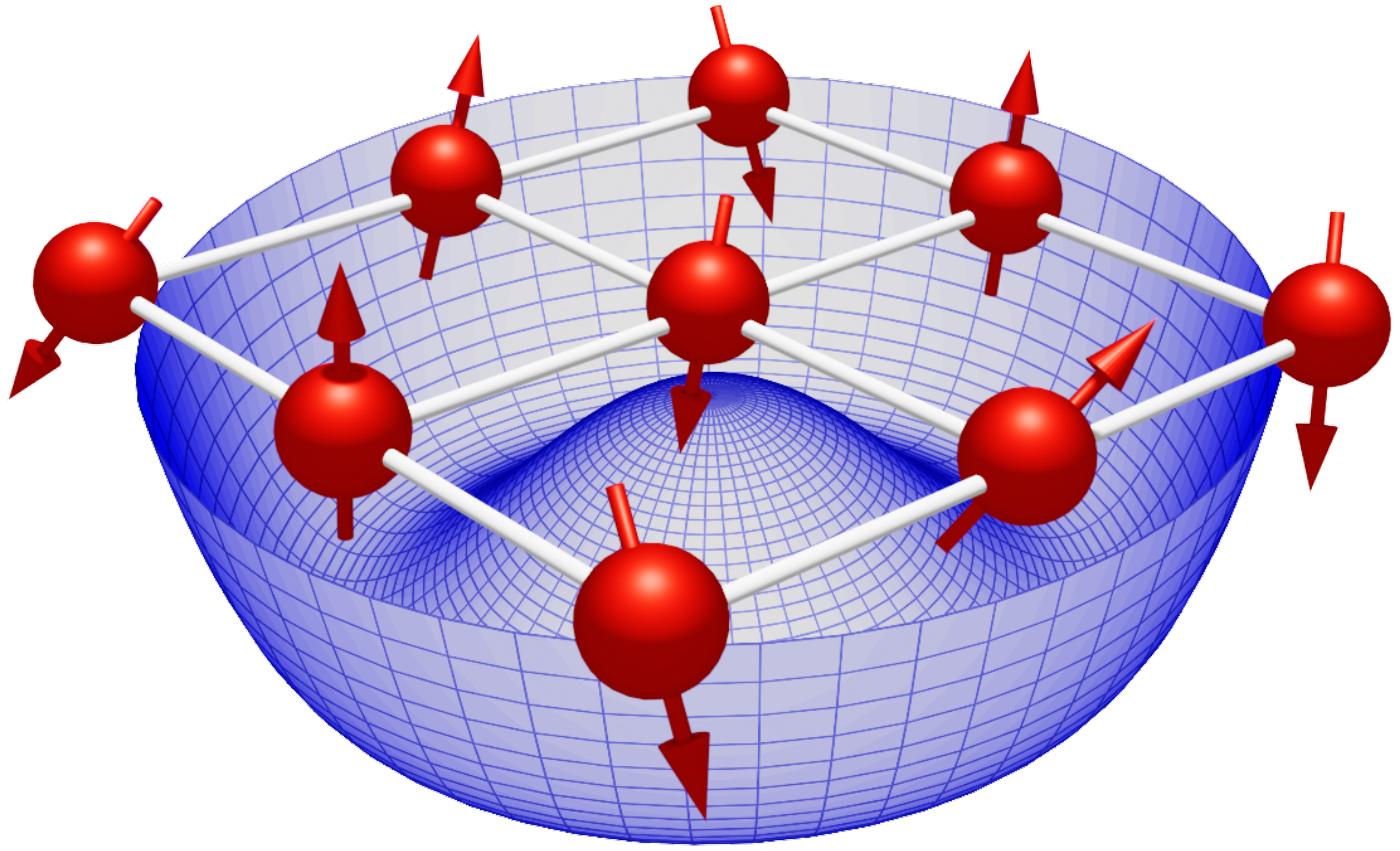
- Due to Gaussian structure, fermionic respectively classical degrees of freedom may be analytic integrated out:

$$\mathcal{S}_\phi = -\,\mathrm{Tr}\ln\left[\mathcal{G}^{-1}_{\mathbf{k}\nu}\delta_{\mathbf{Q},0}\delta_{\sigma,\sigma'} - \sum_{\varsigma}\phi^{\varsigma}_{\mathbf{Q}}\sigma^{\varsigma}_{\sigma\sigma'}\right] - \frac{1}{2}\sum_{\mathbf{Q},\varsigma}\frac{\beta N}{J^{\varsigma}_{\mathbf{Q}}}\phi^{\varsigma}_{\mathbf{Q}}\phi^{\varsigma}_{-\mathbf{Q}} \rightarrow \textbf{Derive free energy}$$

$$\mathcal{S}_c = -\frac{1}{\beta N}\sum_{\mathbf{k},\nu,\sigma} c^*_{\mathbf{k}\nu\sigma}\mathcal{G}^{-1}_{\mathbf{k}\nu}c_{\mathbf{k}\nu\sigma} + \frac{1}{2}\sum_{\mathbf{Q},\varsigma}\frac{J^{\varsigma}_{\mathbf{Q}}}{\beta N}n^{\varsigma}_{\mathbf{Q}}n^{\varsigma}_{-\mathbf{Q}} \qquad \rightarrow \textbf{Employed in variational construction}$$

- Interplay of collective fluctuations are studied through the free energy:

$$\mathcal{F}(\phi^{c}_{\mathbf{Q}}) = -\frac{1}{\beta N}\ln\int D[\phi^{s}_{\mathbf{Q}}]\,\exp\{-\mathcal{S}_\phi[\phi^{c}_{\mathbf{Q}},\phi^{s}_{\mathbf{Q}}]\}$$



A. N. Rubtsov, et. al., PRB 102 224423 (2020)

Stiffness determination

Determination of stiffness parameters $J^{\varsigma}_{\mathbf{Q}}$ based on Peierls-Feynman-Bogoliubov variational principle:

$$\mathscr{F}(J^{\varsigma}_{\mathbf{Q}}) = \mathscr{F}_c(J^{\varsigma}_{\mathbf{Q}}) + \frac{1}{\beta N}\left\langle \mathscr{S} - \mathscr{S}_c \right\rangle_{\mathscr{S}_c}, \qquad \mathscr{F}_c(J^{\varsigma}_{\mathbf{Q}}) = -\ln(Z_c)/\beta N, \qquad \frac{\partial \mathscr{F}(J^{\varsigma}_{\mathbf{Q}})}{\partial J^{\varsigma}_{\mathbf{Q}}} = 0$$

- We exploit a rewriting of the expectation value:

  $\langle \ldots \rangle_{\mathscr{S}_c} = \langle\langle \ldots \rangle_{\mathscr{S}_e}\rangle_{\mathscr{S}_\phi}$ with the Gaussian action $\mathscr{S}_e = -\frac{1}{\beta N}\sum_{\mathbf{k},\nu,\sigma} c^*_{\mathbf{k}\nu\sigma}\mathscr{G}^{-1}_{\mathbf{k}\nu}c_{\mathbf{k}\nu\sigma} + \sum_{\mathbf{Q},\varsigma}\phi^{\varsigma}_{\mathbf{Q}}n^{\varsigma}_{-\mathbf{Q}}$

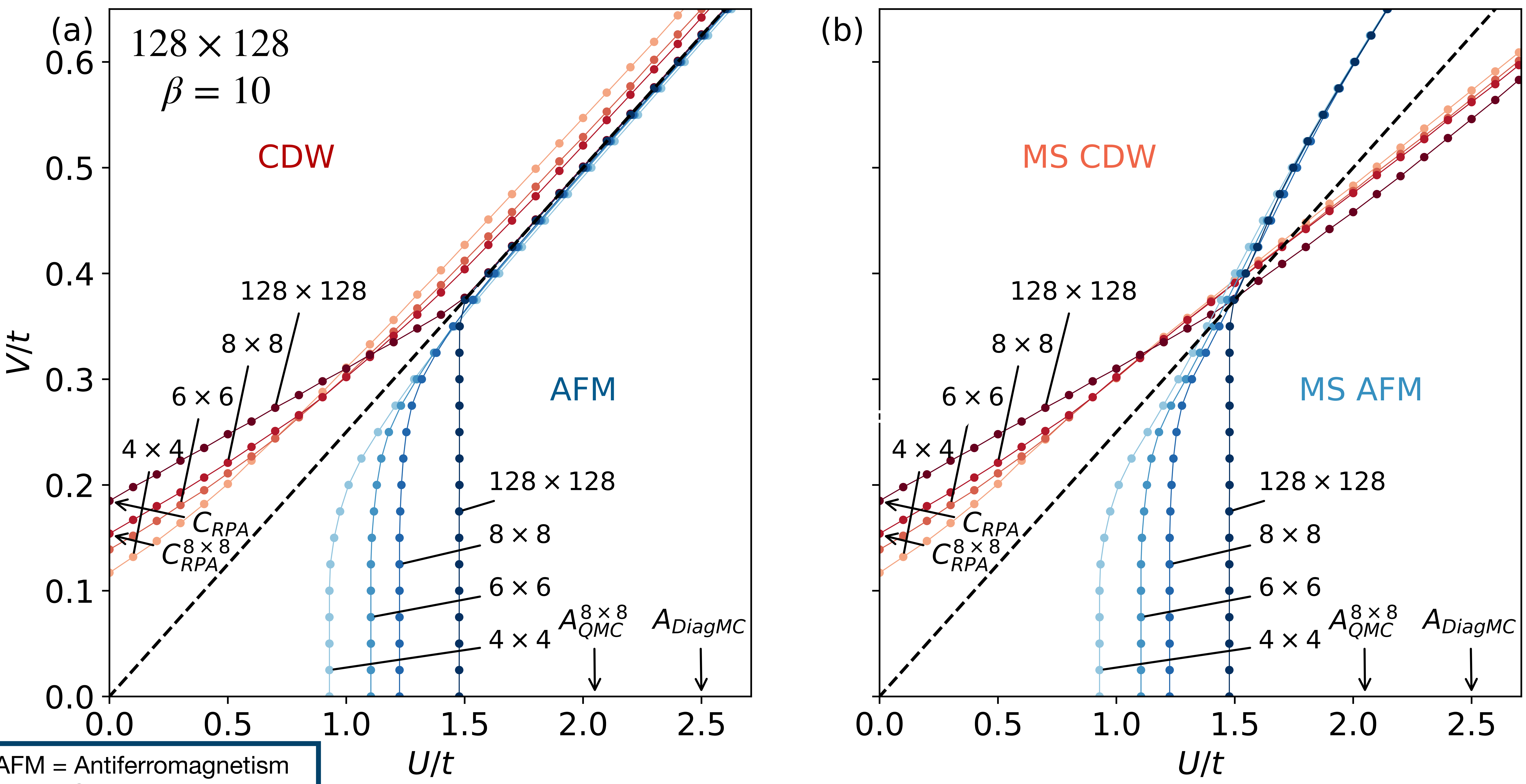
- Functional is approximately rewritten as (dropping sub-leading terms vanishing in the thermodynamic limit):

$$\mathscr{F}(J^{\varsigma}_{\mathbf{Q}}) \approx \mathscr{F}_c(J^{\varsigma}_{\mathbf{Q}}) + \frac{1}{(\beta N)^2}\left(\frac{U}{4} + \frac{V_{\mathbf{Q}}}{2} - \frac{J^c_{\mathbf{Q}}}{2}\right)\left\langle \left\langle n^c_{\mathbf{Q}} \right\rangle_{\mathscr{S}_e} \left\langle n^c_{-\mathbf{Q}} \right\rangle_{\mathscr{S}_e} \right\rangle_{\mathscr{S}_\phi} - \frac{1}{(\beta N)^2}\left(\frac{U}{4} + \frac{J^s_{\mathbf{Q}}}{2}\right)\left\langle \left\langle \vec{n}^s_{\mathbf{Q}} \right\rangle_{\mathscr{S}_e} \left\langle \vec{n}^s_{-\mathbf{Q}} \right\rangle_{\mathscr{S}_e} \right\rangle_{\mathscr{S}_\phi}$$

  allowing to identify: $J^c_{\mathbf{Q}} = \frac{U}{2} + V_{\mathbf{Q}}$ (charge), $J^s_{\mathbf{Q}} = -\frac{U}{2}$ (spin)

Repulsive $U-V$ phase diagram : System size

arXiv:2210.05540 (2022)



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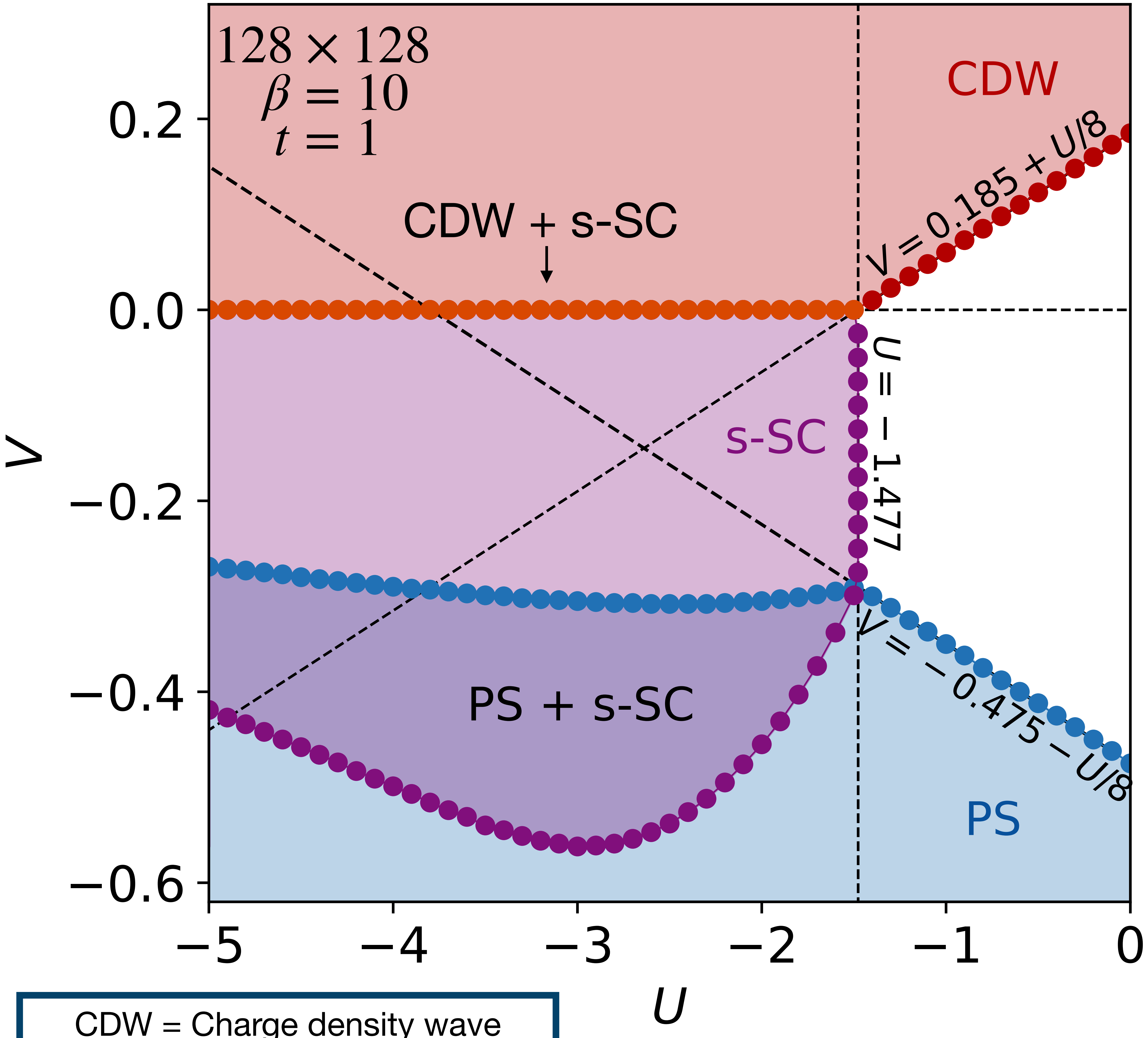

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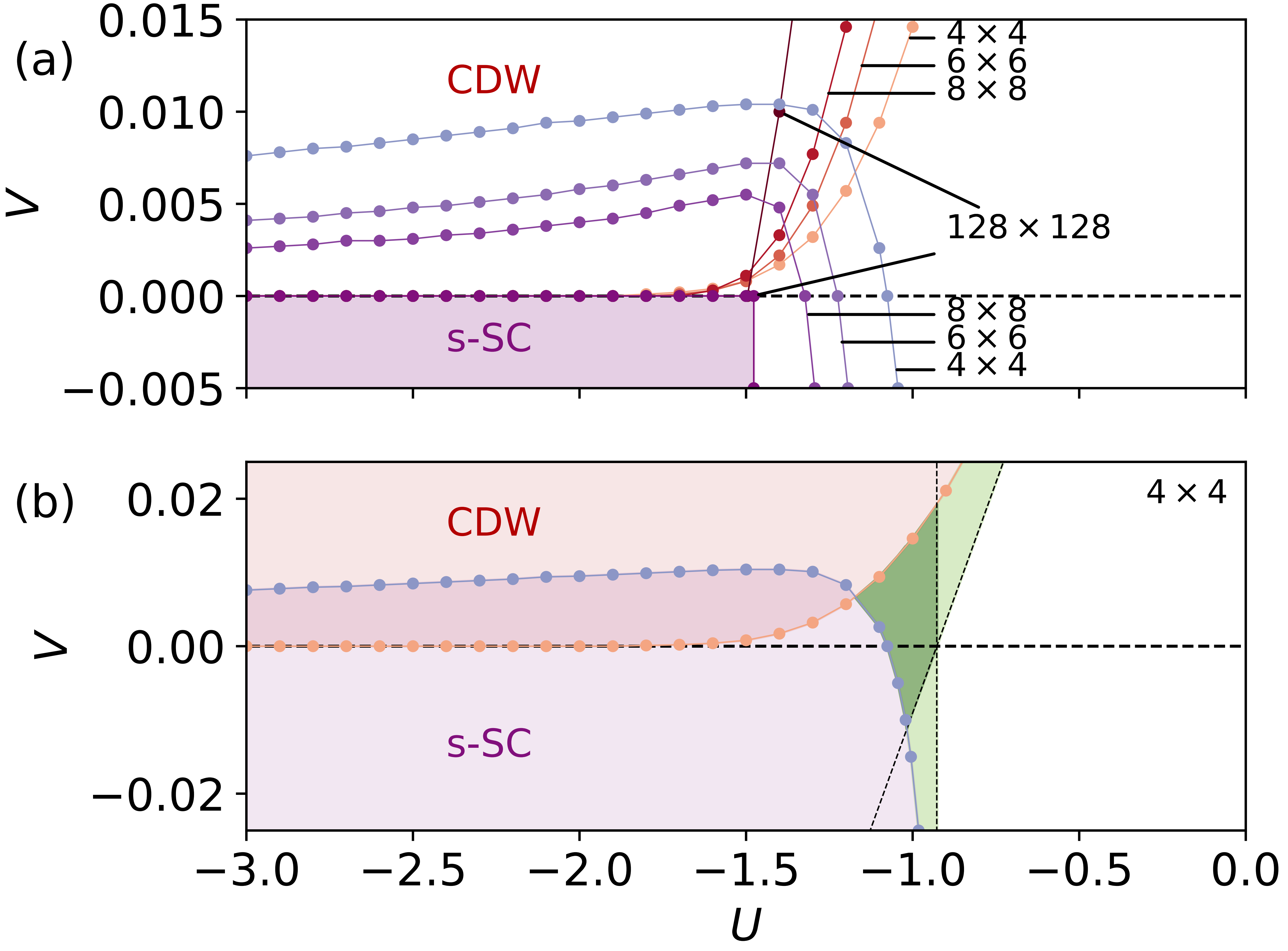
Scaling dependence of the CDW + *s*-SC coexistence phase : Width of phase converges to infinitesimal width in the thermodynamic limit



Regions of separately stable CDW and *s*-SC orderings at small system sizes