

RESEARCH ARTICLE OPEN ACCESS

Surface Functional Renormalization Group for Layered Quantum Materials

Lennart Klebl¹  | Dante M. Kennes^{2,3} 

¹Institute for Theoretical Physics and Astrophysics, Universität Würzburg, Würzburg, Germany | ²Institut für Theorie der Statistischen Physik, RWTH Aachen University and JARA-Fundamentals of Future Information Technology, Aachen, Germany | ³Max Planck Institute for the Structure and Dynamics of Matter, Center for Free Electron Laser Science, Hamburg, Germany

Correspondence: Lennart Klebl (lennart.klebl@uni-wuerzburg.de)

Received: 16 January 2026 | **Revised:** 15 March 2026 | **Accepted:** 25 March 2026

Keywords: functional renormalization group | hubbard model | surface states

ABSTRACT

We present an extension to the 2D functional renormalization group to efficiently treat interactions on the surface or at interfaces of 3D systems. As an application, we consider a semi-infinite stack of 2D square lattices, including a Hubbard interaction on the surface layer and an alternating interlayer coupling. We investigate how strongly correlated states of the decoupled 2D Hubbard model on the surface evolve under inclusion of such an SSH-like interlayer coupling. For large parts of the phase diagram as a function of the interlayer hopping parameters, the physics of the 2D system prevails, with antiferromagnetic, superconducting *d*-wave, and ferromagnetic correlations taking center stage. However, for intermediate interlayer couplings the superconducting state at intermediate interaction strengths separates into two regimes by a small region of incommensurate spin-density-wave and spin-bond order, enabling the potential realization of chiral spin-bond order.

1 | Introduction

One of the most studied models of strongly correlated electrons in condensed matter physics is the 2D Hubbard model [1]. Although being an extremely simplified model, it is believed to capture the essence of the pairing mechanism relevant for high- T_c cuprate superconductors [2–4]. But, even on the level of model physics, obtaining an unbiased characterization of the different regimes at play remains a difficult challenge. Among many other highly developed methods [4–7], one promising contender at small to intermediate interaction strengths is the functional renormalization group (FRG) [8, 9]. Formulated as a diagrammatic technique taking all interchannel feedback into account while successively integrating out the high-energy degrees of freedom, it provides robust and unbiased characterization of ordering tendencies [10–16].

While studies of multi-orbital or spin-orbit coupled models with FRG have been extensively carried out [13, 17–30], performing FRG simulations even in simple, periodic 3D systems remains a numerical challenge [31–33]. Fortunately, electron–electron interactions are often dominant within a single layer [34] at interfaces or on the surface in the case of topological 3D systems [35] or intralayer physics is only weakly perturbed by interlayer couplings, such as in some van der Waals heterostructures. Therefore, it is a promising simplification to study how electron–electron interactions within a single 2D layer (or surface) can induce strongly correlated phases when the kinetic part of the Hamiltonian is 3D.

Here, we develop a variant of momentum space FRG that treats the renormalization of interactions on a surface or a single layer, embedded in a 3D system. We call this variant “surface FRG” in the following. This method efficiently captures intralayer

This is an open access article under the terms of the [Creative Commons Attribution](https://creativecommons.org/licenses/by/4.0/) License, which permits use, distribution and reproduction in any medium, provided the original work is properly cited.

© 2026 The Author(s). *Annalen der Physik* published by Wiley-VCH GmbH

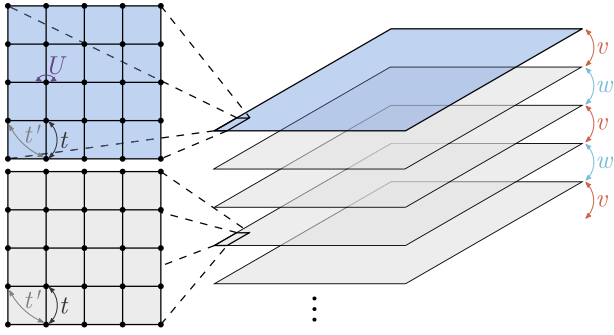


FIGURE 1 | Three-dimensional Hubbard-SSH model. Each of the layers has nearest- and next-nearest-neighbor hopping terms t and t' , respectively (black and gray). The coupling of subsequent layers is given by two alternating hopping amplitudes v (orange) and w (light blue), as in an SSH chain. We treat the renormalization of the two-particle interaction only in the outermost layer, where we include an on-site Hubbard- U term (blue).

interaction effects in an unbiased manner, allowing to study the consequences of 3D embedding of quasi 2D systems with significantly reduced numerical effort. We apply the “surface FRG” to a 3D Su–Schrieffer–Heeger (SSH) model [36]: Figure 1 illustrates the stack of square lattice layers coupled with alternating hoppings in out-of-plane direction. The surface layer (blue) exhibits an on-site Hubbard- U , while all other layers of the semi-infinite “Hubbard-SSH” stack are non-interacting. Using surface FRG, we analyze the effects of electron–electron interactions in the surface layer.

The rest of the paper is structured as follows: We first give an overview of the surface FRG method in Section 2. Thereafter, we introduce the 3D Hubbard-SSH model in greater detail (see Section 3). The results of our surface FRG calculations are presented in Section 4.

2 | Functional Renormalization Group

What most FRG schemes of the two- and four-point vertices have in common is that they require only the vertices at the starting scale $\Lambda_0 = \infty$ and the non-interacting two-point Green's function at renormalization scale Λ as input [11, 37]. Surface Green's functions that include information on the semi-infinite nature of the system can be recursively generated from the bulk couplings [38, 39]. Consequently, investigations on strong correlations arising from surface interactions can be carried out efficiently employing FRG with surface Green's functions as the non-interacting input.

As keeping track of all variables is numerically difficult to achieve, many approximations to and truncations of the FRG equations have been proposed [12, 13, 40–48]. One of these truncations—commonly applied for electrons in 2D systems—is keeping vertices only up to the four-point one, i.e., the two-particle interaction. Additional approximations include going to the static limit (neglecting frequency dependencies) of the vertices (self-energy and interaction) as well as disregarding self-energy feedback [13, 37, 49, 50]. In order to keep the numerical effort of our investigations in the present system tangible, we

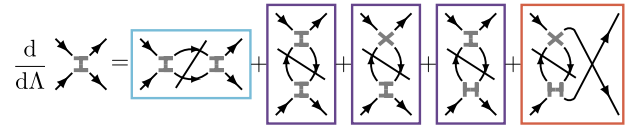


FIGURE 2 | Diagrammatic representation of the flow equation of the four-point vertex. The diagrams are grouped into channels corresponding to distinct transfer momenta, with the particle-particle channel D^Λ in light blue, the direct particle-hole channel C^Λ in purple, and the crossed particle-hole channel C^Λ in orange. Slashed propagator pairs denote a scale derivative ($d/d\Lambda$) of the corresponding propagator pair. The vertices conserve electron spin along the gray lines connecting two in-/out-going electron lines.

hence focus on the renormalization of the static four-point vertex (interactions), while discarding all higher vertices and the two-point vertex (self-energies). We further make use of spin rotational invariance, i.e., $SU(2)$ symmetry and assume translational invariance in the in-plane directions. The effects of out-of-plane hopping are encoded in the propagators G_0 by including an exact self-energy contribution Σ_0 , such that the resulting flow equation of the four-point vertex retains the original diagrammatic structure (see Figure 2):

$$\frac{dV^\Lambda}{d\Lambda} = \frac{d}{d\Lambda} \left(P^{-1}[P^\Lambda] + C^{-1}[C^\Lambda] + D^{-1}[D^\Lambda] \right) \quad (1)$$

$$\frac{dP^\Lambda(q_p, k_p, k'_p)}{d\Lambda} = \int_{\text{BZ}} dk P[V^\Lambda](q_p, k_p, k) \dot{L}^\Lambda(q_p, k) P[V^\Lambda](q_p, k, k'_p) \quad (2)$$

$$\frac{dC^\Lambda(q_c, k_c, k'_c)}{d\Lambda} = \int_{\text{BZ}} dk C[V^\Lambda](q_c, k_c, k) \dot{L}^\Lambda_+(q_c, k) C[V^\Lambda](q_c, k, k'_c) \quad (3)$$

$$\begin{aligned} \frac{dD^\Lambda(q_d, k_d, k'_d)}{d\Lambda} = \int_{\text{BZ}} dk \bigg\{ & -2D[V^\Lambda](q_d, k_d, k) \dot{L}^\Lambda_+(q_d, k) D[V^\Lambda] \\ & (q_d, k, k'_d) + D[V^\Lambda](q_d, k_d, k) \dot{L}^\Lambda_+(q_d, k) C[V^\Lambda] \\ & (q_d, k, k'_d) + C[V^\Lambda](q_d, k_d, k) \dot{L}^\Lambda_+(q_d, k) \\ & D[V^\Lambda](q_d, k, k'_d) \bigg\}. \end{aligned} \quad (4)$$

Here, $V^\Lambda(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3)$ denotes the $SU(2)$ symmetrized four-point vertex function at scale Λ with $\mathbf{k}_1, \mathbf{k}_2$ the 2D in-plane momenta of incoming electron lines and $\mathbf{k}_3, \mathbf{k}_4 = \mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3$ the momenta of outgoing electrons, with spin being conserved along $\mathbf{k}_1 \rightarrow \mathbf{k}_3$ and $\mathbf{k}_2 \rightarrow \mathbf{k}_4$; in order to describe both direct and exchange processes we treat the vertex component $V_{\uparrow\uparrow\uparrow}$ as representative, which results in the five diagrams depicted in Figure 2 [10]. The integral over the Brillouin zone is assumed to be normalized,

$\int_{\text{BZ}} d\mathbf{k} = 1$. Note that we start the flow at $\Lambda = \infty$, where the system is exactly solvable due to suppression of fluctuations, and solve the differential equation for $\Lambda \rightarrow 0$, where the full, interacting description is recovered. As an ordered phase, within the applied truncation scheme, is indicated by a divergence in the four-point vertex at finite $\Lambda_c > 0$, we stop the flow if the maximum element of the vertex surpasses a critical value. Information on the ordered phase is obtained from the vertex at the critical scale Λ_c .

We further define the three channel-projections of the four-point vertex $X[V^\Lambda]$ for each of the channels (particle-particle P , crossed particle-hole C , and direct particle-hole D) as follows:

$$P[V^\Lambda](\mathbf{q}_p, \mathbf{k}_p, \mathbf{k}'_p) = V^\Lambda(\mathbf{k}_p, \mathbf{q}_p - \mathbf{k}_p, \mathbf{k}'_p) \quad (5)$$

$$C[V^\Lambda](\mathbf{q}_c, \mathbf{k}_c, \mathbf{k}'_c) = V^\Lambda(\mathbf{k}_c, \mathbf{k}'_c - \mathbf{q}_c, \mathbf{k}'_c) \quad (6)$$

$$D[V^\Lambda](\mathbf{q}_d, \mathbf{k}_d, \mathbf{k}'_d) = V^\Lambda(\mathbf{k}_d, \mathbf{k}'_d - \mathbf{q}_d, \mathbf{k}_d - \mathbf{q}_d) \quad (7)$$

with $\mathbf{q}_X$ the leading bosonic transfer momentum (Mandelstam variable) corresponding to channel X . The inverse projection can be defined indirectly via

$$X^{-1}[X[V^\Lambda]](\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3) = V^\Lambda(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3) \quad (8)$$

for $X \in \{P, C, D\}$. The fermionic loop integrals depend on the regulator chosen. We here assume the sharp frequency cutoff [51], for which the following holds:

$$\begin{aligned} \dot{L}_\pm^\Lambda(\mathbf{q}, \mathbf{k}) &= \frac{1}{2\pi} [G_0(\pm i\Lambda, \mathbf{k}) G_0(i\Lambda, \pm \mathbf{k} \mp \mathbf{q}) \\ &\quad + G_0(\mp i\Lambda, \mathbf{k}) G_0(-i\Lambda, \pm \mathbf{k} \mp \mathbf{q})] \end{aligned} \quad (9)$$

with $G_0(i\omega, \mathbf{k})$ the free fermionic Green's function at Matsubara frequency $i\omega$ and (in-plane) momentum $\mathbf{k}$.

We stress that when treating surface systems, the structure of $G_0(i\omega, \mathbf{k})$ is highly non-trivial as it includes the effects of out-of-plane hopping as frequency-dependent self-energy $\Sigma_0(i\omega, \mathbf{k})$ [52]. Therefore, in this case, the Matsubara Green's function no longer satisfies its regular functional form and instead $G_0(i\omega, \mathbf{k})^{-1} = i\omega - \epsilon(\mathbf{k}) - \Sigma_0(i\omega, \mathbf{k}) + \mu$ holds. For the evaluation of the loop integrals $\dot{L}_\pm^\Lambda$, it therefore is crucial to use the sharp frequency cutoff—so we only need to evaluate $G_0(\pm i\Lambda, \mathbf{k})$ for a single Λ during each step of the solution of Equation (1).

3 | The 3D Hubbard-SSH Model

We demonstrate how FRG can be applied to surface interactions by constructing a 3D Hubbard-SSH model. Figure 1 visualizes the setup: Within each 2D layer l of the semi-infinite stack, we employ a next-nearest-neighbor tight-binding model on the square lattice with a (kinetic) Hamiltonian

$$H_{2D}^l = \sum_{ij,\sigma} t_{ij} c_{l,i,\sigma}^\dagger c_{l,j,\sigma} \quad (10)$$

where the hopping amplitudes are given by $t_{ij} = t$ for nearest-neighbor sites and $t_{ij} = t'$ for next-nearest-neighbor sites. The operator $c_{l,i,\sigma}^{(\dagger)}$ annihilates (creates) an electron with spin σ at site i in layer l . We couple adjacent sites in subsequent layers as an SSH-chain [36] with alternating hopping amplitudes v and w . As we assume the stack to be semi-infinite, the layer index ranges from $l = 0$ to $l = \infty$ with $l = 0$ denoting the surface layer. We further choose the coupling from the surface to the first bulk layer to be $t_0 = v$. The full non-interacting Hamiltonian thus reads

$$H_0 = \sum_{l=0}^{\infty} \left[H_{2D}^l + \sum_{i,\sigma} t_l (c_{l,i,\sigma}^\dagger c_{l+1,i,\sigma} + \text{h.c.}) \right] \quad (11)$$

with $t_l = v$ for l even and $t_l = w$ for l odd. We can transform the 2D dependency of H_0 to momentum space and write the coupling of subsequent layers as a semi-infinite matrix to arrive at the following instructive representation of H_0 :

$$\begin{aligned} H_0 &= \sum_{\mathbf{k},\sigma} \begin{pmatrix} c_{0,\mathbf{k},\sigma}^\dagger & c_{1,\mathbf{k},\sigma}^\dagger & \cdots \end{pmatrix} \cdot \hat{H}_0(\mathbf{k}) \cdot \begin{pmatrix} c_{0,\mathbf{k},\sigma} \\ c_{1,\mathbf{k},\sigma} \\ \vdots \end{pmatrix} \\ &= \sum_{\mathbf{k},\sigma} \begin{pmatrix} c_{0,\mathbf{k},\sigma}^\dagger & c_{1,\mathbf{k},\sigma}^\dagger & \cdots \end{pmatrix} \cdot \begin{pmatrix} h(\mathbf{k}) & v & & \\ v & h(\mathbf{k}) & w & \\ & w & h(\mathbf{k}) & \\ & & & \ddots \end{pmatrix} \cdot \begin{pmatrix} c_{0,\mathbf{k},\sigma} \\ c_{1,\mathbf{k},\sigma} \\ \vdots \end{pmatrix}, \end{aligned} \quad (12)$$

where we defined the in-plane dispersion

$$h(\mathbf{k}) = -t(\cos(k_x) + \cos(k_y)) - 4t' \cos(k_x) \cos(k_y) \quad (13)$$

For our simulations, we fix the chemical potential to the Van Hove singularity of a single layer, i.e., $\mu = -4t'$ and further set the energy unit as $t = 1$. As indicated in Figure 1, we add a Hubbard-interaction to the surface layer. The interacting part of the Hamiltonian therefore has nonzero components only for $l = 0$ and reads:

$$H_U = U \sum_i n_{0,i,\uparrow} n_{0,i,\downarrow} \quad (14)$$

The renormalization procedure of the surface interactions requires the free surface Green's function at each step of the iteration. We can employ the scheme from Ref. [39] (implemented, e.g., in Ref. [53]) to obtain the surface Green's function $G_0(\omega, \mathbf{k})$ for both real and imaginary frequencies [54]. To use the highly convergent algorithm, we must bring H_0 in a form of periodically repeating couplings $\hat{H}$ on the diagonal and (repeating) tunneling matrices $\hat{\tau}$ between these diagonal couplings. Therefore we define

$$\hat{H}(\mathbf{k}) = \begin{pmatrix} h(\mathbf{k}) & v \\ v & h(\mathbf{k}) \end{pmatrix} \quad (15)$$

$$\hat{\tau} = \begin{pmatrix} 0 & 0 \\ w & 0 \end{pmatrix} \quad (16)$$

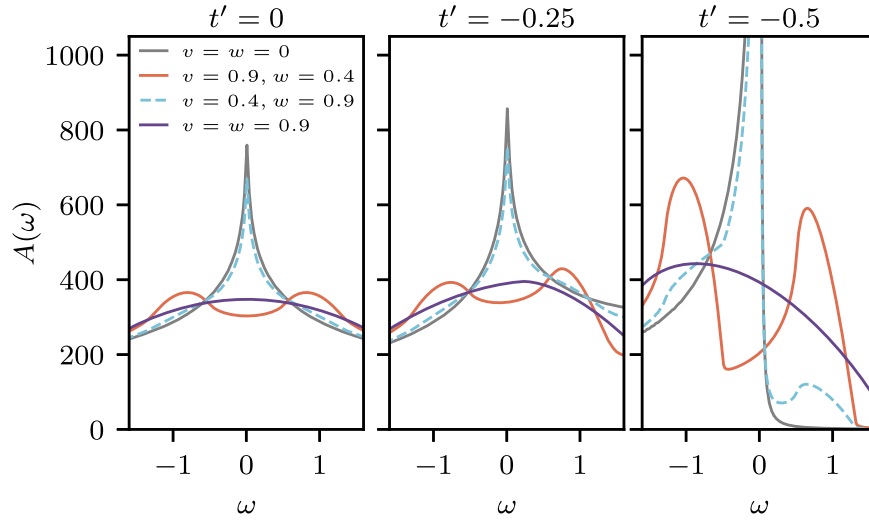


FIGURE 3 | Non-interacting spectral density for three cases of $t' \in \{0, -0.25, -0.5\}$. The chemical potential is fixed at $\mu = -4t'$ such that the system is at Van Hove filling in the layer-decoupled limit (ω is measured with respect to μ). For each panel, the four lines represent four different choices of the out-of-plane hopping parameters v and w : The gray line corresponds to the layer-decoupled system ($v = w = 0$), the orange line to $v = 0.9$ and $w = 0.4$, the dashed cyan line to $v = 0.4$ and $w = 0.9$, and the purple line to an almost isotropic 3D system with $v = w = 0.9$.

and re-introduce the required periodic tridiagonal structure of the tight-binding matrix $\hat{H}_0(\mathbf{k})$:

$$\hat{H}_0(\mathbf{k}) = \begin{pmatrix} \hat{H}(\mathbf{k}) & \hat{\tau} & & \\ \hat{\tau}^\dagger & \hat{H}(\mathbf{k}) & \hat{\tau} & \\ & \hat{\tau}^\dagger & \hat{H}(\mathbf{k}) & \\ & & & \ddots \end{pmatrix} \quad (17)$$

The such obtained surface Green's function $\hat{\mathcal{G}}_0(\omega, \mathbf{k})$ will then be a 2×2 matrix. The (1,1) (top left) component yields the desired Green's function of the top layer: $G_0(\omega, \mathbf{k}) = \mathcal{G}_0^{1,1}(\omega, \mathbf{k})$.

To characterize the non-interacting system, we consider the non-interacting surface spectral function of the 3D Hubbard-SSH model before analyzing the effect of a surface Hubbard- U interaction. The spectral function is given by

$$A(\omega) = \frac{1}{\pi} \text{Im} \int_{\text{BZ}} d\mathbf{k} G_0(\omega + i\eta, \mathbf{k}) \quad (18)$$

where we introduced a broadening parameter η that we set to 10^{-2} . Figure 3 showcases spectral functions for three values of t' and four combinations of $(v, w) \in \{(0, 0), (0.9, 0.4), (0.4, 0.9), (0.9, 0.9)\}$. At $v = w = 0$ the system is effectively 2D leading to the characteristic Van Hove singularity. As long as a surface state is present, i.e., the system is topological where $w > v$, the Van Hove singularity remains at $\omega = 0$ (we measure ω with respect to the chemical potential μ). For the other case, $v \geq w$, the single peak is split into two peaks and smeared out due to the lack of a surface state. Thus we expect the tendency toward correlations driven by electron-electron interactions to be reduced for $v \geq w > 0$.

4 | Results

We carry out FRG simulations for $t' \in \{0, -0.25, -0.5\}$ on a 11×11 grid for $v, w \in [0, 1]$. Moreover, we investigate the two cases $U = 3$ and $U = 5$. We integrate the FRG flow [Equation (1)] using an adaptive Euler scheme and calculate the vertex function on a 20×20 Bravais momentum mesh, refined with 45×45 points in the loop integrals [55]. We consider the flow diverged when the maximum element of the four-point vertex reaches 3×10^1 . The corresponding scale at which the divergence occurs is labeled by Λ_C . With our choice of the sharp cutoff as regulator, the value of Λ_C roughly corresponds to an onset temperature of the order. By inspection of which channel causes the divergence, we can differentiate between spin- and charge-density waves and superconducting instabilities. Analysis of the four-point vertex at the critical scale enables us to obtain more details about the instability, i.e., the leading ordering vector or symmetry of the superconducting state.

Figure 4 shows a v - w false color plot of the critical scale for different values of t' and U , where the red and blue color-maps indicate whether a superconducting or a magnetic instability is dominating. The FRG result for the 2D Hubbard model, i.e., spin-density wave (SDW) instabilities at $t' = 0$ and $t' = -0.5$ as well as a superconducting (SC) instability at $t' = -0.25$ is reproduced for the $v = 0$ case, where the surface layer is decoupled from the bulk. Furthermore, we observe that in most regimes of the phase diagram, the type of instability is independent of v and w , up to the point where the coupling to the bulk becomes strong enough to suppress order entirely for $v > w$. Only for $U = 5$ and $t' = -0.25$, a small area of SDW ordering emerges upon setting v and w to small, nonzero values. Moreover, the presumption of a reduced tendency toward strongly correlated states for $v \geq w$ is mostly fulfilled, except for the $t' = 0$ case, where the SDW instability is strong enough to prevail in the bilayer case (with $w = 0$ and $v = 1$). In addition, we note that in the limit toward a

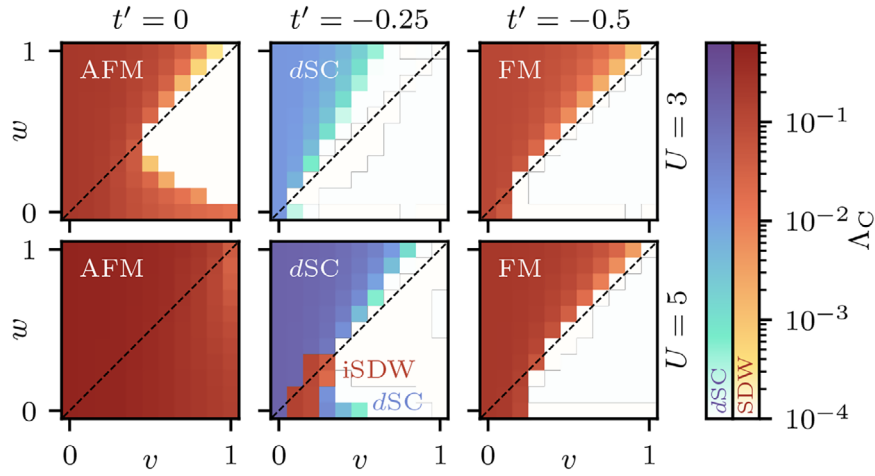


FIGURE 4 | Critical scale Λ_C (approximately onset temperature of the corresponding order) and type of leading instability for $t' \in \{0, -0.25, -0.5\}$ and $U \in \{3, 5\}$. The out-of-plane hopping amplitudes v and w are varied from zero to one on a regular 11×11 grid. The red color-map corresponds to spin-density-wave order (SDW), which includes antiferromagnetism (AFM), incommensurate spin-density-waves/spin-bond-order (iSDW), and ferromagnetism (FM); and the blue color-map to d -wave superconducting order (dSC). Literature results for the 2D Hubbard model are reproduced for $v = 0$, where the surface is decoupled from the bulk.

homogeneous 3D system surface states have a weakened spectral density, which leads to decreased ordering tendencies along the diagonal line in (v, w) phase space. The prevalence of order in the upper left triangle ($w > v$) of the phase diagrams in Figure 4 is tied to the presence of the topological surface state.

We analyze the SDW phases in greater detail by calculating the interacting magnetic susceptibility $\chi_f(\mathbf{q})$ from the vertex at the critical scale Λ_C :

$$\chi_f(\mathbf{q}) = \int_{\text{BZ}} d\mathbf{k} f(\mathbf{k}) \int_{\text{BZ}} d\mathbf{k}' f(\mathbf{k}') \chi_0(\mathbf{q}, \mathbf{k}) C[V^{\Lambda_C}](\mathbf{q}, \mathbf{k}, \mathbf{k}') \chi_0(\mathbf{q}, \mathbf{k}') \quad (19)$$

where we used the non-interacting susceptibility

$$\chi_0(\mathbf{q}, \mathbf{k}) = \frac{1}{\beta} \sum_{i\mathbf{k}_0} G_0(\mathbf{q} + \mathbf{k}) G_0(\mathbf{k}) \quad (20)$$

and set the inverse temperature to $\beta \equiv 1/\Lambda_C$. The formfactors $f(\mathbf{k})$ belong to the C_{4v} symmetrized lattice harmonics of the square lattice [13], see Table 1 for an overview. For $t' = 0$ the interacting susceptibility $\chi_f(\mathbf{q})$ is strongly peaked at $\mathbf{q} = (\pi, \pi)$ for the on-site and next-nearest-neighbor formfactors $f = f_0^{A_1}, f_2^{A_1}$, indicating antiferromagnetic order. At $t' = -0.5$, the dominant contribution originates from $\mathbf{q} = (0, 0)$ pointing toward ferromagnetic order. These two observations are independent on the out-of-plane couplings v and w (with the points considered being those ones where the flow diverges to strong coupling).

For the small area of SDW phases at $t = -0.25$ and $U = 5$ (see the red points in the central lower panel of Figure 4, cf. Appendix A for the stability of this region's presence), incommensurate magnetic instabilities are formed. In Figure 5, we show the corresponding magnetic susceptibilities for the two topologically distinct cases $(v, w) = (0.2, 0.3)$ in (a,b) and $(v, w) = (0.3, 0.2)$ in (c,d). In panels (a,c), we show the constant formfactor ($f =$

TABLE 1 | Symmetrized lattice harmonics for the 2D square lattice with C_{4v} rotational symmetry. Each row corresponds to a different irreducible representation of the formfactor. The columns label the nearest-neighbor shell i needed to generate the formfactor.

irr. rep.	$i = 0$	$i = 1$	$i = 2$
$f_i^{A_1}(\mathbf{k})$	1	$\cos(k_x) + \cos(k_y)$	$\cos(k_x) \cos(k_y)$
$f_i^{A_2}(\mathbf{k})$	—	—	—
$f_i^{B_1}(\mathbf{k})$	—	$\cos(k_x) - \cos(k_y)$	—
$f_i^{B_2}(\mathbf{k})$	—	—	$\sin(k_x) \sin(k_y)$
$f_i^{E_1}(\mathbf{k})$	—	$\sin(k_x)$	$\sin(2k_x)$
$f_i^{E_2}(\mathbf{k})$	—	$\sin(k_y)$	$\sin(2k_y)$

$f_0^{A_1}$) contribution, whereas panels (b,d) depict the contribution of the second-nearest-neighbor formfactor $f = f_2^{A_1}$. Interestingly, we observe a transition of relative weights from the non-trivial formfactor in the topological case (b) to the constant formfactor in the non-topological case (c). The incommensurate nature of the instabilities allows for linear combination of degenerate momenta in the order parameters of a subsequent mean-field decoupling. Combining these incommensurate momenta with non-trivial formfactors in the fermion bilinears as in (b) may lead to a minimization of the free energy by chiral superpositions of order parameters, i.e., a coplanar (instead of collinear) magnetic state.

Superconductivity is observed at $t' = -0.25$ (as expected from the monolayer limit). We find a d -wave symmetric solution $\Delta(\mathbf{k}) \propto f_1^{B_1}(\mathbf{k})$ of the linearized gap equation (see Refs. [20, 22, 51]) for all SC instabilities. In the case of slightly larger $U = 5$, the two superconducting regions for $w \approx 0$ and $v \leq w$ are divided by the SDW region discussed above. Nevertheless, the leading superconducting instability does not differ from one region to the other.

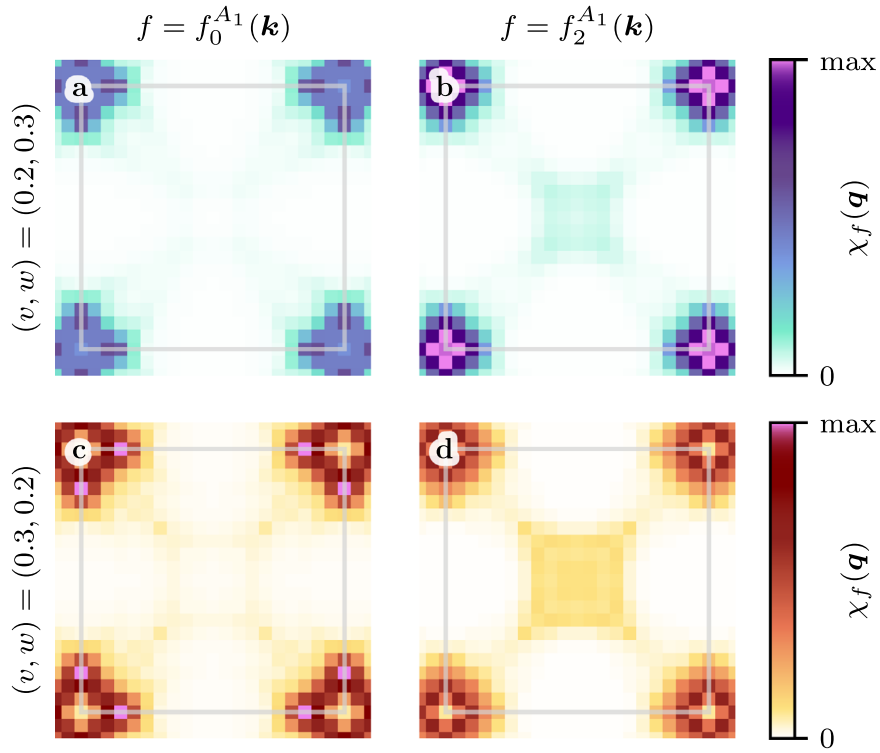


FIGURE 5 | Magnetic susceptibilities $\chi_f(\mathbf{q})$ generated from the vertex at the end of the flow. The Brillouin zone is indicated as a square, with incommensurate peaks (magenta) close to $\mathbf{q} = (\pi, \pi)$ for all cases. In the momentum contraction of fermion bilinears with the vertex, both a constant (a,c) and a nontrivial (b,d) formfactor are used. For the topological case $(v, w) = (0.2, 0.3)$ in (a,b), the susceptibility is slightly stronger for the nontrivial formfactor (b). For the topologically trivial case $(v, w) = (0.3, 0.2)$ in (c,d) the opposite applies and the susceptibility is slightly stronger for the constant formfactor (c). Having a dominant instability with non-trivial formfactor (cf. (b)) can lead to chiral superpositions of degenerate wave-vectors $\mathbf{q}$ in the resulting order parameter.

5 | Conclusion

In this manuscript, we presented a novel application of the momentum space functional renormalization group to study strongly correlated electrons on surfaces. To this end, we conducted a study of a model system of layered square lattices coupled in out-of-plane direction with alternating hoppings v and w (“Hubbard-SSH” model). While obtaining the well-known 2D limit for a decoupled surface layer at $v = 0$, we explore the phase diagram for $0 \leq v, w \leq 1$, interaction strengths $U \in \{3, 5\}$, and various next-nearest-neighbor hoppings t' (all in units of the nearest-neighbor hopping). We find orders inherited from the monolayer limit: An extended antiferromagnetic region at $t' = 0$, superconducting regions at $t' = -0.25$ and ferromagnetism at $t' = -0.5$. In the intermediate coupling regime $U = 5$, the superconducting region is separated by a small area of incommensurate spin-density wave order for weakly coupled layers (i.e., small v and w).

Notably, some of these spin density wave instabilities are peaked at incommensurate transfer momentum $\mathbf{q}$ and at the same time have dominant contributions in non-trivial formfactor shells. The fermion bilinears corresponding to the order are

$$\Delta_{\mathbf{q}}^{\text{SDW}}(\mathbf{k}) \propto f_2^{A_1}(\mathbf{k}) \langle c_{0,\mathbf{k}+\mathbf{q},\sigma}^\dagger c_{0,\mathbf{k},\sigma'} \rangle \quad (21)$$

with equal weight on the degenerate values of $\mathbf{q}$. Such incommensurate spin-density-wave order on the next-nearest-neighbor

formfactor $f_2^{A_1}(\mathbf{k})$ could potentially lead to complex superpositions, i.e., chiral spin-bond order. As a next step, we suggest to scrutinize the chiral spin-density-wave ordering in a mean-field decoupling, potentially combining it with the vertex obtained from FRG. We note that this poses a numerical challenge, as (i) the full 3D structure needs to be considered in order to obtain the free energy at fixed filling and (ii) the value of $\mathbf{q}$ close to (π, π) requires large supercells to render it commensurate.

Furthermore, the current study could be extended by the following points: First, we propose to include longer-ranged interactions. These are known to drive charge-density wave ordering in the 2D case, so we hypothesize that they could transit to charge-bond ordered phenomena (given the behavior of the spin-density-wave). Second, it could be instructive to incorporate frequency dependent self-energies in the flow to analyze the evolution of quasiparticle weights under interactions. Third, one could include interaction effects of the bulk on mean-field level, i.e., use Σ_{MF} instead of Σ_0 for the calculation of the surface Green’s function. In the future, we plan to employ the surface FRG to characterize interaction effects in an unbiased manner in more realistic models, including the renormalization of interactions in correlated subspaces [33]. Some intriguing examples include surface states in Weyl semimetals [56–60] or 3D topological insulators [35, 61, 62]. The incorporation of phonon-induced interactions into the FRG would allow to investigate the interplay of conventional [63, 64] and unconventional mechanisms for

surface superconductivity in systems like PtBi_2 and beyond. Notably, the methodology presented within the scope of this work is straightforwardly applicable to the study of interface effects in 3D heterostructures, and as such could shed light on, e.g., superconductivity at the LAO/STO interface [65, 66].

Acknowledgements

We thank J. B. Profe for useful discussions. We acknowledge funding by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) within the Priority Program SPP 2244 “2DMP”-443274199, the Würzburg-Dresden Cluster of Excellence on Complexity, Topology, and Dynamics in Quantum Matter (ctd.qmat, Project ID 390858490, EXC2147), and through the Research Unit QUASt (Project ID 449872909, FOR5249). In addition, we acknowledge computational resources provided by the Max Planck Computing and Data Facility and through JARA on the supercomputer JURECA [67] at Forschungszentrum Jülich.

Open access funding enabled and organized by Projekt DEAL.

Conflicts of Interest

The authors declare no conflicts of interest.

Data Availability Statement

The code required to produce the data contained in the manuscript is publicly available at Ref. [68].

References

1. J. Hubbard, “Electron Correlations in Narrow Energy Bands,” *Proceedings of the Royal Society of London, Series A, Mathematical and Physical Sciences* 276, no. 1365 (1963): 238–257.
2. P. W. Anderson, “The Resonating Valence Bond State in La_2CuO_4 and Superconductivity,” *Science* 235, no. 4793 (1987): 1196–1198.
3. V. J. Emery, “Theory of High- T_c Superconductivity in Oxides,” *Physical Review Letters* 58 (1987): 2794–2797.
4. D. P. Arovas, E. Berg, S. A. Kivelson, and S. Raghu, “The Hubbard Model,” *Annual Review of Condensed Matter Physics* 13, no. 1 (2022): 239–274.
5. M. Qin, C.-M. Chung, H. Shi, et al., “Absence of Superconductivity in the Pure Two-Dimensional Hubbard Model,” *Physical Review X* 10 (2020): 031016.
6. T. Schäfer, N. Wentzell, F. Šimkovic, et al., “Tracking the Footprints of Spin Fluctuations: A Multimethod, Multimessenger Study of the Two-Dimensional Hubbard Model,” *Physical Review X* 11 (2021): 011058.
7. M. Qin, T. Schäfer, S. Andergassen, P. Corboz, and E. Gull, “The Hubbard Model: A Computational Perspective,” *Annual Review of Condensed Matter Physics* 13, no. 1 (2022): 275–302.
8. C. Wetterich, “Exact Evolution Equation for the Effective Potential,” *Physics Letters B* 301, no. 1 (1993): 90–94.
9. T. R. Morris, “The Exact Renormalization Group and Approximate Solutions,” *International Journal of Modern Physics A* 09, no. 14 (1994): 2411–2449.
10. M. Salmhofer and C. Honerkamp, “Fermionic Renormalization Group Flows: Technique and Theory,” *Progress of Theoretical Physics* 105, no. 1 (2001): 1–35.
11. W. Metzner, M. Salmhofer, C. Honerkamp, V. Meden, and K. Schönhammer, “Functional Renormalization Group Approach to Correlated Fermion Systems,” *Reviews of Modern Physics* 84, no. 1 (2012): 299–352.

12. W.-S. Wang, Y.-Y. Xiang, Q.-H. Wang, F. Wang, F. Yang, and D.-H. Lee, “Functional Renormalization Group and Variational Monte Carlo Studies of the Electronic Instabilities in Graphene near $\frac{1}{4}$ Doping,” *Physical Review B* 85 (2012): 035414.
13. C. Platt, W. Hanke, and R. Thomale, “Functional Renormalization Group for Multi-Orbital Fermi Surface Instabilities,” *Advances in Physics* 62, no. 4–6 (2013): 453–562.
14. D. M. Kennes, J. Lischner, and C. Karrasch, “Strong Correlations and $d + id$ Superconductivity in Twisted Bilayer Graphene,” *Physical Review B* 98 (2018): 241407.
15. L. Classen, C. Honerkamp, and M. M. Scherer, “Competing Phases of Interacting Electrons on Triangular Lattices in Moiré Heterostructures,” *Physical Review B* 99 (2019): 195120.
16. N. Dupuis, L. Canet, A. Eichhorn, et al., “The Nonperturbative Functional Renormalization Group and Its Applications,” *Physics Reports* 910 (2021): 1–114.
17. M. L. Kiesel, C. Platt, and R. Thomale, “Unconventional Fermi Surface Instabilities in the Kagome Hubbard Model,” *Physical Review Letters* 110 (2013): 126405.
18. D. Sánchez de la Peña, “Competing Orders in Honeycomb Hubbard Models with Nonlocal Coulomb Interactions: A Functional Renormalization Group Approach,” (Ph.D. dissertation, RWTH Aachen University, Aachen, 2018).
19. M. Klett, T. Schwemmer, S. Wolf, et al., “From High T_c to Low T_c : Multiorbital Effects in Transition Metal Oxides,” *Physical Review B* 104 (2021): L100502.
20. L. Klebl, Q. Xu, A. Fischer, et al., “Moiré Engineering of Spin-Orbit Coupling in Twisted Platinum Diselenide,” *Electronic Structure* 4, no. 1 (2022): 014004.
21. W. Qin, C. Huang, T. Wolf, N. Wei, I. Blinov, and A. H. MacDonald, “Functional Renormalization Group Study of Superconductivity in Rhombohedral Trilayer Graphene,” *Physical Review Letters* 130 (2023): 146001.
22. L. Klebl, A. Fischer, L. Classen, M. M. Scherer, and D. M. Kennes, “Competition of Density Waves and Superconductivity in Twisted Tungsten Diselenide,” *Physical Review Research* 5 (2023): L012034.
23. J. Beyer, J. B. Profe, L. Klebl, et al., “Rashba Spin-Orbit Coupling in the Square-Lattice Hubbard Model: A Truncated-Unity Functional Renormalization Group Study,” *Physical Review B* 107 (2023): 125115.
24. Y. He, K. Yang, J. B. Profe, E. J. Bergholtz, and D. M. Kennes, “Superconductivity of Repulsive Spinless Fermions with Sublattice Potentials,” *Physical Review Research* 5 (2023): L012009.
25. J. B. Profe, L. Klebl, F. Grandi, et al., “Kagome Hubbard Model from a Functional Renormalization Group Perspective,” *Physical Review Research* 6 (2024): 043078.
26. J. B. Profe, L. C. Rhodes, M. Dürrnagel, et al., “Magic Angle of Sr_2RuO_4 : Optimizing Correlation-Driven Superconductivity,” *Physical Review Research* 6 (2024): 043057.
27. A. Fischer, L. Klebl, V. Crépel, et al., “Theory of Intervalley-Coherent AFM Order and Topological Superconductivity in TwSe_2 ,” *Physical Review X* 15 (2025): 041055.
28. J. Beck, J. Bodky, M. Dürrnagel, et al., “Kekulé Order from Diffuse Nesting near Higher-Order Van Hove Points,” *Physical Review Letters* 136, no. 10 (2026): 106503.
29. M. Dürrnagel, H. Hohmann, A. Maity, et al., “Altermagnetic Phase Transition in a Lieb Metal,” *Physical Review Letters* 135 (2025): 036502.
30. Y. Guo, J. Cenker, A. Fischer, et al., “Angle Evolution of the Superconducting Phase Diagram in Twisted Bilayer WSe_2 ,” *arXiv* (2025), arXiv:2512.06265.
31. J. Ehrlich and C. Honerkamp, “Functional Renormalization Group for Fermion Lattice Models in Three Dimensions: Application to the

- Hubbard Model on the Cubic Lattice,” *Physical Review B* 102 (2020): 195108.
32. J. B. Profe, S. Beck, D. M. Kennes, A. Georges, and O. Gingras, “Competition between d-Wave Superconductivity and Magnetism in Uniaxially Strained Sr₂RuO₄,” *npj Quantum Materials* 9, no. 1 (2024): 53.
33. C. Bigi, M. Dürrnagel, L. Klebl, et al., “Pomeranchuk Instability from Electronic Correlations in CsTi₃Bi₅ Kagome Metal,” *Nature Communications* 17, no. 1 (2025): 325.
34. P. A. Lee, “From High Temperature Superconductivity to Quantum Spin Liquid: Progress in Strong Correlation Physics,” *Reports on Progress in Physics* 71, no. 1 (2007): 012501.
35. S. Rachel, “Interacting Topological Insulators: A Review,” *Reports on Progress in Physics* 81, no. 11 (2018): 116501.
36. W. P. Su, J. R. Schrieffer, and A. J. Heeger, “Solitons in Polyacetylene,” *Physical Review Letters* 42 (1979): 1698–1701.
37. C. Honerkamp and M. Salmhofer, “Temperature-Flow Renormalization Group and the Competition Between Superconductivity and Ferromagnetism,” *Physical Review B* 64 (2001): 184516.
38. D. Kalkstein and P. Soven, “A Green’s Function Theory of Surface States,” *Surface Science* 26, no. 1 (1971): 85–99.
39. M. P. L. Sancho, J. M. L. Sancho, J. M. L. Sancho, and J. Rubio, “Highly Convergent Schemes for the Calculation of Bulk and Surface Green Functions,” *Journal of Physics F: Metal Physics* 15, no. 4 (1985): 851–858.
40. C. Husemann and M. Salmhofer, “Efficient Parametrization of the Vertex Function, Ω Scheme, and the t, t' Hubbard Model at Van Hove Filling,” *Physical Review B* 79 (2009): 195125.
41. J. Lichtenstein, D. Sánchez de la Peña, D. Rohe, E. Di Napoli, C. Honerkamp, and S. Maier, “High-Performance Functional Renormalization Group Calculations for Interacting Fermions,” *Computer Physics Communications* 213 (2017): 100–110.
42. C. Honerkamp, “Efficient Vertex Parametrization for the Constrained Functional Renormalization Group for Effective Low-Energy Interactions in Multiband Systems,” *Physical Review B* 98 (2018): 155132.
43. C. Honerkamp, H. Shinaoka, F. F. Assaad, and P. Werner, “Limitations of Constrained Random Phase Approximation Downfolding,” *Physical Review B* 98 (2018): 235151.
44. C. J. Eckhardt, C. Honerkamp, K. Held, and A. Kauch, “Truncated Unity Parquet Solver,” *Physical Review B* 101 (2020): 155104.
45. C. Hille, F. B. Kugler, C. J. Eckhardt, et al., “Quantitative Functional Renormalization Group Description of the Two-Dimensional Hubbard Model,” *Physical Review Research* 2 (2020): 033372.
46. L. Klebl, D. M. Kennes, and C. Honerkamp, “Functional Renormalization Group for a Large Moiré Unit Cell,” *Physical Review B* 102, no. 8 (2020): 085109.
47. J. B. Profe, C. Honerkamp, S. Achilles, and D. M. Kennes, “Electronic Instabilities in Penrose Quasicrystals: Competition, Coexistence, and Collaboration of Order,” *Physical Review Research* 3 (2021): 023180.
48. J. B. Profe and D. M. Kennes, “TU²FRG: A Scalable Approach for Truncated Unity Functional Renormalization Group in Generic Fermionic Models,” *The European Physical Journal B* 95, no. 3 (2022): 60.
49. C. Honerkamp, M. Salmhofer, N. Furukawa, and T. M. Rice, “Breakdown of the Landau-Fermi Liquid in Two Dimensions Due to Umklapp Scattering,” *Physical Review B* 63 (2001): 035109.
50. C. Honerkamp, “Electron-Doping Versus Hole-Doping in the 2D t - t' Hubbard Model,” *The European Physical Journal B: Condensed Matter and Complex Systems* 21, no. 1 (2001): 81–91.
51. J. Beyer, J. B. Hauck, and L. Klebl, “Reference Results for the Momentum Space Functional Renormalization Group,” *The European Physical Journal B* 95, no. 4 (2022): 65.
52. C. Karrasch, “The Functional Renormalization Group for Zero-Dimensional Quantum Systems in and out of Equilibrium,” (Ph.D. dissertation, RWTH Aachen University, Aachen, 2010).
53. Q. Wu, S. Zhang, H.-F. Song, M. Troyer, and A. A. Soluyanov, “WannierTools: An Open-Source Software Package for Novel Topological Materials,” *Computer Physics Communications* 224 (2018): 405–416.
54. In fact, the implementation provided in Ref. [53] not only provides surface Green’s functions, but at the same time local bulk Green’s functions. The bulk Green’s function can be used in the same manner as the surface Green’s function without further modifications to the FRG equations to study intralayer interactions.
55. For Details on the Numerical Methods See Ref. [51]. The open-source implementation of the Hubbard-SSH model FRG [68] makes use of the publicly available divERGE library [69, 70].
56. M. Laubach, C. Platt, R. Thomale, T. Neupert, and S. Rachel, “Density Wave Instabilities and Surface State Evolution in Interacting Weyl Semimetals,” *Physical Review B* 94 (2016): 241102.
57. N. P. Armitage, E. J. Mele, and A. Vishwanath, “Weyl and Dirac Semimetals in Three-Dimensional Solids,” *Reviews of Modern Physics* 90 (2018): 015001.
58. F. Xiong, X. Han, and C. Honerkamp, “Spin Susceptibilities in Magnetic Type-I and Type-II Weyl Semimetals,” *Physical Review B* 104 (2021): 115151.
59. R. Kundu, H. A. Fertig, and A. Kundu, “Broken Symmetry and Competing Orders in Weyl Semimetal Interfaces,” *Physical Review B* 107 (2023): L041402.
60. Q. Liu, P.-J. Guo, X.-Y. Yue, et al., “Observation of Surface Superconductivity in a 3D Dirac Material,” *Advanced Functional Materials* 32, no. 51 (2022): 2208616.
61. T. Neupert, S. Rachel, R. Thomale, and M. Greiter, “Interacting Surface States of Three-Dimensional Topological Insulators,” *Physical Review Letters* 115 (2015): 017001.
62. R. Lundgren, H. Yerzhakov, and J. Maciejko, “Nematic Order on the Surface of a Three-Dimensional Topological Insulator,” *Physical Review B* 96 (2017): 235140.
63. K. Mæland, M. Bahari, and B. Trauzettel, “Phonon-Mediated Intrinsic Topological Superconductivity in Fermi Arcs,” *Physical Review B* 112 (2025): 104507.
64. K. Mæland, G. Sangiovanni, and B. Trauzettel, “Mechanism for Nodal Topological Superconductivity on PtBi₂ Surface,” *arXiv:2512.09994* (Dec. 2025).
65. S. Gariglio, A. Fête, and J.-M. Triscone, “Electron Confinement at the LaAlO₃/SrTiO₃ Interface,” *Journal of Physics: Condensed Matter* 27, no. 28 (2015): 283201.
66. M. S. Scheurer and J. Schmalian, “Topological Superconductivity and Unconventional Pairing in Oxide Interfaces,” *Nature Communications* 6, no. 1 (2015): 6005.
67. P. Thörnig, “JURECA: Data Centric and Booster Modules Implementing the Modular Supercomputing Architecture at Jülich Supercomputing Centre,” *Journal of Large-Scale Research Facilities* 7 (2021): A182–A182.
68. L. Klebl, “Surface FRG for a Cubic Lattice,” (2025), <https://github.com/alcubierre-drive/surface-frg>.
69. J. B. Profe, D. M. Kennes, and L. Klebl, “divERGE Implements Various Exact Renormalization Group Examples,” *SciPost Physics Codebases* (2024): 26, <https://scipost.org/10.21468/SciPostPhysCodeb.26>.
70. J. B. Profe, D. M. Kennes, and L. Klebl, “Codebase Release 0.5 for divERGE,” *SciPost Physics Codebases* (2024): 26–r0.5, <https://scipost.org/10.21468/SciPostPhysCodeb.26>.

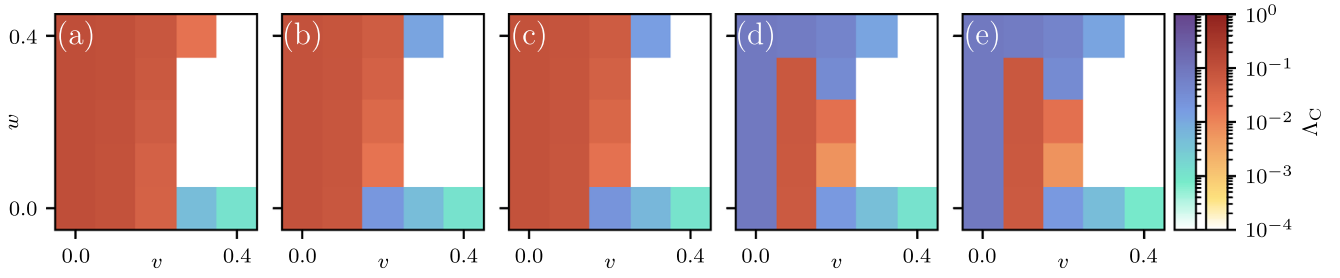


FIGURE A1 | Presence of the iSDW state (red) and the dSC state (blue) in truncated unity FRG [48] for various parameter settings at $t' = -0.25$. For all panels, the coarse momentum grid is fixed at 48×48 points. The fine momentum grid is set to 5×5 (a,b,d) and 15×15 (c,e). Panels (c,d,e) have the divergence threshold set to 60, while it is 30/45 in (a)/(b). The formfactor cutoff distance is 2 in all panels except for (c), where it is 1.

Appendix A: Methods: Robustness of the $t' = -0.25$ iSDW

To clarify that the presence of the iSDW state at $t' = -0.25$ is not a numerical artifact, we perform truncated unity FRG simulations (via the divERGE library [69, 70]) for various momentum resolutions, formfactor cutoff distances, and divergence threshold. Figure A1 demonstrates that irrespective of momentum resolution, the fact that these are truncated unity simulations as opposed to the grid FRG results in the main text, their formfactor cutoff, and their divergence threshold, the iSDW phase occupies a significant region of phase space.