Barkman *et al.* Reply: By using an approximate treatment of a quasiclassical model, the Comment [1] asserts that surface pair-density-wave (PDW) states are not supported by microscopic theory. We demonstrate that the claims of the Comment are incorrect by showing the existence of the surface PDW states in both tight-binding [2] and continuous microscopic Bogoliubov-de Gennes (BdG) approaches. BdG retains microscopic degrees of freedom, which were incorrectly discarded in the Comment [1].

Three questions are raised in the Comment concerning the Ginzburg-Landau (GL) approach. Point (i) highlights that we use $H_{\text{FLO}}(T) \approx H_0(T)$ in Ref. [3], which is justified close to the tricritical point. Indeed, we use that approximation because it is that regime where the GL theory itself can be used justifiably. Moreover, in Ref. [2] we used nonapproximated coefficients Eqs. (2)–(4), which obviously does not make any difference for the question of existence of surface PDW states. Point (ii) highlights the use of truncated gradient expansions. Evidently the GL part of our work, by construction, applies in the vicinity of the tricritical point, where the order parameter varies on macroscopic length scales. Thus, a truncated gradient expansion, is justified for the description of long-wavelength physics in that regime. Moreover, in Ref. [2] we demonstrated the effect fully microscopically without relying on any expansion. Point (iii) highlights that the GL theory we used was obtained with bulk Green's functions. We explicitly pointed that out in Refs. [2,4] along with the ambiguities that arise when employing the phenomenological treatment of boundary conditions. That is why in Ref. [2] we obtained surface states in fully microscopic theory. The discussion on boundary conditions in Ref. [4] was separated from the published version [5] and is now available with the full solution with the microscopically derived GL boundary conditions [6].

There already exists fully microscopic demonstration of the surface states [2]. By contrast the Comment [1] is using a quasiclassical approximation that, as we already pointed out in Ref. [5], in general misses these surface states. Obtaining the surface states within the quasiclassical approach requires a more microscopically accurate treatment of the boundary conditions analogous to the discussion in Ref. [6].

The Comment correctly observes our conclusion in Refs. [2,5] that Fulde-Ferrell-Larkin-Ovchinnikov physics is not the primary mechanism for the enhancement effect and the states exist in the absence of Zeeman splitting. However, the interpretation in terms of the critical temperature of a surface atomic layer in the footnote of the Comment [1] is misleading. In Refs. [2,5] the boundary

FIG. 1. Phase diagram obtained by solving the BdG equations, demonstrating higher critical temperature of surface states. T and h denote temperature and Zeeman splitting energy. The states are found both for a tight-binding (TB) and a continuum (C) model. The inset shows the order parameter profile at points A and B.

states were demonstrated in the standard tight binding model (contrary to the claim in the conclusion of the Comment [1]). The effect was demonstrated also in continuum theory [5]. In both cases the boundary states arise from applying vanishing boundary conditions to the quasiparticle wave functions $u_{\uparrow}(0) = v_{\downarrow}(0) = 0$.

Lastly, we demonstrate the existence of surface states by solving the microscopic BdG equations both in a continuum model and a tight binding lattice model that retain microscopic degrees of freedom discarded in the Comment [1]. The BdG equations for the quasiparticle wave functions read

$$\begin{pmatrix} H_+ & \Delta(x) \\ \Delta^*(x) & -H_- \end{pmatrix} \begin{pmatrix} u_{\uparrow}(x) \\ v_{\downarrow}(x) \end{pmatrix} = E \begin{pmatrix} u_{\uparrow}(x) \\ v_{\downarrow}(x) \end{pmatrix}, \quad (1)$$

where $H_{\pm} = \epsilon - (\mu \pm h)$, with $\epsilon = -\hbar^2 \nabla^2 / (2m)$ in the continuum model, and $\epsilon = -t(\delta_{i,i+1} + \delta_{i,i-1})$ in the tight-binding model. The gap parameter is determined self-consistently through $\Delta(x) = V \langle \Psi_{\uparrow}(x) \Psi_{\downarrow}(x) \rangle$ [7]. The demonstration of surface states in both of these systems, as in Fig. 1, directly disproves the claim in the Comment [1] that the bulk instability is the most favorable one.

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- [2] A. Samoilenka, M. Barkman, A. Benfenati, and E. Babaev, [Phys. Rev. B **101**, 054506 \(2020\)](#).
- [3] M. Barkman, A. Samoilenka, and E. Babaev, [Phys. Rev. Lett. **122**, 165302 \(2019\)](#).
- [4] A. Samoilenka and E. Babaev, [arXiv:1904.10942v1](#).
- [5] A. Samoilenka and E. Babaev, [Phys. Rev. B **101**, 134512 \(2020\)](#).
- [6] A. Samoilenka and E. Babaev, [arXiv:2011.09519](#).
- [7] For the continuum model we set $V = 0.3\pi\hbar v_F$ and for the tight-binding model we set $V = \mu = t$. The bulk critical temperatures in the absence of Zeeman splitting are $k_B T_{c,\text{bulk}} \simeq 0.159 \mu$ in the continuum model, and $k_B T_{c,\text{bulk}} \simeq 0.0147t$ in the tight-binding model.