Strongly interacting holes in Ge/Si nanowires

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We consider holes confined to Ge/Si core/shell nanowires subject to strong Rashba spin-orbit interaction and screened Coulomb interaction. Such wires can, for instance, serve as host systems for Majorana bound states. Starting from a microscopic model, we find that the Coulomb interaction strongly influences the properties of experimentally realistic wires. To show this, a Luttinger liquid description is derived based on a renormalization group analysis. This description in turn allows us to calculate the scaling exponents of various correlation functions as a function of the microscopic system parameters. It furthermore permits us to investigate the effect of Coulomb interaction on a small magnetic field, which opens a strongly anisotropic partial gap.

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I. INTRODUCTION

In the past decades, semiconductor nanowires (NWs) have proven to be a versatile platform for the engineering of nanoscale systems, both as intrinsically one-dimensional (1D) channels, and as hosts for NW quantum dots (QDs). So far, NWs have predominantly been grown using III-V compounds, which can be operated both in the electron regime [1-8] and the hole regime [9]. Recently, a new class of NWs, made of a cylindrical Ge core and a Si shell [10–19], and ultrathin triangular Ge NWs on a Si substrate [20], have emerged as promising alternatives to III-V NWs. The core/shell NWs can be grown with core diameters of 5-100 nm, and shell thicknesses of 1–10 nm. Inside the core, a 1D hole gas accumulates [11,21], and the *p*-wave symmetry of the hole Bloch states results in an unusually large and tunable Rashba-type spin-orbit interaction (SOI) [22]. Applying a magnetic field allows one to access a helical regime [22] susceptible to the formation of Majorana zero-energy bound states (MBS) when the NW is proximity coupled to an s-wave superconductor [23]. Finally, when grown nuclear spin free, these systems have significantly reduced hyperfine induced decoherence effects. Experimentally, high mobilities [12,18], long mean free paths [11], proximity-induced superconductivity [13], and signatures of the tunable Rashba SOI [24] have been identified. Longitudinal confinement has been demonstrated to create tunable single and double QDs [14], with anisotropic and confinement dependent g factors [15,16], short SOI lengths [25], as well as long singlet-triplet relaxation times [19] and hole spin coherence times [26]. Holes confined to such QDs have furthermore been predicted to exhibit strongly anisotropic, tunable g factors and long spin phonon relaxation times [27], and have been proposed as a platform for quantum information processing [28].

In this paper the effects of hole-hole interactions and their Luttinger liquid description in Ge/Si core/shell NWs are, to the best of our knowledge, addressed and quantified for the first time based on a concrete microscopic model. We focus on the single subband regime most relevant for the emergence of MBS. After explicitly evaluating the interaction matrix elements for a realistic geometry, we derive the Luttinger liquid description of the NW, and calculate the interaction dependent scaling exponents of various correlation functions for our microscopic model. The scaling exponents show a weak dependence on the magnitude of an applied electric field, which tunes the SOI strength. This is contrasted by a strong dependence on the NW parameters. The exponents differ substantially from their noninteracting value, thus revealing rather strong interaction effects. As an example for experimental implications of Luttinger liquid physics beyond the scaling of correlation functions, we finally analyze the renormalization of the partial gap around zero momentum resulting from an applied magnetic field. This partial gap precisely corresponds to the helical regime susceptible to the formation of MBS in a superconducting hybrid device [23]. We find that hole-hole interactions lead to a sizable enhancement of the gap (thus implying more stable MBS in an interacting system), which is furthermore strongly anisotropic.

The outline of this paper is as follows. In Sec. II we introduce the effective 1D Hamiltonians describing holes in Ge/Si NWs interacting via Coulomb repulsion and distill an effective lowest-energy Hamiltonian. We bosonize the latter in Sec. III and, in Sec. IV, analyze the exponents of the correlation functions regarding the dependence on the applied electric field and NW parameters. In Sec. V we examine the partial gap opened by an external magnetic field and its dependence on the electric field and the direction of the magnetic field. For technical details we refer to the Appendixes.

II. MODEL

A. 1D hole Hamiltonian

As a first step we derive an effective theory for the single subband regime of a Ge/Si core/shell NW in the presence of Coulomb interactions. Our starting point is a more complex model [22] for a NW with core (shell) radius R (R_s) aligned with the z axis of the coordinate system, and exposed to an electric field perpendicular to the NW axis, $E = E_{\perp}(\cos \varphi_E, \sin \varphi_E, 0)$. A possibly applied magnetic field will be added in a later step. The noninteracting part of this setup is well described by an effective quasi-1D Hamiltonian $H_0 = \int dz \mathcal{H}_0$ with

$$\mathcal{H}_0 = \Psi^{\dagger}(z) [\mathcal{H}_{\mathrm{LK}} + \mathcal{H}_{\mathrm{strain}} + \mathcal{H}_{\mathrm{R}} + \mathcal{H}_{\mathrm{DR}} - \mu] \Psi(z), (1)$$

where μ denotes the chemical potential, and with \mathcal{H}_0 being written in the basis { $\Psi_{g_+}(z), \Psi_{g_-}(z), \Psi_{e_+}(z), \Psi_{e_-}(z)$ }. The indices g_{\pm}, e_{\pm} comprise the band (g, e) and pseudospin

(+,-) labels, and the annihilation operators are given by $\Psi_i(z) = \sum_{k_z} e^{ik_z z} c_{i,k_z}$, with c_{i,k_z} being the annihilation operator of a hole state *i* with momentum k_z along the NW. The Luttinger-Kohn and strain Hamiltonian densities read $\mathcal{H}_{LK} + \mathcal{H}_{strain} = A_+(k_z) + A_-(k_z)\tau_z + Ck_z\tau_y\sigma_x$, with τ_i and σ_i being the Pauli matrices acting in the band and pseudospin space, respectively. Here $A_{\pm}(k_z, \eta) \equiv$ $\hbar^2 k_z^2 (m_g^{-1} \pm m_e^{-1})/4 \pm \Delta/2$, with Planck's constant \hbar , and effective masses $m_g \simeq m_0/(\gamma_1 + 2\gamma_s)$ with and $m_e = m_0/(\gamma_1 + \gamma_s)$. The bare electron mass is denoted by m_0 , and γ_1 and γ_s are the Luttinger parameters in spherical approximation. For Ge, $\gamma_1 = 13.35$ and $\gamma_s = 5.11$ [29]. The level splitting between the g_{\pm} and e_{\pm} states is $\Delta \equiv \Delta_{LK} + \Delta_{strain}(\eta)$ with relative shell thickness $\eta \equiv (R_s - R)/R$, confinement induced $\Delta_{\rm LK} = 0.73\hbar^2/(m_0 R^2)$, and the strain dependent splitting coupling $\Delta_{\text{strain}}(\eta) \simeq 0-30 \text{ meV}.$ The off-diagonal with coupling constant $C = 7.26\hbar^2/(m_0 R)$ is a direct consequence of the strong atomic level SOI. The direct Rashba SOI, $\mathcal{H}_{DR} = eUE_{\perp}(\tau_x \sigma_z \cos \varphi_E - \tau_y \sin \varphi_E)$, where U = 0.15R, results from direct, dipolar coupling of E to the charge of the hole. The conventional Rashba SOI $\mathcal{H}_{\mathrm{R}} = \alpha_{R} E_{\perp} [S(\tau_{x} \sigma_{z} \cos \varphi_{E} - \tau_{y} \sin \varphi_{E}) + B_{+}(k_{z}) +$ reads $B_{-}(k_z)\tau_z$, with $B_{\pm}(k_z) \equiv k_z T(\sigma_x \sin \varphi_E + \sigma_y \cos \varphi_E)/2 \mp$ $3k_z(\sigma_x \sin \varphi_E - \sigma_y \cos \varphi_E)/8$, where T = 0.98, S = 0.36/R, and $\alpha_R = -0.4 \text{ nm}^2 e$ with elementary charge e. Note that $eU/(\alpha_R S) \simeq -1.1 R^2 \text{ nm}^{-2}$, hence \mathcal{H}_{DR} dominates \mathcal{H}_{R} by one to two orders of magnitude for R = 5-10 nm. Diagonalizing the full (4×4) matrix Hamiltonian H_0 yields the eigenenergies $E_{g'_+}$, $E_{g'_-}$, $E_{e'_+}$, and $E_{e'_-}$. The associated annihilation operators are $\Psi_{g'_+}(z)$, $\Psi_{g'_-}(z)$, $\Psi_{e'_+}(z)$, and $\Psi_{e'_-}(z)$, which are linear combinations of the original annihilation operators introduced below Eq. (1). The coefficients of the linear combinations depend strongly on the NW parameters R and Δ , and both magnitude and direction of E. In the following, we assume the chemical potential to be placed below the bottom of the upper bands e'_{\pm} , and therefore focus on the low-energy Hamiltonian in the subspace spanned by $\{\Psi_{g'_{+}}(z), \Psi_{g'_{-}}(z)\}.$

B. Coulomb interaction

Next, we generalize this Hamiltonian to the interacting case. For our concrete microscopic model, we assume the holes to interact via Coulomb repulsion, and take the latter to be screened by mirror charges in the nearby gates. The associated potential for a hole located at r interacting with a hole located at r' in the presence of a mirror charge at r_{mc} is given by

$$V(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}_{\rm mc}) = \frac{e^2}{4\pi\varepsilon_0\varepsilon_r} \left[\frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|} - \frac{1}{|\boldsymbol{r}-\boldsymbol{r}_{\rm mc}|}\right], \quad (2)$$

with vacuum permittivity ε_0 , and relative permittivity ε_r . For Ge, $\varepsilon_r \approx 16$ [30]. In the initial (4 × 4) basis, the interaction Hamiltonian thus reads

$$H_{c} = \frac{1}{2} \sum_{ijkl} \int \int dz dz' \Psi_{i}^{\dagger}(z) \Psi_{j}^{\dagger}(z')$$
$$\times \left[\int dq V_{\rm 1D}^{ijkl}(q) e^{iq[z-z']} \right] \Psi_{k}(z') \Psi_{l}(z), \qquad (3)$$

with $i, j, k, l = g_{\pm}, e_{\pm}$, and q being the wave vector along the NW. The interaction matrix elements $V_{\text{ID}}^{ijkl}(q)$ of H_c are obtained by integrating out the transverse part of $V(\mathbf{r}, \mathbf{r}', \mathbf{r}_{\text{mc}})$ using the three-dimensional wave functions of holes in Ge/Si NWs derived in Ref. [22]. A more detailed sketch of this calculation is given in Appendix A. Finally, we project the full (4×4) interaction Hamiltonian H_c onto the diagonalized low energy subspace $E'_{g_{\pm}}$, thus arriving at the interacting effective model for the single subband regime of a Ge/Si core/shell NW.

III. BOSONIZATION

The low energy excitations of this interacting 1D system are given by collective bosonic density waves rather than individual fermionic quasiparticles [31]. To distill the related Luttinger liquid Hamiltonian, we linearize the noninteracting part of the spectrum, depicted in Fig. 1, around the Fermi points. In this process we only retain low energy excitations by introducing a momentum cutoff \hbar/α relative to the Fermi points, where α denotes the short distance cutoff length. Because of the SOI, the pseudospin bands g'_{+} and g'_{-} are split in momentum space. We decompose the operators $\Psi_{g'_{+}}(z)$ into right (R_j) and left (L_j) moving modes associated with the low energy excitations close to the inner (j = i) and outer (j = o) Fermi points, $\Psi_{g'_{+}}(z) \simeq R_i(z)e^{ik_{F_i}z} + L_o(z)e^{-ik_{F_o}z}$ and $\Psi_{g'_{-}}(z) \simeq R_o(z)e^{ik_{F_o}z} + L_i(z)e^{-ik_{F_i}z}$, where the inner and outer Fermi wave numbers are $k_{F_{i,o}}$. The slopes of the spectrum at these points define the Fermi velocities v_{E_i} and v_{E_o} . These differ because the admixing of the higher energy bands e_{\pm} renders the bands g'_{\pm} nonparabolic. Since we are eventually interested in the renormalization of the partial gap opened by a small magnetic field, we furthermore choose the chemical potential to be pinned to the crossing point of $E_{g'_{\perp}}$ and $E_{g'_{\perp}}$. We emphasize, however, that our model is valid for arbitrary values of μ , with the exception of μ being close to the bottom of the band, where the nonlinearity of the spectrum becomes important for the low-energy excitations.

While the projection of the noninteracting Hamiltonian H_0 on the low-energy modes $R_{i,o}$ and $L_{i,o}$ simply reads $H_0 \approx \int dz \sum_{s=i,o} v_{F_s} (R_s^{\dagger} \partial_z R_s - L_s^{\dagger} \partial_z L_s)$, the interaction Hamiltonian H_c demands a more careful treatment. We project H_c on the low-energy modes $R_{i,o}$ and $L_{i,o}$, thereby dropping

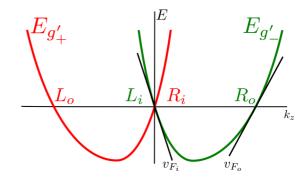


FIG. 1. (Color online) Sketch of the low-energy dispersions $E_{g'_{+}}$ and $E_{g'_{-}}$ as functions of the momentum k_z along the NW for a finite field E_{\perp} . The Fermi velocities v_{F_i} and v_{F_o} for the inner and outer modes differ in the general case, i.e., $v_{F_i} \neq v_{F_o}$.

rapidly oscillating terms, and classify the remaining $V_{\rm 1D}^{ijkl}(q)$ according to the standard *g*-ology [31]. This translates $V_{\rm 1D}^{ijkl}(q)$ to the interaction matrix elements g_{n_f} with indices n = 1, 2, 4, and f = i, o, io, which couple only inner (*i*), only outer (*o*), or inner and outer (*io*) modes. Note that we observe several matrix elements corresponding to g_1 processes coupling the inner and outer modes, we label them $g_{1_{ioj}}$, j = 1, 2, 3, 4, in order of appearance. With these definitions, the projection of H_c reads $H_c = \int dz (\mathcal{H}_1 + \mathcal{H}_2 + \mathcal{H}_4)$, with

$$\mathcal{H}_{2} = g_{2_{i}} \rho_{R_{i}} \rho_{L_{i}} + g_{2_{o}} \rho_{L_{o}} \rho_{R_{o}} + g_{2_{io}} \left(\rho_{L_{i}} \rho_{R_{o}} + \rho_{L_{o}} \rho_{R_{i}} \right), (4)$$

$$\begin{aligned} \mathcal{H}_{4} &= \frac{g_{4_{i}}}{2} \left(\rho_{R_{i}}^{2} + \rho_{L_{i}}^{2} \right) + \frac{g_{4_{o}}}{2} \left(\rho_{R_{o}}^{2} + \rho_{L_{o}}^{2} \right) \\ &+ g_{4_{io}} \left(\rho_{R_{i}} \rho_{R_{o}} + \rho_{L_{i}} \rho_{L_{o}} \right), \end{aligned} \tag{5}$$

$$\begin{aligned} \mathfrak{H}_{1} &= 2g_{I}(R_{i}^{\dagger}L_{i}^{\dagger}L_{o}R_{o} + \mathrm{H.c.}) - g_{1_{io1}}(\rho_{R_{i}}\rho_{L_{o}} + \rho_{R_{o}}\rho_{L_{i}}) \\ &- g_{1_{io2}}(\rho_{L_{o}}\rho_{L_{i}} + \rho_{R_{o}}\rho_{R_{i}}), \end{aligned}$$

$$\tag{6}$$

where $g_I = (g_{1_{io3}} - g_{1_{io4}})/2$, and with $\rho_{r_j} = r_j^{\dagger} r_j$ (r = R, L). Note that we have dropped the terms proportional to g_{1_i} and g_{1_o} because their matrix elements vanish, while we obtain $g_{2_f} = g_{4_f}, g_{1_{io1}} = g_{1_{io4}}$, and $g_{1_{io2}} = -g_{1_{io3}}$.

We thus find that as usual [31] the Coulomb repulsion gives rise to several terms proportional to squares of the fermionic densities ρ_{rj} , plus the term proportional to g_I . We bosonize these interaction terms by expressing the fermionic single-particle operators as $r_s =$ $U_{r,s}e^{-i/2[(1+s)(r\phi_i-\theta_i)+(1-s)(r\phi_o-\theta_o)]}/\sqrt{2\pi\alpha}$, where $r = R, L \equiv$ +1, -1 labels the chirality, and $s = i, o \equiv +1, -1$ denotes the inner/outer pseudospin, while $U_{r,s}$ are Klein factors (unessential for our discussion). The bosonic fields ϕ_s relate to the integrated density of s = i, o particles, while the canonically conjugate fields θ_s are proportional to their current. In terms of the bosonic fields, the Hamiltonian takes the form $H = \int dz (\Psi_{\phi}^{\dagger} \mathcal{H}_{\phi} \Psi_{\phi} +$ $\Psi_{\theta}^{\dagger} \mathcal{H}_{\theta} \Psi_{\theta})/2\pi + \int dz g_I \cos[2(\theta_o - \theta_i)]/(\pi\alpha)^2$, where $\Psi_{\phi} =$ $(\partial_z \phi_o, \partial_z \phi_i)^T, \Psi_{\theta} = (\partial_z \theta_o, \partial_z \theta_i)^T$, and

$$\mathcal{H}_{\phi} = \begin{pmatrix} v_{F_o} + \frac{g_{4_o} + g_{2_o}}{2\pi} & \frac{g_{4_{io}} + g_{2_{io}} - g_{1_{io1}} - g_{1_{io2}}}{2\pi} \\ \frac{g_{4_{io}} + g_{2_{io}} - g_{1_{io1}} - g_{1_{io2}}}{2\pi} & v_{F_i} + \frac{g_{4_i} + g_{2_i}}{2\pi} \end{pmatrix}, \quad (7a)$$
$$\mathcal{H}_{\theta} = \begin{pmatrix} v_{F_o} + \frac{g_{4_o} - g_{2_o}}{2\pi} & \frac{g_{4_{io}} - g_{2_{io}} + g_{1_{io1}} - g_{1_{io2}}}{2\pi} \\ \frac{g_{4_{io}} - g_{2_{io}} + g_{1_{io1}} - g_{1_{io2}}}{2\pi} & v_{F_i} + \frac{g_{4_i} - g_{2_i}}{2\pi} \end{pmatrix}. \quad (7b)$$

The quadratic sector of the Hamiltonian can be diagonalized by a canonical transformation, resulting in effective lowenergy degrees of freedom with velocities u_p and u_m (see Appendix B), while the sine-Gordon term $\sim g_I$ is analyzed using a standard perturbative renormalization group (RG) approach [31]. Because we choose to fix the chemical potential at the crossing point of $E_{g'_+}$ and $E_{g'_-}$, our calculation is restricted to sufficiently large electric fields E_{\perp} such that g_I can be treated as a perturbation $[2g_I/(u_p + u_m) \ll 1]$. For smaller E_{\perp} one of the velocities u_m vanishes, and the dimensionless g_I becomes nonperturbatively large. With this restriction in mind, we find that g_I is an RG irrelevant perturbation in the regime described by our calculation.

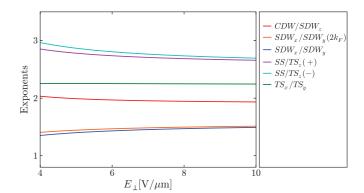


FIG. 2. (Color online) The exponents of the correlation functions as functions of E_{\perp} for R = 10 nm and $\Delta = 8$ meV in the regime where g_I can be treated as perturbation. We fix $\varphi_E = 3\pi/2$ and $\mathbf{r}_{\rm mc} = (0, |\mathbf{r}_{\rm mc}|, 0)$, with $|\mathbf{r}_{\rm mc}| = 100$ nm.

IV. EXPONENTS OF THE CORRELATION FUNCTIONS

After integrating the RG flow of g_I to weak coupling, we evaluate various correlation functions $\langle O_i^{\dagger}(r) O_i(0) \rangle$ for the charge and spin density waves (j = CDW, SDW), and the singlet and triplet superconducting fluctuations (j = SS, TS) [31] (see Appendix B), where the spin is the pseudospin distinguishing the bands g_{\pm}' (as detailed in Appendix B, the correlation functions for $SDW_{x,y}$, SS, and TS_z comprise two terms with slightly different exponents). The scaling exponents of these correlation functions are depicted in Fig. 2 as functions of the applied field E_{\perp} for one concrete set of NW parameters, and exhibit only a weak dependence on E_{\perp} (the same is found for other NW parameters). In Fig. 3 we furthermore plot the scaling exponents for 12 concrete sets of system parameters at a fixed field E_{\perp} . In general, our microscopic model predicts that the exponents of the correlation functions show a strong dependence on the microscopic NW parameters R and Δ , determined by the core and shell radii. The scaling exponents differ substantially from 2, their noninteracting value, thus indicating

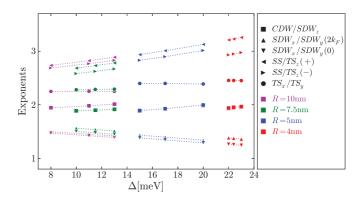


FIG. 3. (Color online) The exponents of the correlation functions as functions of Δ for four different core radii, R = 4 nm (red), R = 5 nm (blue), R = 7.5 nm (green), and R = 10 nm (magenta), where $E_{\perp} = 8V/\mu m$ at fixed $\varphi_E = 3\pi/2$ and $\mathbf{r}_{mc} = (0, |\mathbf{r}_{mc}|, 0)$, with $|\mathbf{r}_{mc}| = 100$ nm. For a fixed *R* and increasing Δ , all exponents besides the ones for the CDW/SDW_z and the TS_x/TS_y become increasingly different from their noninteracting value 2. The dotted lines are a guide to the eyes.

strong interaction effects in Ge/Si core/shell NWs. Exponents differing the most from 2 are found for the NW parameter set with the smallest R, indicating that thin NWs show the strongest interactions. We note that when the field E_{\perp} is tuned to sufficiently small values, such that the system is pushed outside the perturbative regime, the bosonic RG calculation exhibits a Wentzel-Bardeen singularity [32–35]. As a crosscheck for the absence of singularities in the regime well described by our calculation, we have performed a fermionic one-loop RG analysis [36,37], which reproduces the nonsingular behavior of the scaling exponents in the perturbative regime. In the E_{\perp} range where also the fermionic calculation is not valid, the presence or absence of a singularity in the one-loop calculation depends strongly on the chosen NW parameters. For more details we refer the reader to Appendix C.

V. RENORMALIZATION OF THE PARTIAL GAP

As a final example for interaction effects in Ge/Si core/shell NWs, we now turn to the rescaling of the gap opened by a small magnetic field $\boldsymbol{B} = (B_{\perp} \cos \varphi_E, B_{\perp} \sin \varphi_E, B_z).$ This gap, giving rise to the helical regime susceptible to the formation of MBS, is known to be enlarged by Coulomb interaction in an electronic Rashba NW [38,39]. To analyze this effect in our concrete microscopic model with hole-hole interactions, we first introduce the magnetic field Hamiltonian density $\mathcal{H}_B = \mathcal{H}_{B,Z} + \mathcal{H}_{B,orb}$ in the original fermionic (4 × 4) basis of \mathcal{H}_0 with $\mathcal{H}_{B,Z} = [C_+ +$ $C_{-}\tau_{z}\sigma_{z} + [D_{+} + D_{-}\tau_{z}]\sigma_{x}\cos\varphi_{E} - [D_{-} + D_{+}\tau_{z}]\sigma_{y}\sin\varphi_{E}$ $\mathcal{H}_{B,\mathrm{orb}} = F_z \tau_x \sigma_y + F_{\perp} [\tau_y \cos \varphi_E + \tau_x \sigma_z \sin \varphi_E].$ and $C_{\pm} = \mu_B B_z (F \pm G)/2, \quad D_{\pm} = \mu_B B_{\perp} (K \pm M)/2,$ Here $F_z = \mu_B B_z D k_z$, and $F_\perp = \mu_B B_\perp L k_z$, with F = 1.56, G = -0.06, K = 2.89, M = 2.56, D = 2.38R, and L = 8.04R [22]. We focus on a magnetic field **B** in the plane defined by E and the NW axis since a field perpendicular to this plane does not give rise to the helical regime relevant for MBS, but rather to a spin-polarized state. To bring this field to its bosonized form, we first transform \mathcal{H}_B according to the unitary transformation that diagonalizes the fermionic (4×4) Hamiltonian, and then project it to the lower bands. This yields a Hamiltonian density of the form $\mathcal{H}'_B = \mu_B[g_z B_z \sigma_x + g_\perp B_\perp \sigma_y]$, with effective g factors g_z and g_{\perp} , and where $\sigma_{x,y,z}$ acts on the pseudospin distinguishing g'_+ . We finally bosonize \mathcal{H}'_B , and obtain

$$\mathcal{H}'_B = \frac{1}{\pi \alpha} \Delta_Z(\vartheta_B) \cos[2\phi_i - \varphi_B], \qquad (8)$$

with $\Delta_Z(\vartheta_B) = \mu_B(g_z^2 B^2 \cos^2 \vartheta_B + g_\perp^2 B^2 \sin^2 \vartheta_B)^{1/2}$, $B_\perp = B \sin \vartheta_B$, $B_z = B \cos \vartheta_B$, and $\tan \varphi_B = g_z B_z/(g_\perp B_\perp)$. This sine-Gordon term obeys the RG equation $d\Delta_Z/dl = (2 - g_B)\Delta_Z(l)$, where the interaction dependent scaling dimension g_B follows from the diagonalized Hamiltonian. Due to the presence of Coulomb repulsion, we find that g_B is always smaller than its noninteracting value $g_0 = 1$, such that the gap is enhanced by hole-hole interactions. We can thus conclude that hole-hole interactions would stabilize a MBS in the presence of proximity-induced superconductivity, similar to proximitized Rashba NWs for electrons [40,41]. The RG flow is integrated until the running $\Delta_Z(l)$ grows to the value $\Delta_Z(l)/(\hbar v_{F_i}/\alpha) \sim 1$ [31], signaling the opening of the

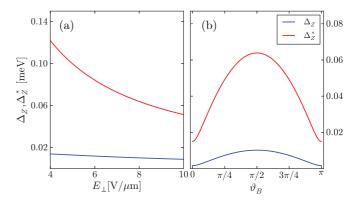


FIG. 4. (Color online) The bare and rescaled helical gaps Δ_Z and Δ_Z^* for B = 0.1T (a) as functions of E_{\perp} for $\vartheta_B = \pi/2$ and (b) as functions of ϑ_B for $E_{\perp} = 8$ V/ μ m. We use the NW parameters R = 7.5 nm and $\Delta = 13$ meV and fix $\varphi_E = 3\pi/2$ and $\mathbf{r}_{\rm mc} = (0, |\mathbf{r}_{\rm mc}|, 0)$, with $|\mathbf{r}_{\rm mc}| = 100$ nm.

helical gap. In physical units, this gap has the size $\Delta_Z^* = \Delta_Z^0 [\hbar v_{F_i}/(2\Delta_Z^0 \alpha)]^{(1-g_B)/(2-g_B)}$ [39]. In Fig. 4(a) we plot both Δ_Z and Δ_Z^* as functions of E_{\perp} for $B_{\perp} = 0.1$ T and $B_z = 0$ T, with $\alpha = 5.65$ Å being the lattice constant of Ge [42]. We find that Δ_Z^* depends much stronger on E_{\perp} than Δ_Z . This can be attributed to the large changes in v_{F_i} for decreasing E_{\perp} . In Fig. 4(b) we finally display Δ_Z and Δ_Z^* for fixed B and E_{\perp} as functions of ϑ_B , i.e., the direction of B with respect to the NW, and find that both Δ_Z and Δ_Z^* are strongly anisotropic.

VI. CONCLUSIONS

In this work we have addressed and quantified the effects of hole-hole interactions and their Luttinger liquid description in Ge/Si core/shell NWs, where we focused on the single subband regime most relevant for the emergence of MBS. We derived the Luttinger liquid description of the NW, and calculated the interaction dependent scaling exponents of various correlation functions. We showed a weak dependence of the scaling exponents on the magnitude of an applied electric field and a strong dependence on the NW parameters. Furthermore, the exponents revealed strong interaction effects since they differ substantially from their noninteracting value with thin NWs showing the strongest deviations. To show the experimental relevance of our results, we analyzed the renormalization of the partial gap around zero momentum resulting from an applied magnetic field which is considerably enhanced by the hole-hole interactions. Additionally, we found that the gap is strongly anisotropic. Regarding the emergence of MBS in the helical regime of a superconducting hybrid device, the enhancement of the gap implies more stable MBS in an interacting system.

In conclusion, hole-hole interactions show sizable effects in Ge/Si core/shell NWs and may lead to the stabilization of emerging MBS by enhancing the partial gap.

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APPENDIX A: CALCULATION OF THE SCREENED COULOMB MATRIX ELEMENTS

To calculate the effective 1D, momentum dependent interaction matrix elements $V_{1D}^{ijkl}(q)$ introduced in Eq. (3) of the main text, we use the transverse part of the real space wave functions of holes confined to the Ge core of the NW [22] $\phi_{g_{\pm}}(\mathbf{r}_{\perp}) = g_{\pm}(r,\varphi)$ and $\phi_{e_{\pm}}(\mathbf{r}_{\perp}) = e_{\pm}(r,\varphi)$, where \mathbf{r}_{\perp} denotes the transverse part of \mathbf{r} . Due to the hard wall confinement assumed for the derivation of $\phi_{g_{\pm}}(\mathbf{r}_{\perp})$ and $\phi_{e_{\pm}}(\mathbf{r}_{\perp})$, the wave functions are proportional to functions of the type $J_n(r)$, where J_n denotes the *n*th Bessel function of the first kind. The interaction matrix elements are given by integrals of form

$$V_{\rm lD}^{ijkl}(q) = \int \int_{\rm NW_{\perp}} d\boldsymbol{r}_{\perp} d\boldsymbol{r}'_{\perp} \phi_i^{\dagger}(\boldsymbol{r}_{\perp}) \phi_j^{\dagger}(\boldsymbol{r}'_{\perp}) V(\boldsymbol{r}, \boldsymbol{r}', \boldsymbol{r}_{\rm mc}) \\ \times \phi_k(\boldsymbol{r}'_{\perp}) \phi_l(\boldsymbol{r}_{\perp}), \tag{A1}$$

with $i, j, k, l = g_{\pm}, e_{\pm}$ and $d\mathbf{r}_{\perp} = rdrd\varphi$ $(d\mathbf{r}'_{\perp} = r'dr'd\varphi')$. Here NW_{\perp} indicates integration over the NW cross section. To perform the integration, we follow the procedure outlined in Ref. [43]. We rewrite the summands of $V(\mathbf{r}, \mathbf{r}', \mathbf{r}_{mc})$ in terms of discrete Fourier transformations along the NW with wave vector $\mathbf{q} = (0, 0, q)$, which brings the position dependent part of the Coulomb potential to the form

$$\frac{1}{|\mathbf{r} - \mathbf{r}'|} = \frac{1}{\sqrt{(z - z')^2 + a^2}} = \sum_{q} 2K_0(aq)e^{iq(z - z')}, \quad (A2)$$

with $a^2 = r^2 + r'^2 - 2rr' \cos(\varphi - \varphi')$, and where $K_m(x)$ denotes the modified Bessel function of the second kind. A similar term is obtained for the position dependent part of the screened potential $1/|\mathbf{r} - \mathbf{r}_{mc}|$. Equation (A2) can be simplified further by applying Graf's addition theorem for Bessel functions [44]

$$K_0(aq) = \sum_{m=-\infty}^{\infty} e^{im(\varphi - \varphi')} K_m(qr_>) I_m(qr_<), \quad (A3)$$

where $r,r' = r_>, r_<$ with $r_> \ge r_<$, while $I_m(x)$ denotes the modified Bessel function of the first kind. We insert the results of Eqs. (A2) and (A3) into Eq. (A1), and integrate out the angular part $\int \int d\varphi d\varphi'$. The remaining nonzero contributions of the sum in Eq. (A3) are the terms corresponding to $m = 0, \pm 1$. However, this result depends strongly on the exact form of the angular dependence of $\phi_{g_{\pm}}(\mathbf{r}_{\perp})$ and $\phi_{e_{\pm}}(\mathbf{r}_{\perp})$. The last step, the radial integration $\int \int rr' dr dr'$ cannot be performed directly in an analytical manner. To circumvent this, we replace the Bessel functions in Eq. (A3), and in the wave functions by Taylor expansions around r,r' = 0 up to appropriate order. This allows us to evaluate the radial integrals analytically. We have checked numerically that our analytical expressions reproduce the exact result very well.

APPENDIX B: OPERATORS AND CORRELATION FUNCTIONS IN THE *i*, *o* BASIS, AND TRANSFORMATION TO THE DIAGONAL BASIS

For the evaluation of correlation functions, it is helpful to change to a basis in which the matrices \mathcal{H}_{ϕ} and \mathcal{H}_{θ} , given in the main text in Eqs. (7a) and (7b), are diagonal. This can be achieved by the basis change $(\phi_i, \phi_o)^T = W_{\phi}(\phi_p, \phi_m)^T$ and

 $(\theta_i, \theta_o)^T = W_{\theta}(\theta_p, \theta_m)^T$, where W_{ϕ} and W_{θ} are matrices with (so far unspecified) real entries $w_{\phi,kl}$ and $w_{\theta,kl}$, and where we have introduced the new fields ϕ_r and θ_r , with r = p, m. For this transformation to be canonical, we demand that the new fields obey the commutation relations $[\phi_r(z), \nabla \theta_{r'}(z')] = i \pi \delta_{z,z'} \delta_{r,r'}$ and $[\phi_r(z), \theta_{r'}(z')] = i \pi/2 \operatorname{sgn}(z - z') \delta_{r,r'}$, which fixes four of the eight parameters in W_{ϕ} and W_{θ} .

The Hamiltonian densities are transformed as $\tilde{\mathcal{H}}_{\phi} = (W_{\phi})^T \mathcal{H}_{\phi} W_{\phi}$ and $\tilde{\mathcal{H}}_{\theta} = (W_{\theta})^T \mathcal{H}_{\theta} W_{\theta}$. The requirement that the transformation diagonalizes the Hamiltonian densities fixes two more parameters in W_{ϕ} and W_{θ} . The remaining two parameters are finally chosen such that

$$\tilde{\mathcal{H}}_{\phi} = \tilde{\mathcal{H}}_{\theta} = \frac{1}{2\pi} \begin{pmatrix} u_p & 0\\ 0 & u_m \end{pmatrix}, \tag{B1}$$

with velocities u_p and u_m .

This diagonal basis is particularly convenient if one is interested in evaluating correlation functions of the charge and spin degrees of freedom, where charge and spin are defined in analogy to a Rashba NW (the band E'_{g_+} , i.e., the modes L_o and R_i , are thus interpreted as left and right moving modes with spin up, while the band E'_{g_-} , i.e., L_i and R_o , are identified with left and right moving spin down modes). The operators describing the integrated charge (ρ) and spin (σ) densities (ϕ_i) and currents (θ_i) are given by

$$\phi_{\sigma} = -\frac{1}{\sqrt{2}}(\theta_i - \theta_o), \quad \theta_{\sigma} = -\frac{1}{\sqrt{2}}(\phi_i - \phi_o), \quad (B2)$$

$$\phi_{\rho} = \frac{1}{\sqrt{2}}(\phi_i + \phi_o), \quad \theta_{\rho} = \frac{1}{\sqrt{2}}(\theta_i + \theta_o). \tag{B3}$$

Using these relations, the operators for the charge density wave (CDW), spin density wave (SDW), singlet superconductivity (SS), and triplet superconductivity (TS) read

$$O_{\text{CDW}}(r) = \frac{1}{\pi \alpha} e^{-ik_{F_o} z} e^{i[\phi_i(r) + \phi_o(r)]} \cos[\theta_i(r) - \theta_o(r)], \quad (B4)$$

$$O_{\text{SDW}}^{x}(r) = \frac{1}{\pi \alpha} e^{-ik_{F_{o}}z} e^{i[\phi_{i}(r) + \phi_{o}(r)]} \cos[\phi_{i}(r) - \phi_{o}(r) + k_{F_{o}}z],$$
(B5)

$$O_{\text{SDW}}^{y}(r) = \frac{1}{\pi \alpha} e^{-ik_{F_o} z} e^{i[\phi_i(r) + \phi_o(r)]} \sin[\phi_i(r) - \phi_o(r) + k_{F_o} z],$$
(B6)

$$O_{\text{SDW}}^{z}(r) = \frac{i}{\pi\alpha} e^{-ik_{F_o}z} e^{i[\phi_i(r) + \phi_o(r)]} \sin[\theta_o(r) - \theta_i(r)], \quad (B7)$$

$$O_{\rm SS}(r) = \frac{1}{\pi \alpha} e^{-i[\theta_i(r) + \theta_o(r)]} \cos[\theta_i(r) - \theta_o(r)], \tag{B8}$$

$$O_{\rm TS}^{x}(r) = \frac{1}{\pi \alpha} e^{-i[\theta_{i}(r) + \theta_{o}(r)]} \cos[\phi_{i}(r) - \phi_{o}(r) + k_{F_{o}}z],$$
(B9)

$$O_{\rm TS}^{y}(r) = \frac{1}{\pi\alpha} e^{-i[\theta_i(r) + \theta_o(r)]} \sin[\phi_i(r) - \phi_o(r) + k_{F_o} z],$$
(B10)

$$O_{\text{TS}}^{z}(r) = \frac{i}{\pi \alpha} e^{-i[\theta_{i}(r) + \theta_{o}(r)]} \sin[\theta_{o}(r) - \theta_{i}(r)].$$
(B11)

A detailed discussion of these operators can be found in Ref. [31]. In the diagonal basis, the associated correlation functions are given by

$$\langle O_{\text{CDW}}^{\dagger}(r) O_{\text{CDW}}(0) \rangle$$

$$= \left\langle O_{\text{SDW}}^{z,\dagger}(r) O_{\text{SDW}}^{z}(0) \right\rangle$$

$$= \frac{1}{(\pi\alpha)^{2}} e^{ik_{F}z} (\alpha/r)^{1/2(u_{a+}^{2}+u_{b+}^{2}+w_{a-}^{2}+w_{b-}^{2})},$$

$$\langle O_{\text{SDW}}^{x,\dagger}(r) O_{\text{SDW}}^{x}(0) \rangle$$

$$(B12)$$

$$= \langle O_{\text{SDW}}^{y,\dagger}(r) O_{\text{SDW}}^{y}(0) \rangle$$

= $\frac{1}{4(\pi \alpha)^{2}} \left[e^{2ik_{F}z} (\alpha/r)^{1/2[(u_{a+}-u_{a-})^{2}+(u_{b+}-u_{b-})^{2}]} + (\alpha/r)^{1/2[(u_{a+}+u_{a-})^{2}+(u_{b+}+u_{b-})^{2}]} \right]$
= $\langle O_{\text{SDW}}^{y,\dagger}(r) O_{\text{SDW}}^{y}(0) \rangle_{(2k_{F})} + \langle O_{\text{SDW}}^{y,\dagger}(r) O_{\text{SDW}}^{y}(0) \rangle_{(0)}, \quad (B13)$
 $\langle O_{\text{SS}}^{\dagger}(r) O_{\text{SS}}(0) \rangle$

$$= \left\langle O_{\rm TS}^{z,\dagger}(r) O_{\rm TS}^{z}(0) \right\rangle$$

= $\frac{1}{4(\pi\alpha)^{2}} \left[(\alpha/r)^{1/2[(w_{a+}+w_{a-})^{2}+(w_{b+}+w_{b-})^{2}]} + (\alpha/r)^{1/2[(w_{a+}-w_{a-})^{2}+(w_{b+}-w_{b-})^{2}]} \right],$
= $\left\langle O_{\rm TS}^{z,\dagger}(r) O_{\rm TS}^{z}(0) \right\rangle_{(+)} + \left\langle O_{\rm TS}^{z,\dagger}(r) O_{\rm TS}^{z}(0) \right\rangle_{(-)},$ (B14)
 $\left\langle O_{\rm TS}^{x,\dagger}(r) O_{\rm TS}^{x}(0) \right\rangle$

$$= \left\langle O_{\rm TS}^{y,\dagger}(r) O_{\rm TS}^{y}(0) \right\rangle$$

= $\frac{1}{(\pi \alpha)^2} (\alpha/r)^{1/2(u_{a-}^2 + u_{b-}^2 + w_{a+}^2 + w_{b+}^2)},$ (B15)

with $u_{a,\pm} = w_{\phi,21} \pm w_{\phi,11}$, $u_{b,\pm} = w_{\phi,22} \pm w_{\phi,21}$, $w_{a,\pm} = w_{\theta,21} \pm w_{\theta,11}$, $w_{b,\pm} = w_{\theta,22} \pm w_{\theta,12}$. Note that the correlation functions for SDW_{*x*,*y*}, SS, and TS_{*z*} each contain two terms with (slightly) different exponents.

APPENDIX C: DIVERGENCES OUTSIDE THE PERTURBATIVE REGIME AND COMPARISON TO A FERMIONIC RG APPROACH

As discussed in the main text, the use of a perturbative RG approach for the coupling g_I restricts our analysis to a regime in which the associated dimensionless coupling satisfies $2g_I/(u_p + u_m) \ll 1$. In this regime, g_I is found to be RG irrelevant. When leaving the perturbative regime, we find that the scaling exponents diverge at a finite field E_{\perp} (solid lines in Fig. 5). These divergences can be traced back to the fact that the off-diagonal matrix elements in the Hamiltonian given in Eq. (7) are so large that the velocity u_m of the diagonalized Hamiltonian vanishes. The system thus seems to exhibit a Wentzel-Bardeen singularity [32–35]. This apparent divergence, however, occurs outside the perturbative regime, and is thus beyond the range of validity of our calculation (we note that during the RG flow, the quadratic sector of the theory is renormalized by corrections of the order $O(g_I^2)$, see Ref. [31]).

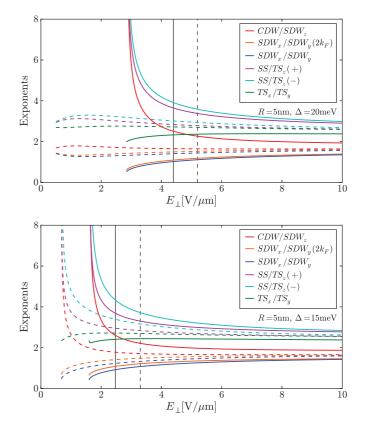


FIG. 5. (Color online) The exponents of the correlation functions for two different sets of NW parameters R and Δ as functions of E_{\perp} , where $\varphi_E = 3\pi/2$ and $\mathbf{r}_{mc} = (0, |\mathbf{r}_{mc}|, 0)$, with $|\mathbf{r}_{mc}| = 100$ nm. We show the exponents obtained by two different RG approaches, a bosonic sine-Gordon RG approach (solid lines), and a fermionic one-Loop RG calculation (dashed lines). The black vertical lines denote where the perturbative regime ends for either of the two RG approaches. In contrast to the bosonic approach, where the scaling exponents always diverge, the presence of a divergence of the scaling exponents for the fermionic approach depends on the NW parameters.

As an independent crosscheck for the absence of singularities in the regime described by our calculation, we compare the scaling exponents of the correlation functions discussed in the main text to the analogous exponents obtained when the system is bosonized only after an initial fermionic one-loop RG treatment, which in particular already describes the flow of g_1 to weak coupling. To this end, we start from the fermionic Hamiltonian with the interactions given in Eqs. (4)–(6), and perform a fermionic one-loop RG analysis following Refs. [36] and [37]. This yields the one-loop RG equations

$$\frac{d\bar{g}_2}{dl} = -\bar{g}_I(l)^2, \quad \frac{d\bar{g}_I}{dl} = -\bar{g}_I(l)\bar{g}_2(l), \tag{C1}$$

where we have introduced the definitions $\pi \bar{g}_2 = g_{2o}/(2v_{F_o}) + g_{2i}/(2v_{F_i}) - 2(g_{2io} - g_{1io1})/(v_{F_o} + v_{F_i})$ and $\pi \bar{g}_I = g_I \sqrt{2(1 + \gamma)}/(v_{F_o} + v_{F_i})$, with $\gamma = (v_{F_o} + v_{F_i})^2/(4v_{F_o}v_{F_i})$. Integrating these RG equations yields the fixed point values $\bar{g}_I^* = 0$ and $\bar{g}_2^* = [\bar{g}_2^2(0) - \bar{g}_I^2(0)]^{1/2}$ [31], from which we find g_{2o}^*, g_{2i}^* , and $g_{2io}^* - g_{1io}^*$. We plug these renormalized interactions back into the fermionic Hamiltonian. The bosonization of this renormalized Hamiltonian in turn yields a purely quadratic bosonic theory, which finally allows us to calculate the exponents of the various correlation functions just as discussed in the main text.

In the perturbative regime, we find that the qualitative behavior of the scaling exponents is identical for both approaches. Outside the perturbative regime, this is not true. There the presence or absence of a divergence of the scaling exponents calculated using the fermionic one-loop approach depends on the NW parameters, while the bosonic approach seems to generically exhibit a singularity.

Most importantly, however, we find that—if present—the divergences always appear outside the range of validity of our calculation. This finding is illustrated in Fig. 5, where we plot

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the exponents obtained in the bosonic sine-Gordon approach (solid lines), and the exponents obtained when bosonizing after the fermionic one-loop RG treatment (dashed lines). The black vertical lines denote the limits of the perturbative regime, i.e., the black solid line indicates where

$$\frac{g_I}{\frac{1}{2}(u_p + u_m)} \approx 1,$$
(C2)

while the black dashed line depicts where

$$\bar{g}_2 = \frac{g_{2_o}}{2\pi v_{F_o}} + \frac{g_{2_i}}{2\pi v_{F_i}} - \frac{2(g_{2_{io}} - g_{1_{io1}})}{\pi (v_{F_o} + v_{F_i})} \approx 1.$$
(C3)

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