

Ground state properties of the doped Kitaev-Heisenberg chain: Topological superconducting and Mott-insulating phases driven by magnetic frustration

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We study the hole-doped Kitaev-Heisenberg chain using the density-matrix renormalization group. In the Kitaev-only limit, the bond-directional exchange itself promotes pairing, favoring spin-singlet and spin-triplet superconducting tendencies for antiferromagnetic and ferromagnetic Kitaev couplings, respectively, together with finite-size Majorana edge correlations suggestive of topological superconductivity. In the full Kitaev-Heisenberg chain, cooperative J - and K exchanges broadly stabilize superconductivity, while competition between J and K induces a strong filling dependence and enables superconductivity even when both J and K are weak. At quarter filling, this competition produces a Mott insulator with spontaneous hopping dimerization. These results identify magnetic frustration as a common mechanism underlying superconducting and interaction-driven insulating phases in doped Kitaev systems.

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Introduction. The Kitaev model is a paradigmatic frustrated spin system that hosts a gapless $\mathbb{Z}_2$ spin liquid at the isotropic point $K_x = K_y = K_z$ [1,2]. In candidate Kitaev materials, additional interactions—most notably Heisenberg exchange and off-diagonal Γ terms—often stabilize magnetic order [3], motivating ongoing efforts to access Kitaev-driven quantum phases by tuning microscopic parameters or by carrier doping [4]. While the undoped Kitaev-Heisenberg (KH) model has been extensively studied [5,6], its doped counterpart remains far less understood.

Early (slave-boson) mean-field studies proposed superconducting (SC) states upon doping, including topological ones, but their detailed character remains unsettled [7–13]. By contrast, beyond-mean-field approaches and recent density-matrix renormalization group (DMRG) studies have revealed strong competing tendencies and a sensitive dependence on geometry, interaction signs, kinetic energy, and doping regime in doped Kitaev systems [14,15]. Recent studies of doped triangular-lattice Kitaev magnets and two-leg Kitaev-Heisenberg ladders further highlight the current interest in carrier-doped Kitaev systems [16,17]. A comprehensive, unbiased characterization of the strictly one-dimensional doped KH model is therefore still lacking.

In this Letter, we present a systematic DMRG study of the hole-doped KH chain. We map out its ground state phase diagram and identify (i) SC regimes whose spin structure depends on the signs of J and K , together with finite-size signatures suggestive of topological superconductivity over a broad parameter range, and (ii) an interaction-driven dimerized Mott insulator at quarter filling ($n = 0.5$) induced by magnetic frustration. Given the established correspondence between one- and two-dimensional phase diagrams in the Mott-insulating KH model [18–21], our results provide useful guidance for doped Kitaev materials and higher-dimensional settings.

Model. We study the hole-doped KH chain described by the projected t - J - K Hamiltonian,

$$\mathcal{H} = -t \sum_{i=1}^L \sum_{\sigma} (f_{i,\sigma}^{\dagger} f_{i+1,\sigma} + \text{H.c.}) + J \sum_{i=1}^L \mathbf{S}_i \cdot \mathbf{S}_{i+1} + K \sum_{i=1}^{L/2} (S_{2i-1}^x S_{2i}^x + S_{2i}^y S_{2i+1}^y), \quad (1)$$

where $f_{i,\sigma}^{\dagger}$ is the electron creation operator with spin σ at site i , acting in the projected Hilbert space with no double occupancy, and $\mathbf{S}_i = (S_i^x, S_i^y, S_i^z)$ is a spin-1/2 operator. The parameters t , J , and K denote the hopping amplitude, Heisenberg exchange, and Kitaev exchange, respectively. As shown in Fig. 1(a), we refer to the bonds $(2i - 1, 2i)$ and $(2i, 2i + 1)$ as the x and y bonds, respectively.

Methods and observables. We investigate Hamiltonian (1) using the DMRG method with open boundaries on chains of length up to $L = 400$. We keep up to $m = 12\,000$ states, with

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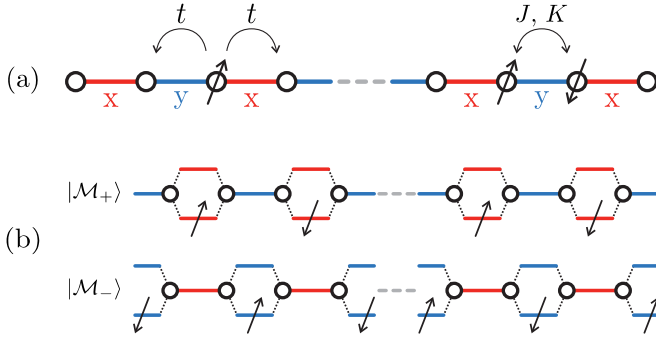


FIG. 1. (a) Lattice structure of the KH chain. (b) Schematic picture of two translation-symmetry-breaking Mott-insulating states, where each bonding orbital is occupied by one fermion.

maximum truncation errors $\lesssim 10^{-4}$, and extrapolate observables to the $m \rightarrow \infty$ limit when necessary.

To map out the ground state phase diagram, we extract the Tomonaga-Luttinger liquid (TLL) parameter K_ρ from the long-wavelength limit of the static charge structure factor $N(q) = \frac{1}{L} \sum_{j,\ell} e^{iq(j-\ell)} \langle (n_j - n)(n_\ell - n) \rangle$ via $K_\rho = \pi \lim_{q \rightarrow 0} N(q)/|q|$ [22]. In a TLL, $K_\rho > 1$ indicates dominant SC correlations. We also compute the pair-binding energy $E_b = 2E_0(N-1) - E_0(N) - E_0(N-2)$, where $E_0(N)$ is the ground state energy in the sector with N electrons. A positive E_b indicates effective attraction between doped holes.

To probe topological SC signatures, we evaluate the end-to-end Majorana correlator $G_{1L} = i \langle \lambda_{1,\sigma} \bar{\lambda}_{L,\sigma} \rangle$, with $\lambda_{j,\sigma} = f_{j,\sigma} + f_{j,\sigma}^\dagger$ and $\bar{\lambda}_{j,\sigma} = f_{j,\sigma} - f_{j,\sigma}^\dagger$ [23]. For finite L , G_{1L} can be nonzero due to edge-mode hybridization, although it vanishes in the thermodynamic limit. Its magnitude and parameter dependence nevertheless provide a useful finite-size diagnostic of regimes with pronounced edge-Majorana character.

To further characterize each phase, we compute the charge gap $\Delta_c = \{E_0(N+2) + E_0(N-2) - 2E_0(N)\}/2$, the connected density and spin correlations $D(r) = \langle n_i n_{i+r} \rangle - \langle n_i \rangle \langle n_{i+r} \rangle$ and $S^\alpha(r) = \langle S_i^\alpha S_{i+r}^\alpha \rangle - \langle S_i^\alpha \rangle \langle S_{i+r}^\alpha \rangle$, and the pair-pair correlations $P_\gamma(r) = \langle \Delta_{\gamma,i+r}^\dagger \Delta_{\gamma,i} \rangle$. Here, $\Delta_{S,i} = (f_{i,\uparrow} f_{i+1,\downarrow} - f_{i,\downarrow} f_{i+1,\uparrow})/\sqrt{2}$ annihilates a spin-singlet pair, while $\Delta_{T1,i} = (f_{i,\uparrow} f_{i+1,\downarrow} + f_{i,\downarrow} f_{i+1,\uparrow})/\sqrt{2}$ and $\Delta_{T2,i}^{(\sigma)} = f_{i,\sigma} f_{i+1,\sigma}$ ($\sigma = \uparrow, \downarrow$) annihilate spin-triplet pairs. Within TLL theory, $D(r) \propto r^{-K_\rho}$ and $P_\gamma(r) \propto r^{-1/K_\rho}$ at long distances.

Pairing induced by Kitaev interactions. While Heisenberg exchange is known to promote superconductivity in doped Mott systems [24,25], the pairing potential of the Kitaev interaction remains largely unexplored. To isolate its effect, we first focus on the $J = 0$ limit and study the doped t - K chain. The resulting ground state phase diagram in the K/t - n plane is shown in Fig. 2, which exhibits an extended region with $K_\rho > 1$, indicating dominant SC correlations within a TLL.

The physical origin of this pairing tendency can already be understood from a local two-particle viewpoint. Consider two carriers occupying neighboring sites, and denote the local two-spin wave function on a bond by $|\psi\rangle$. The Kitaev energy on a γ bond ($\gamma = x, y$) is $e_\gamma = \langle \psi | K S_i^\gamma S_j^\gamma | \psi \rangle$. For antiferromagnetic (AFM) Kitaev exchange ($K > 0$), both e_x and e_y are

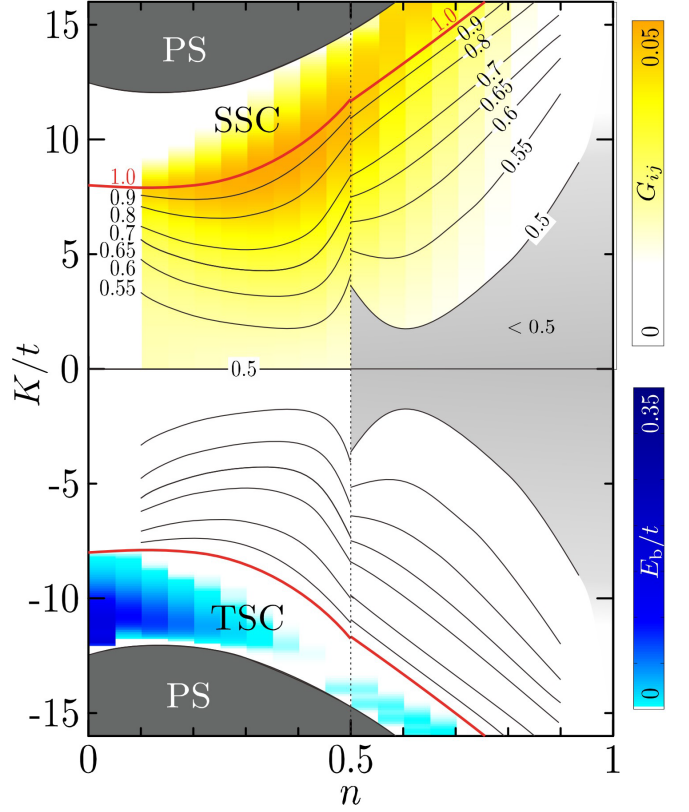


FIG. 2. Phase diagram of the t - K chain ($J = 0$) in the K/t - n plane. Contour lines indicate the TLL parameter K_ρ , while color maps show the end-to-end Majorana correlator G_{1L} and the pair-binding energy E_b/t . Owing to the symmetry under $K \rightarrow -K$, only G_{1L} for $K > 0$ and E_b/t for $K < 0$ are shown (see text). The data for G_{1L} are shown for an open chain with $L = 40$, while those for E_b/t are extrapolated to the thermodynamic limit.

minimized by the singlet $|\psi^-\rangle = (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$, yielding $e_x = e_y = -K/4$. For ferromagnetic (FM) exchange ($K < 0$), the minima are instead achieved by the $S^z = 0$ triplet $|\psi^+\rangle = (|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle)/\sqrt{2}$, again giving $e_x = e_y = -|K|/4$. Thus, the SC regimes for $K > 0$ and $K < 0$ are naturally associated with spin-singlet SC (SSC) and spin-triplet SC (TSC) pairing, respectively. In this sense, the Kitaev interaction provides an effective short-range attraction between neighboring carriers. The SC tendencies in Fig. 2 should therefore be understood as resulting from the competition between this exchange-induced attraction and the kinetic energy of the doped holes; dominant pairing correlations appear only when $|K|/t$ is sufficiently large. Upon further increasing $|K|/t$, however, the attraction eventually becomes too strong and the system undergoes phase separation (PS), as is also well known in the conventional one-dimensional (1D) t - J model.

We note that the Hamiltonians with K and $-K$ are unitarily related by a staggered π -spin rotation, which preserves the energy spectrum while mapping SSC to TSC. Although the present 1D geometry contains only x - and y bonds, it is instructive to note how this local argument extends when a z bond is also present, as in higher-dimensional Kitaev lattices. For a z bond one has $e_z = \langle \psi | K S_i^z S_j^z | \psi \rangle$. Since $\langle \psi^\pm | S_i^z S_j^z | \psi^\pm \rangle = -1/4$, the states $|\psi^\pm\rangle$ minimize e_z only for

$K > 0$. For $K < 0$, the z -bond energy is instead minimized by the equal-spin triplets $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$, for which $\langle S_i^z S_j^z \rangle = +1/4$ and hence $e_z = -|K|/4$. This highlights the bond-selective anisotropy of Kitaev exchange beyond the present 1D setting.

To further characterize the SC regimes in Fig. 2, we show the pair-binding energy E_b/t in the thermodynamic limit and the end-to-end Majorana correlator G_{1L} for an open chain with $L = 40$. While E_b/t is reduced around $n \simeq 0.5$, it remains finite over a broad portion of the pairing-dominated region. The correlator G_{1L} serves as a finite-size diagnostic of edge-Majorana character: it can be nonzero for finite L due to edge-mode hybridization and decreases toward zero in the thermodynamic limit. Nevertheless, the pronounced enhancement of $|G_{1L}|$ at larger fillings, away from the dilute limit, is suggestive of topological superconductivity.

Ground state phase diagram of the doped Kitaev-Heisenberg chain. We now turn to the generic case with both Kitaev and Heisenberg exchanges present. Figure 3 summarizes the ground state phase diagram of the doped KH chain in the K/t - J/t plane for representative fillings $n = 0.1, 0.5$, and 0.9 .

At all doping levels, a robust trend becomes apparent when J and K have the same sign. Here, the two exchanges cooperate to stabilize superconductivity once the overall exchange scale becomes sufficiently large, with relatively weak filling dependence of the phase boundary. For $J, K > 0$ we find an SSC regime, whereas for $J, K < 0$ a TSC regime is realized, as confirmed below by the pair-pair correlations.

By contrast, when J and K have opposite signs, the Kitaev- and Heisenberg-driven tendencies compete strongly, leading to pronounced filling-dependent behavior. Two salient features emerge in this regime. First, at $n = 0.5$, a dimerized Mott-insulating state appears in the narrow region $K > 0$, $J < 0$, and $K + J > 0$, where a finite charge gap Δ_c opens [Fig. 3(b)]. The transition on the small- $|J|$ side is consistent with a transition of the Berezinskii-Kosterlitz-Thouless type, whereas that on the large- $|J|$ side appears to be first order. Second, for $n = 0.9$, superconductivity develops already at relatively small J/t over a broad range of K/t , showing that the competition between J and K can enhance pairing tendencies beyond a simple large-exchange-to-hopping mechanism. In this case, the SC region ($K_\rho > 1$) lies next to a strongly competing metallic regime with a substantially reduced TLL parameter, typically $K_\rho \lesssim 0.5$.

These results suggest that magnetic frustration plays a dual role in the doped KH chain: at commensurate filling it can drive an interaction-induced insulating state, while away from commensuration it enhances SC tendencies near the boundary of the strongly competing regime. More broadly, the pronounced suppression of K_ρ indicates that the competition between Kitaev and Heisenberg exchanges strongly reshapes the low-energy charge response. The unlabeled non-SC regions, except for the PS and commensurate Mott-insulating regimes, are metallic TLL regimes with $K_\rho < 1$, where density-density correlations dominate over pair correlations in the asymptotic TLL sense. The label FMM indicates partial FM polarization within the TSC2 region. Clarifying the microscopic origin of the suppressed K_ρ deep inside

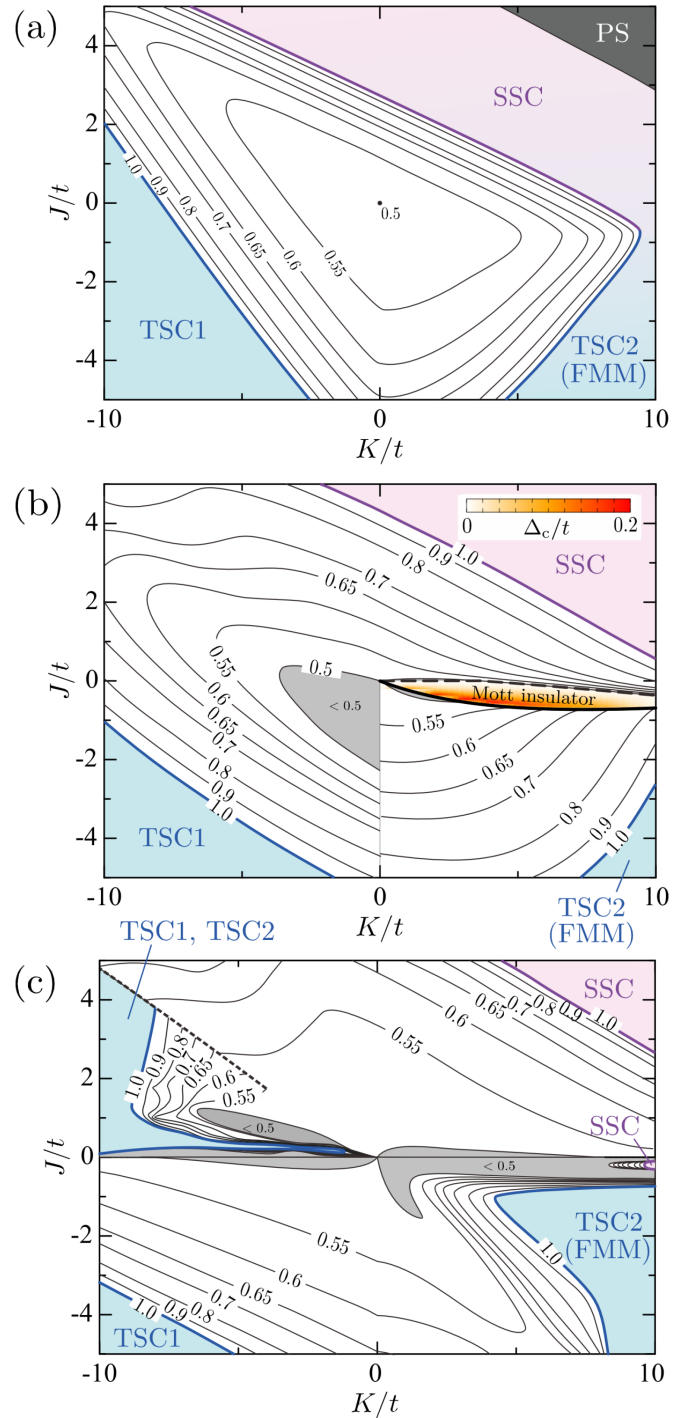


FIG. 3. Phase diagram of the t - J - K chain in the K/t - J/t plane at (a) $n = 0.1$, (b) 0.5 , and (c) 0.9 . A color map of the charge gap Δ_c/t is shown for the Mott-insulating phase at $n = 0.5$. Unlabeled white regions correspond to non-SC metallic TLL regimes with $K_\rho < 1$, except for the phase-separated and Mott-insulating regions indicated explicitly. The label FMM indicates partial FM polarization within the TSC2 region.

the competing metallic regime remains an interesting open problem [14].

In the following, we characterize the dimerized Mott-insulating state in detail and determine the spin structure of the SC regimes by comparing the relevant correlation functions.

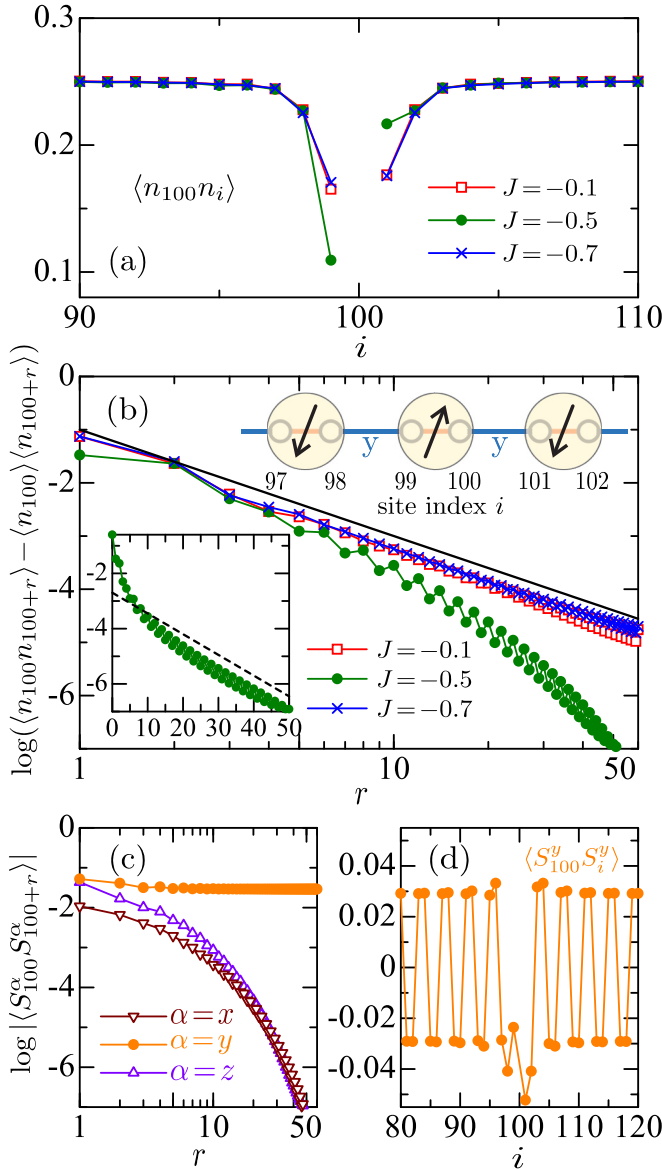


FIG. 4. Results for an open chain of length $L = 200$. (a) Density-density correlation $\langle n_{100}n_i \rangle$ at $K = 5$. (b) Connected density-density correlation $D(r) = \langle n_{100}n_{100+r} \rangle - \langle n_{100} \rangle \langle n_{100+r} \rangle$ at $K = 5$, shown on a log-log scale as a function of distance r . Insets: semilog plot of $D(r)$ (left) and a schematic picture of the dimerized Mott state (right). (c) Spin-spin correlations $|\langle S_{100}^\alpha S_{100+r}^\alpha \rangle|$ for $\alpha = x, y, z$ at $K = 5$ and $J = -0.5$. (d) Real-space profile of the y-component correlation $\langle S_{100}^y S_i^y \rangle$ at $K = 5$ and $J = -0.5$.

Dimerized Mott state at quarter filling. We now examine in more detail the dimerized Mott-insulating state realized at $n = 0.5$ for $K > 0$ and $J < 0$. In this regime, the Kitaev and FM Heisenberg exchanges compete strongly, and the system relieves the resulting frustration by developing a spontaneous dimerization of the kinetic energy, i.e., an alternation of strong and weak bonds.

This dimerization is directly visible in real space from density-density correlations on an open chain. Figure 4(a) shows $\langle n_{100}n_i \rangle$ at $K = 5$ for $J = -0.1, -0.5$, and -0.7 on a chain of length $L = 200$. For $J = -0.1$ and -0.7 , the

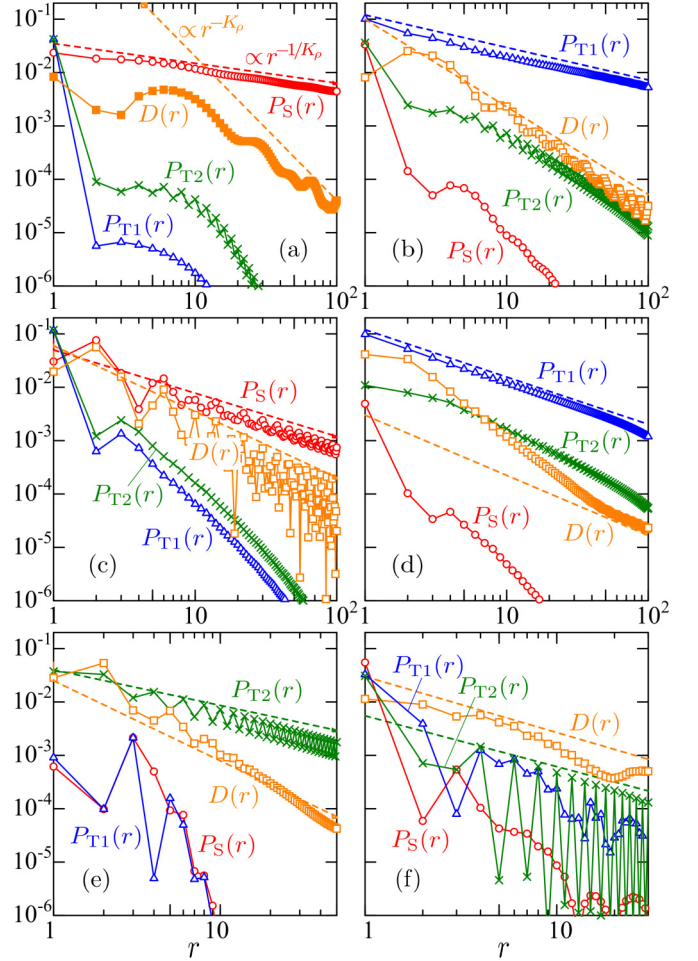


FIG. 5. Pair-pair correlation functions $P_\gamma(r)$ ($\gamma = S, T1, T2$) and density-density correlation functions $D(r)$, plotted on log-log scales for representative parameter sets in the phase diagram: (a) $K = 10.0$, $J = 0.0$, $n = 0.1$ (SSC, $K_\rho = 2.70$); (b) $K = -11.0$, $J = 0.0$, $n = 0.3$ (TSC1, $K_\rho = 1.64$); (c) $K = 5.0$, $J = 3.0$, $n = 0.5$ (SSC, $K_\rho = 1.23$); (d) $K = -5.0$, $J = -4.0$, $n = 0.5$ (TSC1, $K_\rho = 1.13$); (e) $K = 10.0$, $J = -5.0$, $n = 0.5$ (TSC2, $K_\rho = 1.50$); and (f) $K = -10.0$, $J = 2.0$, $n = 0.9$ (TSC1/TSC2, $K_\rho = 1.05$). Panels (a)–(d) are obtained for open chains with $L = 400$, while panels (e) and (f) are for $L = 200$.

correlations remain essentially left-right symmetric around $i = 100$, indicating the absence of bond dimerization. By contrast, for $J = -0.5$ we observe a clear asymmetry between the nearest-neighbor correlations, $\langle n_{100}n_{99} \rangle < \langle n_{100}n_{101} \rangle$, consistent with an alternating strong-weak bond pattern [inset of Fig. 4(b)].

Once such a bond dimerization develops, the strong bonds form bonding and antibonding orbitals. At $n = 0.5$, corresponding to one electron per two sites, the bonding orbitals are effectively half filled, so that a Mott gap opens within the dimerized background. This interpretation is consistent with both the finite charge gap Δ_c and the behavior of the connected density correlation $D(r)$: as shown in Fig. 4(b), $D(r)$ decays algebraically for $J = -0.1$ and -0.7 , as expected for a TLL, whereas for $J = -0.5$ it crosses over to exponential decay, signaling a charge-gapped state.

The dimerization pattern is twofold degenerate, corresponding predominantly to dimers on the x - or y -type bonds, as illustrated in Fig. 1(b). On open chains, the boundaries weakly pin one of these two patterns, producing the observed real-space texture. In addition, within this dimerized Mott phase we find genuine long-range order in the y -spin correlations, $\langle S_i^y S_j^y \rangle$ [Figs. 4(c) and 4(d)], consistent with an effective low-energy description in terms of an Ising-like spin-1/2 chain dominated by the $(K + J)S_i^y S_j^y$ channel.

Pairing symmetry from pair-pair correlations. To identify the dominant SC correlations and their spin structure, we analyze the distance dependence of the pair-pair correlations $P_\gamma(r)$ for the singlet channel $\gamma = S$ and the triplet channels $\gamma = T1, T2$ defined in *Methods and observables*. Within a TLL, the dominant tendency is determined by the slowest-decaying correlation function at long distances. Comparing $P_\gamma(r)$ with the density-density correlation $D(r)$ therefore provides a direct way to identify the leading pairing channel, consistent with the criterion based on K_ρ .

Figure 5 compares $P_S(r)$, $P_{T1}(r)$, $P_{T2}(r)$, and $D(r)$ for representative points in the SC regions of the phase diagram, using open chains with $L = 400$ [Figs. 5(a)–5(d)] and $L = 200$ [Figs. 5(e) and 5(f)]. For comparison, we also show the asymptotic TLL forms r^{-1/K_ρ} and r^{-K_ρ} using the values of K_ρ extracted from $N(q)$.

In the SC regimes stabilized for $J, K > 0$, the singlet correlation $P_S(r)$ decays most slowly and dominates at long distances, identifying an SSC tendency. By contrast, for $J, K < 0$, the leading correlations are triplet, indicating a TSC tendency. In the latter case, the Kitaev exchange further selects the T1 channel over T2. These results also support the energetic classification obtained in the $J = 0$ limit.

More specifically, in the SC phase found for $K > 0$ and $J < 0$ at $n \leq 0.5$, $P_{T2}(r)$ is dominant, while $P_{T1}(r)$ decays much more rapidly. Interestingly, this regime is accompanied by a partially spin-polarized FM metal (FMM), with a magnetization of several tens of percent. By contrast, in the SC regime found for $K < 0$ and $J > 0$ at $n = 0.9$,

$P_{T1}(r)$ and $P_{T2}(r)$ are comparably enhanced and remain nearly degenerate over the accessible distance range. Although $D(r)$ is larger at short distances for this representative point, this mainly reflects a nonuniversal prefactor associated with local charge fluctuations; the slower asymptotic decay of $P_\gamma(r)$ identifies the dominant pairing tendency in the TLL regime.

Overall, these results establish a correlation-based classification of the SSC and TSC regions in Fig. 3.

Summary. We have studied the hole-doped KH chain using DMRG and determined its ground state phase diagram. In the Kitaev-only limit, we found that the Kitaev exchange itself promotes pairing, favoring spin-singlet and spin-triplet SC tendencies for AFM and FM Kitaev couplings, respectively, together with finite-size Majorana edge correlations suggestive of topological superconductivity. In the full Kitaev-Heisenberg chain, cooperative J and K exchanges broadly stabilize superconductivity when the overall exchange scale becomes sufficiently large, while competition between them induces a strong filling dependence and allows superconductivity to emerge even when both J and K couplings are weak. At quarter filling, we identified a Mott-insulating phase with spontaneous hopping dimerization. Our results highlight magnetic frustration as a common mechanism underlying superconducting and interaction-driven insulating phases in doped Kitaev systems.

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Data availability. The data that support the findings of this article are openly available [26].

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