

Zero-energy Majorana states in a one-dimensional quantum wire with charge-density-wave instability

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A one-dimensional lattice with strong spin-orbit interactions (SOIs) and a Zeeman magnetic field is shown to lead to the formation of a helical charge-density-wave (CDW) state near half filling. The interplay between the magnetic field, SOI constants, and the CDW gap seems to support Majorana bound states under appropriate values of the external parameters. An explicit calculation of the quasiparticles' wave functions supports the formation of a localized zero-energy state, bounded to the sample end points. Symmetry classification of the system is provided. The relative value of the density of states shows a precise zero-energy peak at the center of the band in the nontrivial topological regime.

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I. INTRODUCTION

Recently, new exotic topological states of condensed matter, capable of supporting non-Abelian quasiparticles [1], have been suggested [2–5], which can be used as a fault-tolerant platform for topological quantum computation [6,7]. These topological phases reveal chiral Majorana edge particles, being their own antiparticles, which are represented by the non-Abelian statistics with noncommutative fermionic exchange operators.

A suggestion by Read and Green [3] that Majorana states can be realized at the vortex cores of a two-dimensional (2D) $p_x + ip_y$ superconductor has provoked new advances in engineering a semiconductor nanostructure with a zero-energy state. Kitaev showed [2] a possible realization of a single Majorana fermion at each end of a p -wave spinless superconducting wire. The effective p -wave superconductors were shown [8–11] to be realized in a semiconductor film, in which s -wave pairing is induced by the proximity effect in the presence of spin-orbit interactions (SOIs) and a Zeeman magnetic field.

The formation of zero-energy Majorana bound states in a one-dimensional (1D) quantum wire in proximity to an s -wave superconductor and in the presence of SOIs and the magnetic field has been argued recently in Refs. [12,13].

In this paper we predict a different realization mechanism of Majorana quasiparticles in a 1D crystal with charge-density-wave (CDW) instability. We consider the model of a 1D crystal around half filling with strong spin-orbit interactions and in the presence of a Zeeman magnetic field. There is an instability

against the formation of a CDW and spin-density wave (SDW) in a such model. The key to the quantum topological order is the coexistence of SOIs with the CDW or SDW state and an externally induced Zeeman coupling of spins. We show that for the Zeeman coupling below a critical value, the system is a nontopological CDW semiconductor. However, above the critical value of the Zeeman field, the lowest energy excited state is a zero-energy Majorana fermion state for topological CDW crystals. Thus, the system is transmuted into a non-Abelian CDW state by increasing the external magnetic field.

SDW and CDW are broken-symmetry ground states of highly anisotropic, so-called quasi-1D metals which are thought to arise as a consequence of electron-phonon or electron-electron interactions [14,15]. These states have a typical 1D character, and they can be conveniently discussed within the framework of various 1D models [16]. CDW and SDW states are successfully realized in quasi-1D structures such as organic molecules of (TMTSF)₂PF₆, (MDTTF)₂Au(CN)₂, (DMET)₂Au(CN)₂, and Au, In, Ge atomic wires grown by self-assembly on vicinal Si(553), Si(557), or Ge(001) surfaces [17,18].

II. DENSITY-WAVE ORDERING IN THE PRESENCE OF RASHBA AND DRESSSELHAUS SOIs

The model considered here is essentially a 1D Hubbard model with on-site Coulomb interactions in the presence of both Rashba and Dresselhaus SOIs and a Zeeman magnetic field. The noninteracting part \hat{H}_0 of the Hamiltonian $\hat{H} = \hat{H}_0 + \hat{H}_{\text{int}}$ in momentum space reads

$$\hat{H}_0 = \sum_{0 < k < G/2} \sum_{\sigma, \sigma'} \{ \xi_k c_{k, \sigma}^\dagger c_{k, \sigma'} \delta_{\sigma, \sigma'} + \omega_Z c_{k, \sigma}^\dagger (\sigma_x)_{\sigma \sigma'} c_{k, \sigma'} + \alpha_R \sin(kd) c_{k, \sigma}^\dagger (\sigma_z)_{\sigma \sigma'} c_{k, \sigma'} + \alpha_D \sin(kd) c_{k, \sigma}^\dagger (\sigma_y)_{\sigma \sigma'} c_{k, \sigma'} + (k \leftrightarrow k - G/2) \}, \quad (1)$$

where α_R and α_D are constants of the Rashba and Dresselhaus SOIs [19], correspondingly, $\omega_Z = g \hbar \mu_B B/2$ is the Zeeman energy of a magnetic field B , $\xi_k = \epsilon_k - \mu$ with $\epsilon_k = -2t \cos(kd)$, and μ is the Fermi energy. At half filling $\mu = 0$, and the electron-hole symmetry $\xi_{k-G/2} = -\xi_k$ for one-particle states is realized. $G = 2\pi/d$ is the reciprocal lattice vector with d being the unit cell

size. The interaction term H_{int} in the Hamiltonian is written as

$$\hat{H}_{\text{int}} = \frac{1}{2N} \sum_{0 < q < G} \sum_{\sigma} \left\{ \sum_{\substack{-G/2 < k < G/2 - q \\ q - G/2 < k' < G/2}} U(k, k'; q) c_{k+q, \sigma}^{\dagger} c_{k, \sigma} c_{k' - q, -\sigma}^{\dagger} c_{k', -\sigma} + \sum_{\substack{G/2 - q < k < G/2 \\ -G/2 < k' < q - G/2}} U(k, k'; q) c_{k, \sigma}^{\dagger} c_{k+q - G, \sigma} c_{k', -\sigma}^{\dagger} c_{k' - q + G, -\sigma} \right\}, \quad (2)$$

where U is a strength of the Hubbard interaction and N is the number of lattice sites. Note that the momentum summation in Eq. (1) is taken over the positive part of the Brillouin zone, and the first four terms in the Hamiltonian describe the right moving ($k > 0$) particles. The left moving ($k - G/2 < 0$) particles are taken into account by adding the terms with $k \leftrightarrow k - G/2$. The electron-hole order parameter at the density-wave instability is introduced as $\Delta_{\sigma} = \frac{V}{N} \sum_{0 < k < G/2} \langle c_{k - G/2, \sigma}^{\dagger} c_{k, \sigma} \rangle$ under the assumption that $U(k, k', q) = V \delta(q - G/2)$. The complex-conjugate order parameter is obtained by summing the electron-hole pairing over the negative momentum part of the Brillouin zone, $\Delta_{\sigma}^* = \frac{V}{N} \sum_{-G/2 < k < 0} \langle c_{k + G/2, \sigma}^{\dagger} c_{k, \sigma} \rangle$. The CDW and SDW order parameters are defined as $\Delta_{\text{CDW}} = (\Delta_{\uparrow} + \Delta_{\downarrow})/2$ and $\Delta_{\text{SDW}} = (\Delta_{\uparrow} - \Delta_{\downarrow})/2$, respectively. Assuming $\Delta_{\uparrow} = \Delta_{\downarrow}$ for CDW, thereby we eliminate SDW ordering, and $\Delta_{\text{CDW}} = \Delta_{\uparrow} = \Delta_{\downarrow}$. For SDW we assume $\Delta_{\uparrow} = -\Delta_{\downarrow}$, at the same time CDW formation is eliminated, and $\Delta_{\text{SDW}} = \Delta_{\uparrow} = -\Delta_{\downarrow}$. Further, we use a common notation Δ for both CDW and SDW ordering, and replace \hat{H}_{int} in the mean field approximation by $\hat{H}_{\text{int}}^{\text{MF}}$,

$$\hat{H}_{\text{int}}^{\text{MF}} = \sum_{0 < k < G/2, \sigma} \bar{\sigma} \{ \Delta c_{k, \sigma}^{\dagger} c_{k - G/2, \sigma} + \Delta^* c_{k - G/2, \sigma}^{\dagger} c_{k, \sigma} \}, \quad (3)$$

where $\bar{\sigma} = 1$ for CDW ordering, and $\bar{\sigma} = -\sigma = \mp 1$ for the SDW state. The Hamiltonian $\hat{H}_{\text{MF}} = \hat{H}_0 + \hat{H}_{\text{int}}^{\text{MF}}$ is written in the basis $\Psi^{\dagger} = (c_{k, \uparrow}^{\dagger}, c_{k, \downarrow}^{\dagger}, c_{k - G/2, \downarrow}^{\dagger}, -c_{k - G/2, \uparrow}^{\dagger})$ as

$$\hat{H}_{\text{MF}} = \sum_{0 < k < G/2} \{ \Psi^{\dagger} \hat{\mathcal{H}} \Psi + \xi_k + \xi_{-k + G/2} \} + \frac{2}{V} |\Delta|^2, \quad (4)$$

with

$$\hat{\mathcal{H}} = \xi_k \tau_z \otimes \sigma_0 + \alpha_R \sin k \tau_0 \otimes \sigma_z + \alpha_D \sin k \tau_z \otimes \sigma_y + \omega_Z \tau_z \otimes \sigma_x + \tau_j(\Delta) \otimes \sigma_j, \quad (5)$$

where the Pauli matrices σ and τ operate in spin and particle-hole spaces, and \otimes is the Kronecker product of matrices. In the last term, $j = y$ for CDW and $j = x$ for SDW pairing,

$$\tau_y(\Delta) = \begin{pmatrix} 0 & -i\Delta \\ i\Delta^* & 0 \end{pmatrix} \quad \text{and} \quad \tau_x(\Delta) = \begin{pmatrix} 0 & \Delta \\ \Delta^* & 0 \end{pmatrix}. \quad (6)$$

The first term of Eq. (5) in the linearized form $-\hbar \partial_y \tau_z$, with the third Zeeman term $\omega_Z \sigma_x$, constitutes the massive Dirac equation. The charge-density ordering, however, with the last term $\tau_j(\Delta) \sigma_j$, transforms the model into a four-band model.

The pole of the single particle Green's function $G^{-1}(E, k) = E - \hat{\mathcal{H}}$ determines the quasiparticle energy

$$E_{\text{CDW}}^2 = \xi_k^2 + \alpha^2 \sin^2 k + |\Delta|^2 + \omega_Z^2 \pm 2\sqrt{\xi_k^2 \alpha^2 \sin^2 k + \omega_Z^2 |\Delta|^2 + \xi_k^2 \omega_Z^2}, \quad (7)$$

$$E_{\text{SDW}}^2 = (|\xi_k| \pm \sqrt{\alpha^2 \sin^2 k + \omega_Z^2})^2 + |\Delta|^2, \quad (8)$$

for the CDW and SDW states, correspondingly. The SO coupling constant α in the expressions for the energy spectrum is a renormalized constant $\alpha = \sqrt{\alpha_R^2 + \alpha_D^2}$. Equation (8) does not allow a zero-energy mode due to a finite gap Δ at the origin. However, experimental evidences in many quasi-1D materials, e.g., in Bechgaard salt (TMTSF)₂PF₆, suggest a realization of an unconventional SDW with an order parameter $\sim \Delta_1 \sin k$ yielding a zero-energy state. The dispersive CDW or SDW gap can be derived from the extended Hubbard model with a nonlocal interaction [20]. Further, we will discuss only the topological CDW state.

A small deviation from half filling at $T = 0$ was shown by Brazovskii *et al.* [21] to create a band of kink states within the Peierls gap. This picture is changed at finite temperatures. According to the phase diagrams in the temperature-chemical potential (T, μ) and temperature-density (T, n) planes, calculated in Ref. [22] on the basis of Brazovskii *et al.*'s theory [21], for a fixed electron density $1 < n < n_L$, where n_L is Leung's density [23] at the triple point of the normal (N), commensurate (C), and incommensurate (IC) phases, the kink band shrinks with increasing temperature until it vanishes at the IC-C transition. For fixed temperature $0 < T < T_L$ the kink band arises at some electron density $n > 1$ and broadens with increasing density until the kinks become soft. At finite temperatures ($T < T_0$) and for a small deviation of the chemical potential from half filling $|\mu| < T_0 = 1.056 T_c(0) = (2/\pi)\Delta$, where $T_c(0) = (4W e^{\gamma}/\pi) e^{-1/\lambda}$ is the transition temperature at $\mu = 0$ [22], the system is in the C phase with vanishing mismatching between the electronic states k and $G/2 - k$.

The solution of the energy spectrum for different values of $\tilde{\alpha}$, $\tilde{\mu}$, $\tilde{\Delta}$, and $\tilde{\omega}_Z$ is plotted in Fig. 1, where the dimensionless parameters with a tilde are given in the units of the halved bandwidth $2t$. The solution of Eq. (7) $\alpha_R = \alpha_D = \Delta = \omega_Z$ yields a usual cosine band in the reduced Brillouin zone. The SOI results in two shifted cosine bands along the k axes, whereas Zeeman splitting doubles the band along the energy axes, opening a gap at the anticrossing point [see Fig. 1(a)]. The formation of the density wave opens a gap at the boundary of the Brillouin zone.

The energy spectrum at the center of the Brillouin zone for the topological CDW with gapped "bulk" states and zero-energy end states can be written as

$$E_{\text{CDW}}^{(0)} = E(0) = |\omega_Z - \sqrt{\mu_t^2 + |\Delta|^2}|, \quad (9)$$

where $\mu_t = -2t - \mu$. A magnetic-field-dominated gap at the center of the band for $\omega_Z^2 > |\Delta|^2 + \mu_t^2$ turns to the pairing-dominated one for $\omega_Z^2 < |\Delta|^2 + \mu_t^2$ [Figs. 1(d) and 1(b), correspondingly]. A quantum phase transition from a

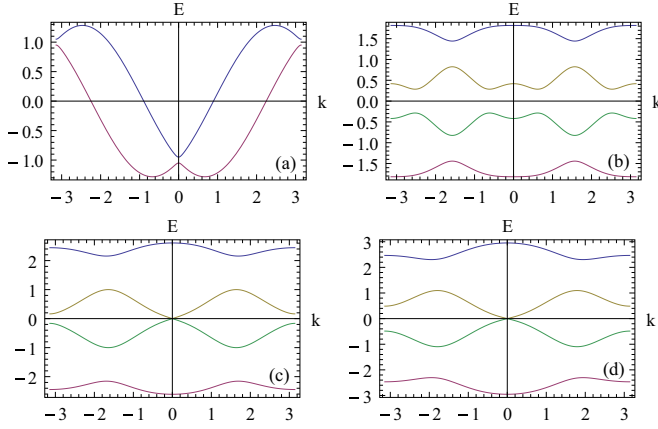


FIG. 1. (Color online) The energy spectrum is plotted according to Eq. (7) for fixed values of $t = 0.5$, $\tilde{\alpha} = 0.8$, and for the following values of the dimensionless parameters: (a) $\tilde{\Delta} = 0.0$, $\tilde{\omega}_Z = 0.05$, $\tilde{\mu} = 0.0$; (b) $\tilde{\Delta} = 0.5$, $\tilde{\omega}_Z = 0.7$, $\tilde{\mu} = 0$; (c) $\tilde{\Delta} = 0.7$, $\tilde{\omega}_Z = \sqrt{1.3}$, $\tilde{\mu} = -0.1$; and (d) $\tilde{\Delta} = 0.7$, $\tilde{\omega}_Z = \sqrt{2.18}$, $\tilde{\mu} = -0.3$.

topological nontrivial to trivial phase occurs at $\omega_Z^2 = |\Delta|^2 + \mu_t^2$. The gap at $k = 0$ vanishes under this condition, with emerging Majorana fermion states at the ends of the wire, which is plotted in Fig. 1 for the dimensionless parameters $\tilde{\alpha} = 0.8$, $\tilde{\Delta} = 0.7$, $\tilde{\omega}_Z = \sqrt{1.3}$, and $\tilde{\mu} = -0.1$.

It is possible to check that the Hamiltonian $\hat{\mathcal{H}}$ respects time-reversal symmetry (TRS) $U_T \hat{\mathcal{H}}^*(k) U_T^{-1} = \hat{\mathcal{H}}(-k)$ with the TRS operator $T = U_T K$ in the absence of the magnetic field, and particle-hole symmetry (PHS) $U_P \hat{\mathcal{H}}^*(k) U_P^{-1} = -\hat{\mathcal{H}}(-k)$ with the PHS operator $P = U_P K$. Here, K is the complex conjugate operator, $U_T = \sigma_0 \otimes i\sigma_y$, and $U_P = \sigma_x \otimes \sigma_0$, satisfying $T^2 = -1$ and $P^2 = 1$. The TRS operator transforms $k \rightarrow -k$ as well as $c_{k\uparrow} \leftrightarrow c_{k\downarrow}^\dagger$ and $c_{k\downarrow} \leftrightarrow -c_{k\uparrow}^\dagger$, resulting in $\Delta \leftrightarrow \Delta^*$ for the order parameter and keeping the excitation spectrum unchanged, $\xi_{-k} = \xi_k$. Instead, the PHS operator transforms

$$c_{k\uparrow} \leftrightarrow c_{k-G/2\downarrow}^\dagger \quad \text{and} \quad c_{k\downarrow} \leftrightarrow -c_{k-G/2\uparrow}^\dagger, \quad (10)$$

keeping the order parameter Δ unchanged. PHS entails an energy spectrum symmetric about the Fermi level. According to symmetry classification the system belongs to the DIII class, which can be topologically nontrivial [24] provided that both TRS and PHS are satisfied. An external magnetic field breaks TRS and drives the system from DIII to the D class, which possesses a single Majorana zero-energy mode at each end of the wire.

III. MAJORANA FERMIONS

The main feature of a Majorana fermion is that it is its own ‘‘antiparticle.’’ This property can be proved for a 1D unconventional CDW model [14,20] with a dispersive and complex order parameter $\Delta_k = \Delta_0 \sin(kd)$ by mapping it to the Kitaev model [2] for the p -wave superconductor. The Hamiltonian of a 1D unconventional CDW model becomes invariant under the particle-hole transformations $c_k^v \equiv c_k \leftrightarrow c_k^\dagger \equiv c_{k-G/2}^\dagger$ and $c_k^{v\dagger} \leftrightarrow c_k^c$ in momentum space or $d_n^v \leftrightarrow d_n^{c\dagger}$ and $d_n^{v\dagger} \leftrightarrow d_n^c$ in site representation, where the spin index is

neglected due to the spin degeneration. The PHS transforms it to Kitaev’s one,

$$\hat{H}_0 = \sum_n \left\{ -2t(d_n^{v\dagger} d_{n+1}^v + d_{n+1}^{v\dagger} d_n^v) + 2i\Delta_0 d_n^{v\dagger} d_{n+1}^{v\dagger} + 2i\Delta_0^* d_{n+1}^v d_n^v \right\}, \quad (11)$$

which reveals the Majorana end states. It is easy to show that the PHS conditions (10) transform our Hamiltonians (1) and (3) to the form, describing the s -wave type superconductor with misaligned spins but with the same momenta k of Cooper pairs, which should reveal again the Majorana quasiparticles.

A. Wave functions of Majorana bound states

Majorana bound states arise at the interface of trivial and topological regions under certain conditions by varying the parameters of the 1D wire. In order to understand the localized character of the zero-energy state, we rewrite the Hamiltonian in the real coordinate space. We linearize the cosine energy spectrum around the Fermi level $k_F = G/4$ as $\xi_k = \epsilon_k - \mu = 4t \sin(\frac{(k+k_F)d}{2}) \sin(\frac{(k-k_F)d}{2}) \approx v_F \hbar(k - k_F) \rightarrow v_F \hbar(-i\frac{\partial}{\partial y} - k_F)$ for the right mover, and $\xi_{k-G/2} \approx -v_F \hbar(k + k_F) \rightarrow -v_F \hbar(i\frac{\partial}{\partial y} - k_F)$ for the left mover, and the SO coupling term $\sin(dk) \rightarrow -id\frac{\partial}{\partial y}$. One can see that $\mu_z = v_F k_F \hbar$; at half filling $\mu = 0$ and $\mu_t = v_F k_F \hbar = 2t$. The Schrödinger equation, corresponding to zero energy, reads

$$\begin{aligned} \left[-\mu_t - i(v_F \hbar + v_\sigma \alpha_R) \frac{\partial}{\partial y} \right] \psi_\sigma^R + \left(\omega_Z - v_\sigma \alpha_D \frac{\partial}{\partial y} \right) \psi_{-\sigma}^R \\ + \Delta \psi_\sigma^L = 0, \\ \left[\mu_t + i(v_F \hbar + v_\sigma \alpha_R) \frac{\partial}{\partial y} \right] \psi_\sigma^L + \left(\omega_Z + v_\sigma \alpha_D \frac{\partial}{\partial y} \right) \psi_{-\sigma}^L \\ + \Delta^* \psi_\sigma^R = 0, \end{aligned} \quad (12)$$

where $-\sigma = \downarrow, \uparrow$, and $v_\sigma = \pm$ for $\sigma = \uparrow, \downarrow$, correspondingly. For a long enough wire $L \gg 1$, we choose the magnetic field $\omega_Z^2 < \mu_t^2 + |\Delta|^2$ for $y \in [0, L]$ and $\omega_Z^2 > \mu_t^2 + |\Delta|^2$ outside this interval. By choosing the wave functions $\Psi^T(y) = \exp\{iky\}(b_\uparrow^R, b_\downarrow^R, b_\downarrow^L, -b_\uparrow^L)^T$, one gets the determinant equation $\det|\bar{\mathbf{H}}| = 0$ to find k , where

$$\begin{aligned} \mathbf{H} = v_F \hbar(k - k_F) \tau_z \otimes \sigma_0 + \alpha_R k \tau_0 \otimes \sigma_z \\ + \omega_Z \tau_z \otimes \sigma_x + \alpha_D k \tau_z \otimes \sigma_y + \Delta \sigma_y \otimes \tau_y. \end{aligned} \quad (13)$$

The allowed values of k are obtained from the equation $(v_F^2 \hbar^2 - \alpha^2)k^2 - 2k(\mu_t v_F \hbar \pm i|\Delta|\alpha) - \mathcal{L} = 0$, where $\mathcal{L} = \omega_Z^2 - |\Delta|^2 - \mu_t^2$. For $\mathcal{L} = 0$ this equation has a real root $k = 0$, corresponding to a single allowed state in the gap. Since there is no other state for a quasiparticle to move, this state is localized and it seems to be protected against local perturbations. For $\mathcal{L} \neq 0$, k takes complex values, signaling on the realization of a gapped state. In this case the wave function decays exponentially in both sides of $y = 0$ but with different localization lengths. The general solution for k

reads

$$k_v = \frac{k_F \pm i|\bar{\Delta}|\bar{\alpha} + v\sqrt{(k_F\bar{\alpha} \pm i|\bar{\Delta}|)^2 + \bar{\omega}_Z^2(1 - \bar{\alpha}^2)}}{1 - \bar{\alpha}^2}, \quad (14)$$

where $\bar{\alpha} = \frac{\alpha}{v_F\hbar}$, $\bar{\Delta} = \frac{\Delta}{v_F\hbar}$, $\bar{\omega}_Z = \frac{\omega_Z}{v_F\hbar}$, and $v = \pm$. The wave function decays exponentially if, generally speaking, $|\Delta|, \alpha \neq 0$. For $\alpha = 0$, $k_{\pm} = \frac{\mu_t \pm \sqrt{\omega_Z^2 - |\Delta|^2}}{v_F\hbar}$, and the trivial CDW state is gapped for $\omega_Z < |\Delta|$, which is destroyed for $\omega_Z > |\Delta|$.

B. Domain wall formation

The Majorana bound state is formed by varying the parameters Δ , ω_Z , and μ . We consider a linearized Hamiltonian, Eq. (13), for the relevant momenta near $k = 0$ and $\mu_t = 0$, assuming a spatial variation of the magnetic field $\omega_Z = \Delta + by$ near $y = 0$, which crosses a constant gap $\Delta > 0$. For simplicity, the Dresselhaus SOI is neglected, $\alpha_D = 0$, and Δ is chosen to be real. Following Oreg *et al.* [13], the squared, due to the particle-hole symmetry, Hamiltonian (13), \mathbf{H}^2 , is reduced to the diagonal form by means of the unitary operator $U = \frac{1}{2}(\tau_z + i\tau_y + i\sigma_x\tau_z + \sigma_x\tau_y)$,

$$\begin{aligned} \tilde{\mathbf{H}} &= U\mathbf{H}^2U^\dagger \\ &= [\omega_Z^2 + \Delta^2 + (\alpha_R k)^2] - \alpha_R \hbar b \sigma_z \tau_z + 2\omega_Z \sigma_z \tau_0, \end{aligned} \quad (15)$$

with the spectrum $E^2 = (\omega_Z \pm \Delta)^2 \pm \alpha_R \hbar b$. The term, proportional to $b\sigma_z$, appears in the Hamiltonian due to the topological defect at the ends of the wire, which bridges the two edges of the conduction and valence bands. The bound state may form if Δ varies in space and crosses ω_z .

IV. DENSITY OF STATES AND ZERO-BIAS ANOMALY

The zero-energy Majorana state in the Peierls gap can be experimentally detected from the tunneling experiments, where the conductivity of the tunneling contact is expressed through the one-particle density of states (DOS), $\rho(\epsilon, T)$, as

$$\frac{\delta G(V, T)}{G^{(0)}} = \int_{-\infty}^{+\infty} \frac{d\epsilon}{4T} \frac{\delta\rho(\epsilon)}{\rho^{(0)}} \left[\frac{1}{\cosh^2 \frac{\epsilon - eV}{2T}} + \frac{1}{\cosh^2 \frac{\epsilon + eV}{2T}} \right]. \quad (16)$$

At $T = 0$ this expression is written $\delta G(\epsilon)/G^{(0)} = [\rho(\epsilon, 0) - \rho^{(0)}]/\rho^{(0)} = \delta\rho(\epsilon)/\rho^{(0)}$, where $\rho^{(0)}$ is the DOS of a pure system. The DOS is found from the conventional expression $\rho(\epsilon) = \int_{-\pi}^{\pi} \frac{dk}{2\pi} \sum_n \delta(\epsilon - E_n(k))$, where $E_n(k)$ is the energy spectrum for $n = 1, 2, 3, 4$ given by Eq. (7). The delta function is regularized for numerical calculations, replacing it with the Lorentzian function $\delta(\epsilon - E_n(k)) = \eta / \{[\epsilon - E_n(k)]^2 + \eta^2\}$, where η is the rate of inelastic processes. A formation of the Majorana quasiparticle in the center of the band is clearly seen in the relative value of the DOS, $\delta\rho(\epsilon)/\rho^{(0)}$. The evolution of the central peak in $\delta\rho(\epsilon)/\rho^{(0)}$ is depicted in Fig. 2, where the central peak emerges only for special values of the external parameters satisfying the critical condition $\omega_Z^2 = |\Delta|^2 + \mu_t^2$. Note that midgap states have been observed recently in a topological superconducting phase by Mourik *et al.* [25] and by Das *et al.* [26] in zero-bias measurements on InSb and

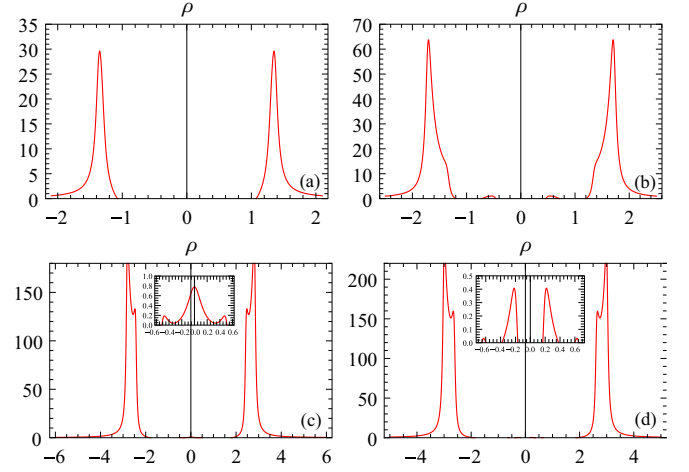


FIG. 2. (Color online) The relative change in the DOS, $\delta\rho(\epsilon, V)/\rho^{(0)}(\epsilon)$, for (a) $\bar{\alpha} = 0.8$, $\bar{\Delta} = 0.0$, and $\bar{\omega}_Z = 0.3$, (b) $\bar{\alpha}_R = 0.6$, $\bar{\Delta} = 0.7$, and $\bar{\omega}_Z = 0.5$, (c) $\bar{\alpha}_R = 0.3$, $\bar{\Delta} = 1.0$, and $\bar{\omega}_Z = \sqrt{2.0}$, and (d) $\bar{\alpha}_R = 0.3$, $\bar{\Delta} = 1.0$, and $\bar{\omega}_Z = 1.6$. The inelastic scattering rate is chosen to be $\tilde{\eta} = 0.05$. The inset in (c) shows a zero-energy peak, corresponding to the Majorana quasiparticle, which disappears in the inset in (d) by destroying the condition.

InAs nanowires, contacted with one normal (gold) and one superconducting electrode.

An artificial string of Au, In, Ge, and Pb atoms on vicinal Si(557), Si(553), and Ge(001) surfaces seems to be suitable for experimental realizations. These structures with a large lateral chain spacing (~ 1.6 nm) can be built [27] by placing metallic atoms side by side on a nonconducting template by using, e.g., a scanning tunneling microscope. Angle-resolved photoemission data indicate a 1D electron pocket with very weak transverse dispersion in these structures. The ratio of the parallel and transverse hopping integrals t_{\parallel}/t_{\perp} was determined from a tight-binding fit to the Fermi contour to be larger than 60 [18]. Therefore, the structures are three dimensional with practically in-wire motion of particles. These structures exhibit a Peierls instability below ~ 150 – 200 K. Recently, a spin polarized CDW has been observed [28] in Pb/Si(557), where the Fermi surface nested charge-density instability occurs by an appropriate choice of band filling, spin-orbit coupling, and external parameters. The Rashba parameter in this structure was found to be 1.9 eV \AA for the value of the Rashba splitting 0.2 \AA^{-1} . High values of the band gap and the SOI constants may allow one to realize a topological CDW phase at higher temperatures, making a significant step compared to previous mechanisms to detect the Majorana state in topological superconductors.

V. CONCLUSIONS

In this paper, we showed a possible realization of a zero-energy Majorana state in the CDW phase of a 1D crystal. The CDW state in a 1D crystal is realized due to the nesting of the Fermi level. The wave function of this state “mixes” an electron state $\psi_{k,\sigma}$ with a momentum $k > 0$ above the Fermi level with a hole state $\psi_{k-G/2,\sigma}$ with a momentum $k - G/2 < 0$ below the Fermi level, which resembles the Bogolyubov–de Gennes

wave function with mixed electron and hole states, too. A quasiparticle excitation in the topological CDW state emerges as a localized zero-energy state in the middle of the Brillouin zone. Since the CDW phase is realized at higher temperatures, this mechanism facilitates an observation of Majorana particles and their implementation for quantum computations.

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