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

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One-dimensional lattice with strong spin-orbit interactions (SOI) and Zeeman magnetic field is shown to lead to the formation of a helical charge-density wave (CDW) state near half-filling. Interplay of the magnetic field, SOI constants and the CDW gap seems to support Majorana bound states under appropriate value of the external parameters. Explicit calculation of the quasi-particles’ wave functions supports a formation of the localized zero-energy state, bounded to the sample endpoints. Symmetry classification of the system is provided. Relative value of the density of states shows a precise zero-energy peak at the center of the band in the non-trivial topological regime.

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

Suggestion by Read and Green\textsuperscript{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 zero-energy state. Kitaev showed\textsuperscript{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\textsuperscript{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 (SOI) and Zeeman magnetic field.

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

In this Letter we predict a new realization mechanism of Majorana quasi-particles 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 Zeeman magnetic field. There is an instability against formation of CDW and spin-density wave (SDW) in a such model. The key to the quantum topological order is the coexistence of SOI with 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 non-topological CDW semiconductor. However, above the critical value of Zeeman field, the lowest energy excited state is a zero-energy Majorana fermion state for topological CDW crystal. Thus, the system is transmuted into a non-Abelian CDW state with 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 the consequence of electron-phonon or electron-electron interactions\textsuperscript{14,15}. These states have typical 1D character, and they can be conveniently discussed within the framework of various 1D models\textsuperscript{16}. CDW and SDW states are successfully realized in quasi-1D structures such as organic molecules of $(TMTSF)_2PF_6$, $(MDTF)_2Au(CN)$_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\textsuperscript{17,18}.

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

$$
\hat{H}_0 = \sum_{0<k<\frac{G}{2}} \sum_{\sigma,\sigma'} \left\{ \xi_k c^\dagger_{k,\sigma} c_{k,\sigma'}^\dagger \delta_{\sigma,\sigma'} + \omega_Z c^\dagger_{k,\sigma} (\sigma_z) \sigma' c_{k,\sigma'} + \alpha_R \sin(kd) c^\dagger_{k,\sigma} (\sigma_x) \sigma' c_{k,\sigma'} + \alpha_D \sin(kd) c^\dagger_{k,\sigma} (\sigma_y) \sigma' c_{k,\sigma'} + (k \leftrightarrow -k - \frac{G}{2}) \right\},
$$

(1)

where $\alpha_R$ and $\alpha_D$ are constants of Rashba and Dresselhaus SOI\textsuperscript{19}, correspondingly, $\omega_Z = g\hbar \mu_B B/2$ is Zeeman energy of a magnetic field $B$, $\xi_k = \epsilon_k - \mu$ with $\epsilon_k = -2t \cos(kd)$, and $\mu$ 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. Interaction term $\hat{H}_{\text{int}}$ in the Hamiltonian is written

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

(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 positive part of the Brillouin zone, and the first four terms in 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 \( \Delta = \frac{\nu}{N} \sum_{0 \leq k \leq G/2} \langle c_{k+G/2,\sigma}^\dagger c_k \rangle \) under assumption that \( U(k, k') = 0 \) for all \( k' \neq k \). The complex-conjugate order parameter is obtained by summing the electron-hole pairing over negative momentum part of the Brillouin zone, \( \Delta^* = \frac{\nu}{N} \sum_{-G/2 < k < 0} \langle c_k^\dagger c_{k+G/2,\sigma} \rangle \). CDW and SDW order parameters are defined as \( \Delta_{CDW} = (\Delta^* + \Delta) / 2 \) and \( \Delta_{SDW} = (\Delta^* - \Delta) / 2 \), respectively. Assuming \( \Delta = \Delta^* \) for CDW, thereby we eliminate SDW ordering, and \( \Delta_{CDW} = \Delta_{SDW} = 0 \). For SDW we assume \( \Delta = \Delta^* \), at the same time CDW formation is eliminated, and \( \Delta_{CDW}^* = \Delta_{SDW}^* = \Delta^* \). Further we use a common notation \( \Delta \) for both CDW and SDW ordering, and replace \( H_{int} \) in the mean field approximation by \( H_{int}^{MF} \)

\[
H_{int}^{MF} = \sum_{0 < k < G/2, \sigma} \bar{\sigma} \{ \Delta c_{k,\sigma}^\dagger c_{k-G/2,\sigma} + \Delta^* c_{k-G/2,\sigma}^\dagger c_k \},
\]

where \( \bar{\sigma} = 1 \) for CDW ordering, and \( \bar{\sigma} = -\sigma = \pm 1 \) for SDW state. Hamiltonian \( H_{MF} = H_0 + H_{int}^{MF} \) is written in the basis \( \Psi = (c_{k,\sigma}^\dagger c_{k+G/2,\sigma}^\dagger c_k^\dagger c_{k-G/2,\sigma}) \) as

\[
H_{MF} = \sum_{0 < k < G/2} \{ \Psi^\dagger \mathcal{H} \Psi + \xi_k + \xi_{-k+G/2} \} + \frac{2}{\lambda^2} \Delta^2,
\]

with

\[
\mathcal{H} = \xi_k \tau_z \otimes \sigma_0 + \alpha_R \sin k \tau_0 \otimes \sigma_z + \alpha_D \sin k \tau_z \otimes \sigma_y + \omega_2 \tau_z \otimes \sigma_z + \tau_j(\Delta) \otimes \sigma_j;
\]

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

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

The first term of Eq. (5) in the linearized form, \(-\hbar \partial_\Delta \tau_x \), with the third Zeeman term, \( \omega_2 \sigma_x \), constitutes the massive Dirac equation. The charge density ordering, however, with the last term \( \tau_j(\Delta) \sigma_j \) transforms the model to the four-band model.

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

\[
E_{CDW}^2(k) = \xi_k^2 + \alpha^2 \sin^2 k + |\Delta|^2 + \omega_2^2 \pm 2\sqrt{\xi_k^2 \alpha^2 \sin^2 k + \omega_2^2 |\Delta|^2 + \xi_k^2 \omega_2^2} \pm 2\sqrt{\xi_k^2 \alpha^2 \sin^2 k + \omega_2^2 |\Delta|^2 + \xi_k^2 \omega_2^2};
\]

\[
E_{SDW}^2 = \left( |\xi_k| \pm \sqrt{\alpha^2 \sin^2 k + \omega_2^2} \right)^2 + |\Delta|^2,
\]

for CDW and SDW states, correspondingly. SO coupling constant \( \alpha \) 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 \( \Delta \) at the origin. However, experimental evidences in many quasi-1D materials, e.g. in Bechgaard salt \((TMTSF)_2PF_6\), suggest a realization of an unconventional SDW with an order parameter \( \sim \Delta \sin k \) yielding a zero-energy state. The dispersive CDW or SDW gap can be derived from the extended Hubbard model with 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 \((T, \mu)\) and temperature-density \((T, n)\) planes, calculated in Ref.[22] on the base of Brazovskii et al. theory\(^21\), for 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 small deviation of the chemical potential from half-filling \( |\mu| < T_0 = 1.056T_c(0) = (2/\pi)\Delta \), where \( T_c(0) = (4We^*/\pi)e^{-1/\Lambda} \) is the transition temperature at \( \mu = 0 \)\(^22\), the system is in C-phase with vanishing mismatching between the electronic states \( k \) and \( G/2 - k \).

Solution of the energy spectrum for different values of \( \alpha, \mu, \Delta, \) and \( \omega_2 \) is plotted in Fig. 1, where the dimensionless parameters with tilde are given in the unit of the halved band width \( 2t \). Solution of Eq. (7)
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

$$E_{CDW}^{(0)} = E(0) = |ω_Z - \sqrt{\mu_1^2 + |Δ|^2}|,$$

where $μ_1 = -2t - μ$. A magnetic-field-dominated gap at the center of the band for $ω_Z^2 > |Δ|^2 + μ_1^2$ turns to the pairing-dominated one for $ω_Z^2 < |Δ|^2 + μ_1^2$. The gap at $k = 0$ vanishes under this condition emerging Majorana fermion states at the ends of the wire, which is plotted in Fig. 1 for the dimensionless parameters $\tilde{α} = 0.8$, $Δ = 0.7$, $\tilde{ω} = 1.3$, and $μ = -0.1$.

It is possible to check that the Hamiltonian $\mathcal{H}$ respects time-reversal symmetry (TRS) $U_T\mathcal{H}^*(k)U_T^{-1} = \mathcal{H}(-k)$ with TRS operator $T = U_T K$ in the absence of the magnetic field, and particle-hole symmetry (PHS) $U_P\mathcal{H}^*(k)U_P^{-1} = -\mathcal{H}(-k)$ with PHS operator $P = U_P K$. Here, $K$ is the complex conjugate operator, $U_T = σ_0 ⊗ σ_y$ and $U_P = σ_x ⊗ σ_0$ satisfying $T^2 = -1$ and $P^2 = 1$. The TRS operator transforms $k → -k$ as well as $c_k \leftrightarrow c_{-k}^\dagger$ and $c_{-k} \leftrightarrow -c_{-k}^\dagger$, resulting in $Δ \leftrightarrow Δ^*$ for the order parameter and keeping the excitation spectrum unchanged $ξ_k = ξ_{-k}$. Instead, the PHS operator transforms

$$c^\uparrow_{k} \leftrightarrow c^\dagger_{k-G/2\uparrow} \quad \text{and} \quad c^\downarrow_{k} \leftrightarrow -c^\dagger_{k-G/2\downarrow},$$

keeping unchanged the order parameter $Δ$. PHS entails an energy spectrum symmetric about the Fermi level. According to symmetry classification the system belongs to $DIII$ class which can be topologically nontrivial\(^2\) provided that both TRS and PHS are satisfied. An external magnetic field breaks TRS and drives the system from $DIII$ to $D$ class, which possesses a single Majorana zero-energy mode at each end of the wire.

The main feature of Majorana fermion is that it is own ‘anti-particle’. This property can be proved for a $1D$ unconventional CDW model\(^{2,3,9}\) with dispersive and complex order parameter $Δ_k = Δ_0 \sin(kd)$ by mapping it to the Kitaev’s model\(^2\) for the $p$-wave superconductor. Hamiltonian of a $1D$ unconventional CDW model becomes invariant under the particle-hole transformations $c^\dagger_{k} \equiv c_k \leftrightarrow c^\dagger_{k-G/2}$ and $c_{k} \leftrightarrow c^\dagger_{k}$ in momentum space or $d^\dagger_{n} \leftrightarrow d^\dagger_{n+1}$ and $d_{n} \leftrightarrow d_{n+1}$ in site-representation, where the spin index is neglected due to the spin degeneration. The PHS transforms to the Kitaev’s one

$$\hat{H}_0 = \sum_{n} \{-2t(d^\dagger_{n+1}d_{n+1} + d^\dagger_{n}d_{n}) + 2iΔ_0d^\dagger_{n}d^\dagger_{n+1} + 2iΔd^\dagger_{n+1}d_{n} \},$$

which reveals the Majorana end states. It is easy to show that the PHS conditions (10) transform our Hamiltonian (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 quasi-particles.

Majorana bound states arise at the interface of trivial and topological regions under certain condition by varying the parameters of $1D$ wire. In order to understand the localized character of the zero energy state we rewrite Hamiltonian in the real coordinate space. We linearize the cosine energy spectrum around the Fermi level $k_F = G/4$ as $ξ_k = ε_k - μ = 4t^2(\sin(k+F_0))d^2 \sin((k-F_0)d)^2 \approx v_F\hbar(k - k_F) → v_F\hbar(-i\frac{∂}{∂y} - k_F)$ for right-mover, and $ξ_{k-G/2} = -v_F\hbar(k + k_F) → v_F\hbar(i\frac{∂}{∂y} - k_F)$ for left-mover, and the SO coupling term $\sin(dk) → -iν\frac{∂}{∂y}$. One can see that $μ_2 = v_Fk_Fh$; at half-filling $μ = 0$ and $μ_1 = v_Fk_Fh = 2t$. Schrödinger equation, corresponding to zero energy, reads

$$-\mu - iv_Fh + ν_σαR \frac{∂}{∂y} \psi^σ_R + \left(ω_Z - ν_σα_D \frac{∂}{∂y} \right) \psi^σ_R + \Delta_σ^R \psi^σ_R = 0,$$

$$-\mu + iv_Fh + ν_σα_R \frac{∂}{∂y} \psi^σ_L + \left(ω_Z + ν_σα_D \frac{∂}{∂y} \right) \psi^σ_L - Δ^* \psi^σ_L = 0,$$

outside this interval. By choosing the wave functions $Ψ^σ(y) = \exp(iky)\{b^\uparrow, \bar{b}^\uparrow, b^\downarrow, -b^\downarrow\}^T$, one gets the determinant equation $det|H| = 0$ to find $k_f$, where

$$H = v_F\hbar(k - k_F) τ_z ⊗ σ_0 + α_Rk τ_0 ⊗ σ_z + ω_Z τ_2 ⊗ σ_x + α_Dk τ_z ⊗ σ_y + Δ σ_2 ⊗ τ_y.$$  

The allowed values of $k_f$ are obtained from the equation, $(v_F^2h^2 - α^2)k^2 = 2k(μ_1ν_σh ± i|Δ|α) - L = 0$, where $L = \tilde{ω}_Z - |Δ|^2 - μ_1^2$. For $L = 0$ 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 quasi-particle to move, this state is localized and it seems to be protected against local perturbations. For $L \neq 0$, $k$ takes complex values, signaling on realization of a gapped state. In this case the wave function decays exponentially in both sides of $y = 0$ but with different localization lengths. General solution for $k_f$ reads

$$k_F = \frac{L ± i|Δ|α + ν\sqrt{(k_F^2α^2 ± i|Δ|^2)^2 + \tilde{ω}_Z^2(1 - α^2)}}{1 - α^2},$$

where $α = \frac{\tilde{ω}_Z}{v_F\hbar}, \tilde{Δ} = \frac{Δ_0}{v_F\hbar}, \tilde{ω}_Z = \frac{ω_Z}{v_F\hbar}$, and $ν = ±$. The wave function decays exponentially if, generally speaking $|Δ|, α \neq 0$. For $α = 0, k_F = \frac{μ_1\pm\sqrt{2μ_1^2 - |Δ|^2}}{v_F\hbar}$ and the trivial CDW state is gapped for $ω_Z < |Δ|$, which is destroyed for $ω_Z > |Δ|$.
diagonal form by means of the unitary operator following Oreg et al.\(^<5>\). The delta-function is regularized for the Fermi level with an hole state \(\psi_{\text{ks}}\). Since the Fermi level is 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 CDW phase is realized at higher temperatures, this new mechanism facilitates an observation of Majorana particles and their implementation for the quantum computations.

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