Metal-insulator transition in a quantum wire driven by a modulated Rashba spin-orbit coupling

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We study the ground-state properties of electrons confined to a quantum wire and subject to a smoothly modulated Rashba spin-orbit coupling. When the period of the modulation becomes commensurate with the band filling, the Rashba coupling drives a quantum phase transition to a nonmagnetic insulating state. Using bosonization and a renormalization-group approach, we find that this state is robust against electron-electron interactions. The gaps to charge and spin excitations scale with the amplitude of the Rashba modulation with a common interaction-dependent exponent. An estimate of the expected size of the charge gap, using data for a gated InAs heterostructure, suggests that the effect can be put to practical use in a future spin transistor design.

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I. INTRODUCTION

Progress in the control and manipulation of spin degrees of freedom in semiconductors holds great promise for the development of future spintronics devices.¹ Much of current work in the field is inspired by various proposals for spin transistors. In what has become the prototype for a spintronics device scheme, the Datta-Das spin transistor,² spinpolarized electrons are injected from a ferromagnetic source into a quasi-one-dimensional (1D) ballistic channel ("quantum wire") formed in a semiconductor heterostructure. The structure inversion asymmetry of the heterostructure produces a Rashba spin-orbit coupling that makes the spins of the electrons precess with a rate controllable via a gate. In a simplified picture, an electron with the same spin projection as that of the magnetized drain is accepted by the drain, or else the electron is scattered away. This realizes an "on-off" current switch, controllable by the gate bias. The scheme is yet to be realized, however. One obstacle is the inefficiency of present techniques for injecting spin-polarized electrons from a ferromagnet into a quantum wire. Alternative ideas for developing a current switch based on a Rashba coupling are thus in high demand.

In an analysis of 1D spin transport, Wang³ suggested a design for a spin transistor where the electrons experience a spatially periodic Rashba spin-orbit coupling. In this scheme segments of a quantum wire with a uniform Rashba coupling are connected in series to segments with no coupling. A Fabry-Pérot-like interference between electron waves scattered at the interfaces between two segments leads to a transmission gap with a complete blocking of the charge current over a range of energies when the number of segments becomes sufficiently large. By tuning the electron density-and hence the Fermi level-by a supplementary gate, the flow of current in the wire can then be controlled effectively. As pointed out by Gong and Yang,⁴ the effect is fully operative for electrons with no spin polarization. By utilizing a periodically modulated Rashba coupling, one may thus envision a spin transistor without the injection of spin-polarized electrons into the current-carrying channel.⁵

This intriguing prospect motivates a closer investigation. In the present Rapid Communication we address two issues: first, how robust is the opening of a charge excitation gap against smoothening of the boundaries between regions with different strengths of the Rashba coupling? In particular, if the Rashba strength varies continuously on the scale of the underlying lattice, can a gap still appear? If so, under what conditions? Second, how do electron-electron interactions influence the gap opening? This question is crucial in view of applications as electron interactions in 1D can dramatically change the physics expected from an independent-electron picture.⁶ As we shall see, by "locking" the band filling to the periodicity of the Rashba modulation, a gap to charge excitations-as well as to spin excitations-does open up for a smooth Rashba interaction and it persists even when electron interactions are included. This gap-opening mechanism is very different from that based on repeated potential scattering in Refs. 3 and 4, the only common ingredient being the presence of a periodic Rashba modulation. In fact, we find that in the experimentally relevant parameter range, electron interactions increase the size of the charge gap, thus assisting the use of a gate-controlled modulated Rashba coupling as a current switch.

II. NONINTERACTING ELECTRONS

We consider a Rashba spin-orbit interaction H_R , which can be split into a uniform and a harmonically varying piece,

$$H_R = \left(\alpha_0 k_x + \frac{\alpha_1}{2} \{\cos(Qx), k_x\}\right) \sigma^{y}.$$
 (1)

Here α_0 and α_1 are constants, Q is a wave number, k_x is the electron wave number along the wire, and σ^y is a Pauli matrix. The anticommutator $\{\cos(Qx), k_x\}$ ensures that the interaction is Hermitian. The structure of Eq. (1) may be used in an attempt to qualitatively capture the effect of a piecewise modulated Rashba coupling in a quantum wire where distortions and stray electric fields smoothen the sharp interface

between two consecutive segments of the wire (each of extension $l_0=2\pi/Q$) with different values of the coupling. The real *raison d'être* for our choice in Eq. (1), however, is that it allows for a well-controlled analysis of a modulated Rashba coupling, also in the presence of electron interactions.

To set the stage, let us first focus on the case of noninteracting electrons. We shall assume that only the lowest-energy subband is partly filled as this is the case most relevant for an experimental realization. Making use of a tight-binding lattice formulation, we represent the kinetic energy by

$$H_0 = -t \sum_{n,\mu} \left(c_{n,\mu}^{\dagger} c_{n+1,\mu} + \text{H.c.} \right).$$
(2)

Here *t* is the hopping amplitude and $c_{n,\mu}^{\uparrow}(c_{n,\mu})$ are electron creation (annihilation) operators on site *n* with spin projection $\mu = \uparrow, \downarrow$ along the \hat{z} axis. The role of the Rashba interaction in Eq. (1) is taken by

$$H_{R} = -i \sum_{n,\mu,\nu} [\gamma_{0} + \gamma_{1} \cos(Qna)] (c_{n,\mu}^{\dagger} \sigma_{\mu\nu}^{y} c_{n+1,\nu} - \text{H.c.}),$$
(3)

where $\gamma_j = \alpha_j a^{-1} (j=0,1)$, with *a* as the lattice spacing. It is useful to introduce spin-rotated operators $b_{n,+} \equiv (c_{n,\downarrow} - ic_{n,\uparrow})/\sqrt{2}$ and $b_{n,-} \equiv (c_{n,\uparrow} - ic_{n,\downarrow})/\sqrt{2}$, and write the Hamiltonian $H = H_0 + H_R$ as

$$H = -\sum_{n,\tau} \left[(t + i\tau\gamma_0) b^{\dagger}_{n,\tau} b_{n+1,\tau} + \text{H.c.} - i\gamma_1 \cos(Qna) (\tau b^{\dagger}_{n,\tau} b_{n+1,\tau} - \text{H.c.}) \right], \tag{4}$$

with $\tau = \pm$ labeling the eigenstates of the σ_y operator, i.e., the spin projections on the axis along which the effective momentum-dependent Rashba field is pointing. When $\gamma_1=0$, the Hamiltonian in Eq. (4) describes a 1D system of noninteracting electrons in the presence of a uniform Rashba spin-orbit coupling. For this case the Hamiltonian is readily diagonalized in momentum space, and one finds that the spindegenerate band in the absence of Rashba coupling gets shifted horizontally into two distinct branches,

$$E_{\tau}^{0}(k) = -2\tilde{t}\cos[(k - \tau q_{0})a], \qquad (5)$$

where $q_0 = a^{-1} \arctan(\gamma_0/t)$ and $\tilde{t} = \sqrt{t^2 + \gamma_0^2}$. Note that we here consider an *ideal* 1D quantum wire, thus avoiding the complication of energy-band deformations produced by a spin-orbit interaction in the presence of a soft transverse confining potential.⁷

At band filling $\nu = N_e/N_0$, with $N_e[N_0]$ being the number of electrons [lattice sites], the system is characterized by the four Fermi points $k_{F,R}^{\tau} = k_F^0 + \tau q_0$, $k_{F,L}^{\tau} = -k_F^0 + \tau q_0$ ($\tau = \pm$), where $k_F^0 = \pi \nu/2a$. To simplify the analysis we linearize the spectrum around these Fermi points and pass to a continuum limit with $na \rightarrow x$. By decomposing the lattice operators $b_{n,\tau}$ into right- and left-moving fields $R_{\tau}(x)$ and $L_{\tau}(x)$,

$$b_{n,\tau} \to \sqrt{a} (\mathrm{e}^{i(k_F^0 + \tau q_0)x} R_{\tau}(x) + \mathrm{e}^{-i(k_F^0 - \tau q_0)x} L_{\tau}(x)),$$

the lattice Hamiltonian in Eq. (4) takes the form $H=\int dx(\mathcal{H}_++\mathcal{H}_-)$, with

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$$\mathcal{H}_{\tau} = -iv_F(:R_{\tau}^{\dagger}(x)\partial_x R_{\tau}(x):-:L_{\tau}^{\dagger}(x)\partial_x L_{\tau}(x):)$$
$$-2\Delta_R \cos(Qx)(e^{-2ik_F^0(x+a/2)}R_{\tau}^{\dagger}(x)L_{\tau}(x) + \text{H.c.}), \quad (6)$$

where $v_F = 2a\sqrt{t^2 + \gamma_0^2}$ and $\Delta_R = \gamma_1 \sin(q_0 a)$, and where we have omitted rapidly oscillating terms, which vanish upon integration. The normal ordering :...: is carried out with respect to the filled Dirac sea.

III. BOSONIZATION

To make progress we bosonize the theory, using $R_{\tau}(x) = \eta_{\tau} \exp(i\sqrt{\pi} [\varphi_{\tau}(x) + \vartheta_{\tau}(x)])/\sqrt{2\pi a}$ and $L_{\tau}(x) = \overline{\eta}_{\tau} \exp(-i\sqrt{\pi} [\varphi_{\tau}(x) - \vartheta_{\tau}(x)])/\sqrt{2\pi a}$, where $\varphi_{\tau}(x)$ and $\vartheta_{\tau}(x)$ are dual bosonic fields satisfying $\partial_{t}\varphi_{\tau} = v_{F}\partial_{x}\vartheta_{\tau}$, and where η_{τ} and $\overline{\eta}_{\tau}$ are Klein factors which keep track of the fermion statistics for electrons in different branches.⁸ Inserting the bosonized forms of $R_{\tau}(x)$ and $L_{\tau}(x)$ into Eq. (6), and introducing the charge (c) and spin (s) fields $\varphi_{c} \equiv (\varphi_{+} + \varphi_{-})/\sqrt{2}$ and $\varphi_{s} \equiv (\varphi_{+} - \varphi_{-})/\sqrt{2}$, we arrive at the bosonized Hamiltonian

$$H = \int dx \left(\frac{v_F}{2} \sum_{i=c,s} \left((\partial_x \varphi_i)^2 + (\partial_x \vartheta_i)^2 \right) - \frac{2\Delta_R}{\pi a} \sum_{j=\pm 1} \sin([Q + 2jk_F^0]x + k_F^0 a + \sqrt{2\pi}\varphi_c)\cos(\sqrt{2\pi}\varphi_s) \right).$$

.

When $Q-2k_F^0 \simeq \mathcal{O}(1/a)$, both Rashba terms $\sim \Delta_R$ are rapidly oscillating and average to zero. Thus, in this limit the model describes free charge and spin bosons, i.e., a metallic phase with gapless spin excitations.

In contrast, when $Q-2k_F^0 \ll \mathcal{O}(1/a)$ the j=-1 component of the modulated Rashba coupling comes into play. For this case it is useful to perform a transformation, $(Q-2k_F^0)x+k_F^0a+\sqrt{2\pi\varphi_c} \rightarrow \pi/2+\sqrt{2\pi\varphi_c}$, and rewrite the Hamiltonian density as

$$\mathcal{H} = \frac{\partial_F}{2} \sum_{i=c,s} \left((\partial_x \varphi_i)^2 + (\partial_x \vartheta_i)^2 \right) - \mu_{\text{eff}} \partial_x \varphi_c - \frac{2\Delta_R}{\pi a} \cos(\sqrt{2\pi}\varphi_c) \cos(\sqrt{2\pi}\varphi_s),$$
(7)

where $\mu_{\text{eff}} \equiv v_F \sqrt{2/\pi} (Q - 2k_F^0)$ is an effective "chemical potential," which, when tuned to zero, "locks" the band filling to commensurability with the Rashba modulation. For this case, i.e., with $\mu_{\text{eff}}=0$, the Hamiltonian describes two bosonic charge and spin fields coupled by the strongly [renormalization-group (RG)] relevant operator $\cos(\sqrt{2\pi\varphi_c})\cos(\sqrt{2\pi\varphi_s})$. This operator pins the charge and spin fields at their ground state expectation values

$$\langle \varphi_c \rangle = \langle \varphi_s \rangle = \sqrt{\pi/2}n \quad n = 0, \pm 1, \pm 2, \dots.$$
 (8)

and as a result both spin and charge excitations develop a gap.⁹ Thus, when $\mu_{eff}=0$, the system turns into a nonmagnetic insulator.

To study the properties of the insulating state, specifically the size of the charge excitation gap, we use a mean-field decoupling of charge and spin in Eq. (7) and write the

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Hamiltonian as $H = \int dx (\mathcal{H}_c + \mathcal{H}_s)$, where (for i = c, s)

$$\mathcal{H}_i = \frac{v_F}{2} [(\partial_x \varphi_i)^2 + (\partial_x \vartheta_i)^2] - \frac{m_i}{\pi a} \cos(\sqrt{2\pi}\varphi_i), \qquad (9)$$

with

$$m_c \equiv \Delta_R \langle \cos(\sqrt{2\pi}\varphi_s) \rangle, \quad m_s \equiv \Delta_R \langle \cos(\sqrt{2\pi}\varphi_c) \rangle.$$
 (10)

Note that the mean-field decoupling is here under control since the pinning [Eq. (8)] implies that field fluctuations are strongly suppressed. As seen from Eq. (9), the mean-field theory at $\mu_{eff}=0$ is equivalent to two commuting sine-Gordon models with $\beta^2 = 2\pi$, and with "bare" masses defined by Eq. (10). From the exact solution of the sine-Gordon model it is known that for this case the excitation spectrum is gapped and consists of solitons and antisolitons with mass $M_{c/s}$ and soliton-antisoliton bound states ("breathers") with the lowest breather mass also equal to $M_{c/s}$.¹⁰ As M_c determines the charge gap caused by the modulated Rashba coupling, we shall derive an expression for M_c that allows us to estimate its size in a given experimental setting. Before doing so, however, let us show how the analysis above can be extended so as to take into account the electron-electron interactions.

IV. INTERACTING ELECTRONS

Since Umklapp scattering is absent in a ballistic quantum wire, one is left with backscattering $(\sim g_{1\pm})$, dispersive scattering $(\sim g_{2\pm})$, and forward scattering $(\sim g_{4\pm})$, controlled by

$$\mathcal{H}_{\text{int}} = g_{1-} : R_{\tau}^{\dagger} L_{\tau} L_{\tau}^{\dagger} R_{-\tau} R_{-\tau} : + \widetilde{g}_{2\tau} : R_{+}^{\dagger} R_{+} L_{\tau}^{\dagger} L_{\tau} :$$
$$+ \frac{g_{4\tau}}{2} (: R_{+}^{\dagger} R_{+} R_{\tau}^{\dagger} R_{\tau} :+ R \leftrightarrow L), \qquad (11)$$

with $\tau = \pm$ summed over, $\tilde{g}_{2\tau} \equiv g_{2\tau} - \delta_{\tau+} g_{1\tau}$, and $(+,-) \leftrightarrow (\parallel, \perp)$ in the standard "g-ology" notation.⁶

The strength of the electron interaction in a semiconductor structure is typically much smaller than the band width. For this weak-coupling case the backscattering $\sim g_{1-}$ is marginally irrelevant and renormalizes to zero at low energies (just as for a 1D electron system in the absence of spin-orbit coupling).¹¹ From now on we therefore consider an effective model where the backscattering has been renormalized away. The bosonized mean field theory, including electron interactions, then takes the form $H = \int dx \left[\mathcal{H}_c + \mathcal{H}_s \right]$, where (for i = c, s)

$$\mathcal{H}_i = \frac{v_i}{2} [(\partial_x \varphi_i)^2 + (\partial_x \vartheta_i)^2] - \frac{m_i}{\pi a} \cos(\sqrt{2\pi K_i} \varphi_i).$$
(12)

For weak interactions, v_i and K_i can be explicitly parametrized in terms of the amplitudes in Eq. (11).⁶ Note that also the bare masses m_i get renormalized by the interaction, with $\varphi_i \rightarrow \sqrt{K_i}\varphi_i$ in Eq. (10). It is also important to note that the breaking of spin-rotational invariance by the Rashba interaction implies that the RG fixed-point value of K_s is not slaved to unity⁶ but can take larger values.¹²

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V. CHARGE AND SPIN EXCITATION GAPS

We can now derive an expression for the charge excitation gap—identified as the physical soliton mass M_c in the charge sector of Eq. (12)—with the electron interactions included. The mass M_c and the corresponding mass M_s in the spin sector are related to the (bare) mass parameters m_c and m_s , respectively, by¹³

$$M_i = C_1(K_i)\Lambda(m_i/\Lambda)^{2/(4-K_i)}, \quad i = c, s,$$
 (13)

where Λ is an energy cutoff, and $C_1(K_i) \equiv [\pi\Gamma(1-K_i/4)/\Gamma(K_i/4)]^{2/(4-K_i)}[2\Gamma(\xi_i/2)/\sqrt{\pi}\Gamma(1/2-\xi_i/2)],$ with $\xi_i = K_i/(4-K_i)$. The ground-state expectation values entering the bare masses m_i are in turn related to the physical masses M_i by¹⁴

$$\langle \cos(\sqrt{2\pi K_i}\varphi_i)\rangle = C_2(K_i)(M_i/\Lambda)^{K_i/2}, \quad i = c,s$$
(14)

with

$$C_{2}(K_{i}) \equiv \left[(1 + \xi_{i})\pi \Gamma(1 - K_{i}/4) / 16 \sin(\pi\xi_{i})\Gamma(K_{i}/4) \right] \\ \times \left[\Gamma(1/2 + \xi_{i}/2)\Gamma(1 - \xi_{i}/2) / 4\sqrt{\pi} \right]^{(K_{i}/2) - 2} \\ \times \left[2 \sin(\pi\xi_{i}/2) \right]^{K_{i}/2}.$$

Combining Eqs. (10), (13), and (14), some elementary algebra yields for the charge excitation gap,

$$M_c = \mathcal{C}_c \Lambda (\Delta_R / \Lambda)^{2/(4 - K_c - K_s)}, \qquad (15)$$

where

$$\begin{split} \mathcal{C}_{c}^{16-4K_{c}-4K_{s}} &\equiv \mathcal{C}_{1}(K_{c})^{(4-K_{c})(4-K_{s})} \\ & \times \mathcal{C}_{2}(K_{c})^{2K_{s}} \, \mathcal{C}_{1}(K_{s})^{(4-K_{s})K_{s}} \, \mathcal{C}_{2}(K_{s})^{2(4-K_{s})}. \end{split}$$

The spin gap M_s is given by the same expression but with $c \leftrightarrow s$.

The opening of the charge gap at a band-filling commensurate with the period of the Rashba modulation leads to a reduction in the ground state energy and pins the band filling at this value until the chemical potential reaches the bottom of the upper band. The competition between the chemical potential μ and the commensurability energy drives a continuous quantum phase transition from a gapped (insulating) phase at $\mu < \mu_c = M_c$ to a gapless (metallic) phase at $\mu > \mu_c$.^{15,16} Such a transition belongs to the universality class of a commensurate-incommensurate metal-insulator transition.⁶ The critical conductivity σ , proportional to the doping of the upper band, scales as $\sigma \sim (\mu - \mu_c)^{1/2}$, while the compressibility κ diverges as $\kappa \sim (\mu - \mu_c)^{-1/2}$ before dropping to zero on the insulating side. In the gapless phase the ground-state expectation value $\langle \cos(\sqrt{2\pi K_c \varphi_c}) \rangle$ vanishes and, as follows from Eq. (10), this implies that also the bare mass m_s vanishes. As a consequence, the quantum phase transition in the charge sector at $\mu = \mu_c$ is accompanied by a similar transition in the spin sector, with the system showing Luttinger liquid behavior with gapless spin and charge excitations for $\mu > \mu_c$.

VI. IMPLICATIONS

Our main result, Eq. (15), boosts the proposal^{3,4} that a controllable and modulated Rashba coupling may serve as a

current switch in a quantum wire. It is here important to emphasize that our scheme exploits a nontrivial commensurability property, encoded in the condition $Q=2k_F$, and is hence different from that in Refs. 3 and 4, which is based on a picture of repeated single-particle scattering. For an implementation one would need a configuration of switchable top gates that produce the modulation, as well as a tunable back gate by which the band filling can be adjusted. While a challenging quest in quantum engineering, our analysis testifies to the soundness of the scheme as it shows that a Rashbainduced charge gap is robust against electron-electron interactions. In fact, as revealed by Eq. (15), in the experimentally relevant range $K_c+K_s<2$,⁶ the gap grows with the strength of the electron interactions.

As for the size of the gap, we may take as illustration a quantum wire patterned in an InAs heterostructure, which, due to its strong spin-orbit coupling and large electron mean-free path, is favored in spintronics applications.¹ Using data for a heterostructure grown by molecular-beam epitaxy,¹⁷ with Rashba parameter $\hbar \alpha \approx 2 \times 10^{-11}$ eV m, carrier density $n_e \approx 1 \times 10^{12}$ cm⁻², effective mass $m^* \approx 0.4m_e$, and lattice spacing $a \approx 5$ Å, we have that $\hbar \Delta_R \approx 4$ meV, taking $\alpha_1 \approx \alpha$. A rough estimate of the charge and spin stiffness parameters, assuming a well-screened interaction¹⁸ with $\epsilon \approx 15\epsilon_0$,¹⁹ yields that $K_c \approx 0.6$ and $K_s \approx 1.2$. With $\Lambda = \hbar v_F / a \approx 0.5$ eV, it follows from Eq. (15) that $M_c \approx 1 \times 10^2$ meV, corresponding to a threshold voltage of approximately 100 mV in a spin transistor application.

Using the estimate of M_c above, the characteristic length scale $\xi \sim \hbar v_F / M_c$ at which the gap starts to open up is given by $\xi \approx 5$ nm. This number fits easily within the quantum ballistic regime of an InAs quantum wire, with an estimated mean-free path of $\gtrsim 1.5 \ \mu m$,¹⁹and one thus expects the gap to open up fully. In this context one should realize that an implementation of a gate-controlled Rashba modulation with a well-defined periodicity is an experimental challenge and must probably await further progress in device technology. It

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is here important to note that a periodic gate bias will modulate also the electron density, thus favoring a build-up of charge density wave correlations. While this effect is expected to assist the opening of the Rashba gap, its precise influence needs to be studied in a more complete theory.

VII. SUMMARY

To conclude, we have shown that a smoothly modulated Rashba spin-orbit coupling in a quantum wire drives a commensurate-incommensurate metal-insulator transition at a critical value of the band filling. The charge excitation gap (as well as the associated spin gap) is found to scale with the amplitude of the Rashba modulation γ_1 as $\gamma_1^{2/(4-K_c-K_s)}$, where K_c and K_s are the charge and spin stiffness parameters that encode electron interaction effects. In a next step one should try to refine the analysis of the problem and go beyond the minimal model employed here. In particular, effects from local variations in the electron density and from electron back scattering at very low densities¹¹ are important to explore. Also, the question of what happens for more general periodic profiles of the Rashba modulation is an important issue. With a more complete theory, and with advances in device technology, a low-bias spin transistor based on a switchable and modulated Rashba coupling may well become a reality.

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