Dressed Majorana fermion in a hybrid nanowire

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The low-energy theory of hybrid nanowire systems fails to define Majorana fermion (MF) in the strong tunneling and magnetic field strength. To address this limitation, we propose a holistic approach to define MF in which the quasi-excitation in nanowire and superconductor constitutes together its own “antiparticles”. This definition is general, beyond the constraint presented in the low-energy theory. It reveals that the Majorana phase depends not only on the chemical potential and Zeeman energy in nanowire but also on those of superconductor, and that the mismatch of chemical potential leads not to observe MF. Such a broader perspective provides more specific experimental guidance under various conditions.

Introduction.—The observation of Majorana fermion (MF) in condensed matter systems is a prerequisite for realizing topological quantum computation [1–5]. As one of the promising platforms, the semiconductor nanowire with appreciable spin-orbit coupling coupled to an s-wave superconductor (SC), as considered to display MF [6–8], mainly based on a low-energy effective theory [3, 9, 10]. Such a low-energy effective theory predicts that the topological phase of MF can be implemented in experiments by only adjusting the chemical potential and applied magnetic field in the nanowire, directly independent on the proximity superconducting materials.

The above low-energy effective theory is derived by eliminating the virtual process of exchange of electron in nanowire between Bogoliubov quasi-particles in SC, and a constant s-wave pairing is induced in the nanowire. But the validity of the low-energy theory is limited due to the following three approximations [9–11]:

(i) the s-wave SC is assumed at a periodic boundary to ignore the boundary effect, which indicates that the edge state of MF is only localized at two ends of the nanowire;

(ii) the energy-independent coupling spectral between the nanowire and SC in wide-band limit results in the induced constant pairing term;

(iii) only low-energy effects of superconducting self-energy correction are considered, which limits the effective theory to the weak tunneling strength between the nanowire and SC.

What is more, it has also been pointed out that the effective Kitaev model cannot be reduced when the Zeeman splitting and tunneling strength are comparable to the superconducting gap due to the failure of perturbation method [12], which leaves unresolved the question whether MF can be defined in the strong magnetic field and coupling region.

However, in the mainstream hybrid system used to observe MF experimentally such as InSb/InAs nanowire partially or fully covered by aluminum film, the coupling strength between nanowire and SC has reached the intermediate or even strong coupling schemes under the strong magnetic field [4, 13–16]. Besides, some artificially experimental signature of MF fitting a phase diagram given by the above low-energy theory have caused great controversy and were even retracted so that the validity of the low-energy theory should be doubted [15–18]. Therefore, it is necessary to address the following issues:

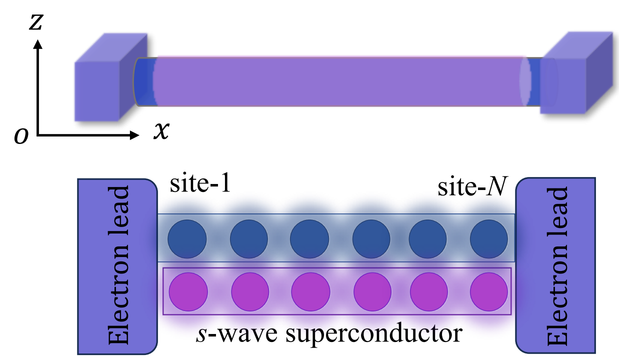

FIG. 1. The semiconductor nanowire is partially or fully covered by the superconducting shell, which can be characterized by the one-dimensional lattice model of nanowire coupled to an s-wave superconductor. And the spectrum of its differential conductance is obtained by connecting electron leads at the ends of the nanowire.

(i) how to generally define MF in a hybrid system at any magnetic field and tunneling strength ?

(ii) what is universal Majorana topological phase like? Does it also depend on the relevant parameters of SC ?

(iii) under what conditions, the topological phase of MF obtained by the low-energy effective Hamiltonian is valid ?

In this paper, by a minimal hybrid model [4] that a one-dimensional semiconductor nanowire couples to a one-dimensional s-wave SC [Fig. 1], we propose a holistic perspective to define the dressed Majorana fermion (DMF), namely, DMF is composed of the electron and hole excitations in nanowire dressed by quasi-excitations in SC. Here, we treat the excitations in nanowire and SC equally, rather than directly eliminating quasi-excitation in SC, as has been done in the low-energy effective theory. Therefore, such a definition of DMF holds for any tunneling and magnetic field strength.

The edge state of DMF in open boundary is localized not only at two ends of nanowire but also of SC, and its distribution in nanowire and SC is determined by the tunneling strength. As a signature of DMF, we show that the $2e^2/h$ zero-bias peak in the differential conductance spectrum is also obtained by connecting electron leads to nanowire.

We demonstrate that the universal Majorana phase depends not only on the chemical potential and Zeeman energy in nanowire but also in SC. The low-energy phase diagram given by the effective theory [*it depends only on chemical potential and magnetic field in nanowire*] is only an approximate result of the universal Majorana phase in the weak tunneling scheme.

Lastly, the universal Majorana phase is applied to the experimental hybrid InSb/InAs-Al system, and it is suggested that the mismatch of chemical potentials between nanowire and SC hinders the observation of MF.

Theoretical Model.—The semiconductor nanowire with the Rashba spin-orbit coupling α_w is described by N-sites lattice model as [9, 19, 20]

$$\begin{aligned} H_w = &\sum_{n=1}^{N} d_n^\dagger \left[(t_w - \mu_w)\sigma_0 + h_w\sigma_x\right] d_n \\ &- \sum_{n=1}^{N-1} d_n^\dagger \left(\frac{t_w}{2}\sigma_0 + \frac{i\alpha_w}{2}\sigma_y\right) d_{n+1} + \text{H.c.}, \end{aligned} \tag{1}$$

where $d_n := [d_{n\uparrow}, d_{n\downarrow}]^T$ is a annihilation operator of the electron in site-n with spin $\uparrow, \downarrow$, and $\sigma_{0,x,y}$ are the 2×2 identity and Pauli matrices. Here, μ_w is the chemical potential, t_w is the hopping strength between nearest sites in the nanowire, and h_w is the Zeeman splitting caused by an external magnetic aligned with the nanowire axis.

The semiconductor nanowire is in contact with an s-wave SC or wrapped by superconducting shell (such as Al [13, 15] and Pb [21, 22] shell), and such a SC is also characterized by the one-dimensional lattice model: [23]

$$\begin{aligned} H_s = &\sum_{n=1,\sigma}^{N} (t_s - \mu_s) c_{n,\sigma}^\dagger c_{n,\sigma} - \frac{t_s}{2}[c_{n,\sigma}^\dagger c_{n+1,\sigma} + \text{H.c.}] \\ &+ \sum_{n=1}^{N} [\Delta_s c_{n,\uparrow}^\dagger c_{n,\downarrow}^\dagger + h_s c_{n\uparrow}^\dagger c_{n\downarrow} + \text{H.c.}]. \end{aligned} \tag{2}$$

Similarly, μ_s is the chemical potential, t_s is hopping strength, h_s is the Zeeman energy [24–27] and Δ_s is a pairing strength for the s-wave SC.

And the interaction between nanowire and SC is via single electron tunneling: $H_t = -\sum_{n,m,\sigma} T_{nm}[d_{n\sigma} c_{m\sigma}^\dagger + c_{m\sigma} d_{n\sigma}^\dagger]$, with the tunneling strength T_{nm} between the site-n of the nanowire and site-m in SC. Below, we consider that the tunneling strength for the same sites $n = m$ is equal but ignored between different sites $n \neq m$, i.e., $T_{nm} \equiv \delta_{mn} T$.

Notice that the Hamiltonian of the hybrid nanowire can be diagonalized as $H = H_w + H_s + H_t = 1/2 \sum_E E\, \eta_E^\dagger \eta_E$, and the corresponding quasi-particle operator is

$$\eta_E = (\mathbf{u}_E^w)^\dagger \cdot \mathbf{d} + (\mathbf{v}_E^w)^\dagger \cdot (\mathbf{d}^\dagger)^T + (\mathbf{u}_E^s)^\dagger \cdot \mathbf{c} + (\mathbf{v}_E^s)^\dagger \cdot (\mathbf{c}^\dagger)^T, \tag{3}$$

where $\mathbf{d} := [d_1, \ldots, d_N]^T$ and $\mathbf{c} := [c_1, \ldots, c_N]^T$ with $c_n := [c_{n\uparrow}, c_{n\downarrow}]^T$. And the eigen-wave function is $\Psi_E = [\mathbf{u}_E, \mathbf{v}_E]^T$ with $\mathbf{u}_E = [\mathbf{u}_E^w, \mathbf{u}_E^s]^T$ and $\mathbf{v}_E = [\mathbf{v}_E^w, \mathbf{v}_E^s]^T$, where $\mathbf{o}_E^\alpha = [\mathrm{o}_{E,1}^\alpha, \ldots, \mathrm{o}_{E,N}^\alpha]^T$ with $\mathrm{o}_{E,n}^\alpha = [\mathrm{o}_{E,n\uparrow}^\alpha, \mathrm{o}_{E,n\downarrow}^\alpha]^T$ respctively represent the wave function of electrons $\mathrm{o} \equiv \mathrm{u}$ and holes $\mathrm{o} \equiv \mathrm{v}$ in the nanowire and SC for $\alpha = w, s$.

Dressed MF.—We define the dressed Majorana fermion as

$$\eta_E = \eta_E^\dagger \Longrightarrow \mathbf{u}_E^w = (\mathbf{v}_E^w)^*,\ \mathbf{u}_E^s = (\mathbf{v}_E^s)^*, \tag{4}$$

where the quasi-excitation constitutes its own "antiparticles". Further, the particle-hole symmetry requires $(\mathbf{u}_{-E}^w)^* = \mathbf{v}_E^w$ and $(\mathbf{u}_{-E}^s)^* = \mathbf{v}_E^s$. Thus it is proved that only the zero-energy quasi-particle is Majorana fermion [11]. Then, we need to give the conditions for the existence of such a zero-energy wave function.

For the zero-enrgy wave function $E = 0$ ($\mathbf{u} = \mathbf{v}^*$, where subscript "0" is omitted), we decompose $\mathbf{u}$ into real and imaginary parts $\mathbf{u} = \mathbf{u}^{(r)} + i\mathbf{u}^{(i)}$. It is easy to verify that the electron wave function's real and imaginary parts in nanowire satisfy

$$[(\mathbf{H}_s + \lambda \mathbf{P}_s) \cdot \mathbf{H}_w - \mathbf{T}^2] \cdot \mathbf{u}_w^{(\lambda)} = 0, \tag{5}$$

and the electron wave function in SC is $\mathbf{u}_s^{(\lambda)} = -\mathbf{T}^{-1} \cdot \mathbf{H}_w \cdot \mathbf{u}_w^{(\lambda)}$. Here, $\lambda = \pm 1$ corresponds to the real and imaginary parts of $\mathbf{u}_\alpha^{(\lambda)}$, that is $\mathbf{u}_\alpha^{(1)} \equiv \mathbf{u}_\alpha^{(r)}$ and $\mathbf{u}_\alpha^{(-1)} \equiv \mathbf{u}_\alpha^{(i)}$ with $\alpha = w, s$. And the $2N \times 2N$ Hamiltonian matrices of the nanowire $\mathbf{H}_w$, tunneling interaction $\mathbf{T}$ and SC ($\mathbf{H}_s$ and $\mathbf{P}_s$) are given in *supplemental materials* [11].

We assume that $\mathrm{u}_{w,n}^{(r)} \equiv \xi^n [a_\uparrow, a_\downarrow]^T, 1 \le n \le N$, where ξ is a complex number, and $a_\uparrow, a_\downarrow$ are undetermined coefficients. By substituting $\mathrm{u}_{w,n}^{(r)}$ into Eq. (5), it is proved that ξ is root of 8-order equation of one variable $f_\lambda(\xi) = 0$ with $\lambda = 1$, and $a_\uparrow, a_\downarrow$ are determined for an given ξ [11]. Thus such a electron wave function in nanowire becomes $\mathrm{u}_{w,n}^{(r)} = \sum_{j=1}^{8} \alpha_j \xi_j^n [a_{j\uparrow}, a_{j\downarrow}]^T$, where α_j are arbitrary superposition coefficients.

The boundary and normalization conditions of the zero-energy wave function $\mathbf{u}^{(r)}$ require that $f_1(\xi) = 0$ must have three roots less than 1 as the total site number approaches infinity $N \to \infty$, namely

$$f_1(\xi_j) = 0, \exists\, \xi_j, j = 1, 2, 3,\ |\xi_j| < 1 \tag{6}$$

At this time, $\mathbf{u}_w^{(r)}$ is uniquely determined, and the wave function in SC is obtained by $\mathbf{u}_s^{(r)} = -\mathbf{T}^{-1} \cdot \mathbf{H}_w \cdot \mathbf{u}_w^{(r)}$.

Similarly, the imagine part of the wave function $\mathbf{u}_w^{(i)}$ is obtained as $\mathrm{u}_{w,n}^{(i)} = \sum_{j=1}^{3} \beta_j \xi_j^{-N+n+1} [b_{j\uparrow}, b_{j\downarrow}]^T$ for the given β_j and $b_{j\sigma}$ with $\sigma = \pm 1$, and $\mathbf{u}_s^{(i)} = -\mathbf{T}^{-1} \cdot \mathbf{H}_w \cdot \mathbf{u}_w^{(i)}$. Here, we have utilized the function relation $f_{\lambda=1}(\xi) = f_{\lambda=-1}(1/\xi) = 0$ with $\xi \neq 0$ [11].

Known $\mathbf{u}^{(r)}$ and $\mathbf{u}^{(i)}$, DMF is rewritten as

$$\begin{aligned} \gamma_1 &= \sum_{n\sigma} \mathrm{u}_{w,n\sigma}^{(r)} (d_{n\sigma} + d_{n\sigma}^\dagger) + \mathrm{u}_{s,n\sigma}^{(r)} (c_{n\sigma} + c_{n\sigma}^\dagger), \\ \gamma_N &= \sum_{n\sigma} \mathrm{u}_{w,n\sigma}^{(i)} (i[d_{n\sigma}^\dagger - d_{n\sigma}]) + \mathrm{u}_{s,n\sigma}^{(i)} (i[c_{n\sigma}^\dagger - c_{n\sigma}]). \end{aligned} \tag{7}$$

It is seen from Eqs. (6, 7) that γ_1 and γ_N correspond to the localized edge state at site-1 and site-N of the nanowire and SC. Such a MF is a compsite of electron and hole exication in nanowire dressed by the quasi-exication of SC [the last two terms of (7)], and it is different from MF defined by the low-energy effective theory, where the quasi-excitation in SC has been eliminated.

Apparently, there is another case where the real and imaginary part of zero-energy wave function are respetively localized near site-N and site-1 of the nanowire and SC [$|\xi_j| > 1$ in Eq. (6)]. In short, a zero-energy wave function exists only when the function $f_1(\xi)$ has three complex roots, and their magnitudes are greater than or less than 1. Thus, the parameter range in the presence of the edge state of DMF is

$$\prod_k [(h_w + Z_k h_s)^2 - (\epsilon_k^w - \mu_w - Z_k(\epsilon_k^s - \mu_s))^2 - (Z_k \Delta_s)^2] < 0, \tag{8}$$

where $\epsilon_k^s := t_\alpha(1 - \cos k)$, and k only takes 0 and π. The correction factor $Z_k := T^2/(E_{k,+}^s E_{k,-}^s)$ embodies the dressed effect of SC for the nanowire, where the excitation energy of quasi-particle in SC is included as $E_{k,\pm}^s = \sqrt{[\epsilon_k^s - \mu_s]^2 + \Delta_s^2} \pm h_s$ [3]. Such a edge state of DMF depends not only on the chemical potential μ_w and Zeeman energy h_w of the nanowire, but also on the chemical potential μ_s and Zeeman energy h_s in SC. And it can be proved that the conditions for the existence of the Majorana edge state (8) is consistent with the topological phase of DMF (Majorana phase) given by the topological invariant $\mathrm{sgn}(\mathrm{Pf}[\mathscr{H}_\gamma(0)])\mathrm{sgn}(\mathrm{Pf}[\mathscr{H}_\gamma(\pi)]) < 0$ [11].

In this Majorana phase, the energy spectrum of hybrid system indeed displays the zero-energy modes of DMF, and there is a gap between the zero and excitation energy [Fig. 2(a)]. The edge state of DMF is not only localized at two ends in the nanowire, but also in SC [Fig. 2(c, d)]. And the proportion of zero-energy wave function distributed in the nanowire and SC $\mathrm{P_{SC}}/\mathrm{P_{NW}}$ increases with the enhance of tunneling strength T , where the zero-energy wave function of the nanowire and SC are measured by $\mathrm{P_{NW}} = \sum_{n\sigma} |\mathrm{u}_{w,n\sigma}|^2 + |\mathrm{v}_{w,n\sigma}|^2$ and $\mathrm{P_{SC}} = \sum_{n\sigma} |\mathrm{u}_{s,n\sigma}|^2 + |\mathrm{v}_{s,n\sigma}|^2$ with normalization condition $\mathrm{P_{SC}} + \mathrm{P_{NW}} = 1$ [Fig. 2(b)]. This shows that the more zero-energy wave function penetrates SC from the nanowire as the tunneling strength increases. However, the low-energy effective theory has ignored the zero-energy wave function in SC since the superconductor is considered as a periodic boundary. In the intermediate, especially strong tunneling schemes $T > \Delta_s$, the zero-energy wave function in SC is comparable to that in nanowire [$T \sim 2\Delta_s$, $\mathrm{P_{SC}}/\mathrm{P_{NW}} \sim 30\%$], and the boundary effect of SC cannot be ignored.

It is known that MF determined by the low-energy theory will result in the zero-bias peak (ZBP) with the height $2e^2/h$ at zero temperature [12, 28, 29]. For DMF in the hybrid nanowire, the $2e^2/h$ ZBP as a signature of DMF also appears by connecting electron leads at the ends of the nanowire [see Fig. (1) and Fig. 2(e)] [11].

Typically, the bandwidth of the nanowire and SC as the maximum energy scale is much larger than their Zeeman energy, chemical potential and the superconducting gap $t_\alpha \gg \mu_\alpha, h_\alpha, \Delta_s$ with $\alpha = w, s$. Then the universal Majorana phase (8) becomes

$$(h_w + Z_0 h_s) > \sqrt{(\mu_w - Z_0\mu_s)^2 + (Z_0\Delta_s)^2}. \tag{9}$$

When the dressed effect of SC for the nanowire (the correction factor Z_0) is small so that $Z_0 h_s, Z_0\mu_s \ll 1$, the Majorana phase returns to the low-energy phase diagram $h_w > \sqrt{\mu_w^2 + \Delta^2}$ with $\Delta := Z_0\Delta_s$ [3, 4]. In this regard, the correction factor can be regraded as the ratio of the induced pairing strength Δ to the superconducting gap $Z_0 = \Delta/\Delta_s$, which characterizes the different tunneling schemes. By increasing the tunneling strength between nanowire and SC, the correction factor gradually achieves a stronger tunneling scheme $Z_0 \to 1$ so that the Zeeman energy $\tilde{h}_w := h_w + Z_0 h_s$ and chemical potential $\tilde{\mu}_w := \mu_w - Z_0\mu_s$ in the nanowire is significantly modified. This results in the Majorana phase deviating significantly from the previous low-energy phase diagram, especially for the more considerable superconducting chemical potentials and Zeeman energy [Fig. 2(f)]. Therefore, the Majorana phase (9) is more general, the fragile low-energy

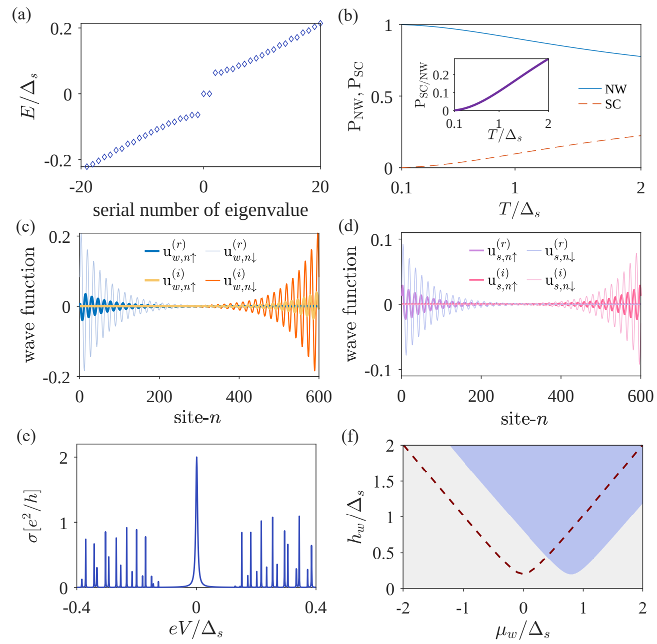

FIG. 2. (a) The zero-energy and excitation-energy modes in the hybrid system. (b) The zero-energy wave function $\mathrm{P_{SC}}, \mathrm{P_{NW}}$ in nanowire and SC, and their proportion $\mathrm{P_{SC}}/\mathrm{P_{NW}}$ change as the tunneling strength enhances. (c, d) The distribution of the localized zero-mode wave functions at each site-n in nanowire and SC. (e) The zero bias peak in differential spectrum by connecting electron leads at the ends of the nanowire. The parameters are set as $N = 600, t_w = 12\Delta_s, t_s = 10\Delta_s, \mu_w = 0, \mu_s = 4\Delta_s, h_w = 1.5\Delta_s, h_s = 0, \alpha_w = T = 1.5\Delta_s$. (f) The general Majorana phase (light purple region) deviates from the phase diagram determined by the low-energy theory (red dashed line) in $\mu_w - h_w$ space with the correction factor $Z_0 = 0.2$ and $h_s = 0.1h_w$.

topological phase is just an approximate result of which in weak tunneling scheme $Z_0 \ll 1$.

It is worth noting that the low-energy phase diagram *depends only on chemical potential* μ_w *and magnetic field* h_w *in nanowire*, which is considered as the solid theoretical basis to observe MF in experiments so far. However, the universal Majorana phase also depends significantly on the chemical potential μ_s and magnetic field h_s in SC [see Eq. (9)], and it does have an impact on the observation of MF in an actual hybrid nanowire system.

Dependence of Majorana phase on the chemical potential and magnetic field in SC—For the hybrid InSb/InAs-Al system, the superconducting gap of aluminum film is $\Delta_s = 0.34\,\mathrm{meV}$, and the Zeeman splitting in SC is an order of magnitude smaller than that in the nanowire due to the difference in Landé factor $h_s \sim 0.05 - 0.15 h_w$ [4, 21, 26, 27]. From the induced energy gap observed in experiments $\Delta = 0.2\,\mathrm{meV}$ [15], the correction factor can be estimated as $Z_0 = \Delta/\Delta_s \simeq 0.6$. Therefore the magnetic field required for the Majorana phase by (9) is obtained as

$$B > \frac{2\sqrt{(\mu_w - 0.6\mu_s)^2 + (0.6\Delta_s)^2}}{\mu_\mathrm{B}(\mathrm{g}_w + 0.6\mathrm{g}_s)}. \tag{10}$$

with the Bohr magneton μ_B and the Landé factor $\mathrm{g}_\alpha, \alpha = w, s$ of nanowire and SC. Since the critical magnetic field of the aluminum film is $2\,\mathrm{T}$ [21], the maximum difference in chemical potential between the nanowire and SC cannot be greater than $|\mu_w - 0.6\mu_s| < 2.4/0.9\,\mathrm{meV}$ for the InSb\InAs nanowire, where the Landé factors are taken as $\mathrm{g}_\mathrm{InSb} = 40, \mathrm{g}_\mathrm{InAs} = 15$ and $\mathrm{g}_s = 2$ [4, 21]. For example, if the superconducting chemical potential is $1\mathrm{eV}$ [30], the chemical potential of the InSb\InAs nanowire must be adjusted to $597/599 \lesssim \mu_w \lesssim 602/600\,\mathrm{meV}$. Only within such a small range of the chemical potential, MF is possibly observed. The smaller the external magnetic field, the smaller the above window of chemical potential of nanowire for the Majorana phase. Therefore, the mismatch of the chemical potentials in nanowire and SC will prevent the Majorana topological phase. This may understand why the signature of zero-bias peak in the current hybrid nanowire systems is non-topological [14, 15, 31].

Based on the above facts, there are some remarks for observing MF in experiments. (i) The magnetic field should be modest strength. An excessively large magnetic field will inhibit the superconducting gap [32–35], while a smaller magnetic field will require higher control accuracy of the chemical potential in nanowire and SC. (ii) The mismatch of chemical potential highlighted above requires that the chemical potential in the nanowire is adjusted in an extensive range to achieve the Majorana phase, which may produce the current between the nanowire and SC due to the drastic change of their potential difference. This is not conducive to observe MF. (iii) The instability of (especially the larger) superconducting chemical potential as other experimental parameters are adjusted also destroys the signature of MF. Therefore, it is almost impossible to observe the prominent MF signature robust to the large-range external magnetic field and the gate voltage in the huge mismatch of chemical potential.

Conclusion.—We define the dressed Majorana fermion (DMF) in any tunneling strength and magnetic field for the hybrid nanowire. Under the open boundary, the edge state of DMF is localized at both ends of the nanowire and superconductor (SC). And we obtain the general topological phase of DMF, which is determined by the magnetic field and the chemical potential in the nanowire and SC. We clarify the validity of the low-energy phase diagram. Namely, it is only an approximate result of the DMF phase in the weak tunneling scheme. We also point out that in the mainstream hybrid InSb/As-Al system, the mismatch in chemical potential between nanowire and SC makes MF challenging to observe [4, 13–15].

Our theory provides a new method to define MF in the hybrid system analytically. Namely, we treat the quasi-excitation in the nanowire and superconductor equally instead of treating SC as an environment to provide the proximity effect for the nanowire. Therefore, such a definition of DMF is general and applicable to any parameters of any chosen nanowire and SC materials, including the strong tunneling strength and magnetic field.

Note that although s-wave SC is described by a one-dimensional lattice model in the above discussion, such a method of defining Majorana fermion can be generalized to more hybrid systems, such as the two-dimensional multi-band nanowire coupled to superconducting shell [9, 23, 36, 37], and two-dimensional topological insulator-superconductor system [38–40].

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[11] See supplemental material for details: The approximate conditions of low-energy effective theory and the phase diagram determined by it in Sec. I; The definition of the dressed Majorana fermion and the conditions under which it exists in Sec. II A; The topological phase of dressed Majorana fermion in Sec. II B ; Proof that the dressed Majorana fermion results in a zero-bias peak Sec. II C.

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