Midgap States and Generalized Supersymmetry in Semi-infinite Nanowires

Bor-Luen Huang¹, Shin-Tza Wu², and Chung-Yu Mou¹,³

¹. Department of Physics, National Tsing Hua University, Hsinchu 30043, Taiwan
². Department of Physics, National Chung-Cheng University, Chiayi 621, Taiwan
³. National Center for Theoretical Sciences, P.O.Box 2-131, Hsinchu, Taiwan

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Edge states of semi-infinite nanowires in tight binding limit are examined. We argue that understanding these edge states provides a pathway to generic comprehension of surface states in many semi-infinite physical systems. It is shown that the edge states occur within the gaps of the corresponding bulk spectrum (thus also called the midgap states). More importantly, we show that the presence of these midgap states reflects an underlying generalized supersymmetry. This supersymmetric structure is a generalized rotational symmetry among sublattices and results in a universal tendency: all midgap states tend to vanish with periods commensurate with the underlying lattice. Based on our formulation, we propose a structure with superlattice in hopping to control the number of localized electronic states occurring at the ends of the nanowires. Other implications are also discussed. In particular, it is shown that the ordinarily recognized impurity states can be viewed as disguised midgap states.

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I. INTRODUCTION

The one-dimensional (1D) wire has been of great theoretical and experimental interests in the past. This is because of not only the wide variety of fascinating phenomena it exhibits, but also the testing grounds it offers for ideas that may become applicable in higher dimensions. In practice, 1D wires need not be physically one dimension. It may result from projection after a partial Fourier transformation from higher dimensional models. For instance, a superlattice structure can be reduced to an equivalent 1D structure after a partial Fourier transformation along the direction normal to the layers. Similar examples include d-wave superconductors, graphite sheet, and many other systems. Therefore, understanding the 1D wire is an ideal first step toward the understanding of any higher dimensional problems. Further boost for studying 1D wires comes from recent advances achieved in nanotechnology. Here the feasibility for bottom-up assembly of single nanowires has made direct investigation of finite 1D wires possible. Nevertheless, conventional studies of the 1D wire have mostly been focused on its bulk properties, whereas assembled nanowires can only have finite lengths and must terminate at some sites (the ends, or the edges). It is therefore desirable to reconsider the effects of the ends to the properties of the nanowires.

The commonly recognized edge (or surface) effects in the physics of nanostructures are concerned with the large volume fraction of the boundaries. However, from either fundamental or practical viewpoints, the possible occurrence of edge modes and its influences on the properties of the system poses a much more interesting problem. For example, when applying carbon nanotubes as emitters for screen displays, the occurrence of edge states may change the density of electrons at the edge and thus affects the threshold working potential. It is therefore of great technological interest if one could devise a way to engineer the number of edge states. From the fundamental viewpoint, the elegant role of edge excitations in the physics of Quantum Hall systems is a well known example that illustrates the importance of edge states. Generally speaking, the edge states occur within the gap of the bulk energy spectrum and are called the midgap states. The existence of these states causes anomalous properties near the end which can manifest in tunneling measurements. A recently discovered example is the zero-bias conductance peak observed in the measurement of the metal-d-wave superconductor junctions. When electron-electron interactions are present, as occurs for an externally-implemented magnetic impurity, "intrinsic" Kondo effects may also arise due to these localized states, causing zero-bias anomaly near the Fermi energies. Furthermore, if the system is finite, coupling between edge states can not be neglected. An example is the anomalous paramagnetic behavior observed in carbon nanoribbons, where we have recently shown that there are residual antiferromagnetic couplings between edge spins in this system. All these examples clearly illustrate the important role of edge states in the physics and applications of nanostructures.

In previous work, applying the Green’s function approach, we have shown that broken reflection symmetry is a necessary condition for the occurrence of edge states, and the energies of edge states are the roots to the Green’s functions. In this work, resorting to the supersymmetric method, we further develop a systematic way to determine the wavefunctions and the precise energies of the edge states.

Conventionally, the usage of the supersymmetric method in the condensed matter physics has been focused on applying the supersymmetry (SUSY) quantum field theory to disorder systems. The application of the corresponding (0+1) dimensional limit - the SUSY quan-
quantum mechanics, however, is quite limited. Nevertheless, it has been realized that the zero-bias anomaly in d-wave superconductors is closely related with the SUSY quantum mechanics. These studies, however, are done in in the continuum limit, using the semi-classical approximation, while the more relevant limit for high Tc superconductors and many other systems is the tight binding limit. Furthermore, the zero-energy state was the primary focus, while not all the states localized at the edge have zero energy. It is therefore important to see if the idea of SUSY quantum mechanics can be generalized to understand the finite-energy midgap states, in particular those in the discrete condensed matter systems, as well.

In this work, we shall show that indeed, this is possible. We shall first show that the semi-infinite tight-binding d-wave superconductors belongs to a more general class, the bipartite system, and which can be well described by the conventional SUSY quantum mechanics. Here the supersymmetric partners are two sublattices of the same system and the SUSY is characterized by a hermitian supercharge $Q$ and the SUSY Hamiltonian $H^S = \{Q, Q\}/2$ with $[H^S, Q] = 0$. For bipartite systems with nearest neighbor hoppings, $Q$ is identical to the physical Hamiltonian ($= H_2$) and hence $H^S$ is a quadratic functional of $H_2$. Furthermore, the zero-energy state is annihilated by the supercharge, which then constitutes one of the conditions for determining the zero-energy state; while the other condition is to require it to decay from the edge. It is found that this conventional SUSY quantum mechanics can be appropriately extended to describe the semi-infinite $p$-partite systems with nearest neighbor hoppings. First, when $p \geq 3$, the original supercharge splits into two: In addition to the physical Hamiltonian $H_2$, a second supercharge $Q_p$ can be formed. They both commute with the SUSY Hamiltonian $H_S$. Furthermore, only when $p = 2$, $H_S \approx H^S$ is a quadratic functional of $H_2$. In general, $H_S$ is a polynomial functional of $H_2$. This is a reminiscence of the fractional SUSY quantum mechanics in which the SUSY Hamiltonian is generalized to be integer power of the supercharge. Nevertheless, our model is different and provides more realistic generalization of the conventional SUSY. The upshot of this generalization shows that, in addition to the zero-energy state, all the midgap states, including finite energy ones, are annihilated by the supercharge $Q_p$. The wavefunctions of the midgap states thus obtained tend to vanish with the same period commensurate with $p$: $\Psi_0 \approx (\cdots, 0, \cdots, 0, \cdots, 0, \cdots)$. These zeroes cut the original Hamiltonian into smaller ones so that the energies of the midgap states are determined by the eigenvalues of the Hamiltonian within each period. As a result, the matrix for determining the energies of midgap states is of size much smaller than the size of the original Hamiltonian. This reduction in matrix size heavily reduces the computation for determining the occurrence of the midgap states and provides a way to control the occurrence of the midgap states. As an application, we propose a structure with superlattice in hopping with period $p$ to control the number of localized electronic states occurring at the end of nanowires. In that case, the number of edge states is simply $p - 1$.

As the period $p$ goes to infinity, the ensemble of configurations of hopping forms a semi-infinite disorder chain. This limit has been extensively investigated during the past since Dyson’s seminal work in which it was pointed out that the average density of state (DOS) is enhanced at zero energy. From our point of view, this enhancement also reflects that the system has high probabilities to take the above-mentioned form for the ground state. The presence of the boundary breaks translational invariance. Thus, unlike the bulk case where the DOS at zero energy has no spatial dependence, the enhance DOS at zero energy for semi-infinite disordered wires has the largest amplitude near the edge. Even for slight disorders, the effects of enhanced DOS at zero-energy are still observable. This offers a possible explanation for many unexpected zero-bias anomalies observed in tunneling experiments because, unless extremely carefully controlled, junction qualities are usually rather poor and disorders can easily set in near the junctions.

Other implications and extensions of our generalized SUSY quantum mechanics will also be discussed. In particular, we shall demonstrate that by appropriate mappings, the ordinarily recognized impurity state can be viewed as a disguised midgap state. Such mapping provides a simple way to construct the impurity wavefunction and the corresponding energy. In addition to this application, possible extension to include the electron-electron interactions will also be discussed at the end of this paper.

This paper is organized as follows. In Sec. II, we lay down the basic tight binding model considered in this work and illustrate the SUSY quantum mechanics for the bipartite systems. In Sec. III, we generalize the supercharge and supersymmetric Hamiltonian to the $p$-partite systems and discuss the disorder limit. We also point it out of how to engineer the number of edge states by using a superlattice structure. By applying the SUSY quantum mechanics, we illustrate in Sec. IV how an impurity state can be viewed as a midgap state. In Sec. V we conclude and discuss possible generalization to include electron-electron interactions. Appendices A and B are devoted to technical details of superalgebra and computation of commutators.

II. THEORETICAL FORMULATION AND SUPERSYMMETRIC QUANTUM MECHANICS

We start by considering the 1D atomic chain as illustrated in Fig. II. This is the most general 1D atomic chain in which reflection symmetry with respect to the edge point is broken and, consequently, edge states might arise. In the tight-binding limit, we consider the follow-
ing Hamiltonian to model this system:

\[
H_p = \sum_{i=1}^{\infty} t_i c_i^\dagger c_{i+1} + h.c. + v_i c_i^\dagger c_i.
\]  

Here the subscript \(p\) indicates the period of the lattice and \(i\) is the site index; \(t_i\) is the hopping amplitude between site \(i\) and its nearest neighbors, \(c_i (c_i^\dagger)\) is the electron annihilation (creation) operator, and \(v_i\) is the local potential at site \(i\). We shall assume that both \(t_i\) and \(v_i\) are periodic with period \(p\), namely \(t_{p+i} = t_i\) and \(v_{p+i} = v_i\). In real systems, this Hamiltonian may correspond to an assembly of \(p\) different atoms repeatedly arranged into a line (see Fig. 1). For wires composed of atoms of a single species, \(H_p\) may describe systems which exhibit density-wave order. This includes polyacetylene\(^\dagger\), which has a dimerized structure and corresponds to \(p = 2\), and polymers with higher commensurability charge density waves\(^\dagger\). In the following, we shall call \(p = 2\) the \(t_1\)-\(t_2\) model, and similarly for models with higher periods. As mentioned in the introduction, \(H_p\) may also represent the reduced model of a higher dimensional structure after partial Fourier transformation. For example, for a semi-infinite graphite sheet with zig-zag edge, since the system is translationally invariant along the edge, a partial Fourier transformation can be applied along this direction, leading to an effective 1D model. In this case, it is identical to the \(t_1\)-\(t_2\) model except that now \(t_1\) and \(t_2\) are \(k\)-dependent:\(^\dagger\) \(t_1 = 2t_0 \cos(\sqrt{3}k_ya/2), t_2 = t_0\), where \(a\) is the lattice constant and \(k_y\) represents the Fourier mode. This approach has been successfully applied to understand the anomalous properties near the edge in carbon ribbons.\(^\dagger\) As a final example, we note that the operator \(c_i\) in \(H_p\) needs not be restricted to be the electron annihilation operator. For example, after applying the Jordan-Wigner transformation, one can map a 1D quantum XY spin chain to a 1D model described by \(H_p\). Specifically, we have \(t_i\) replaced by the exchange coupling for nearest neighbors \(J_i/2\), and \(v_i\) replaced by the local magnetic field \(h_i\). It is clear from these examples that \(H_p\) is quite general and captures the physics of many interesting systems.

To investigate the behavior of \(H_p\) near the edge, as a first step, we calculate the local density of states at the end point using the generalized method of image developed in Ref. 3. Fig. 2 shows typical local density of states at the end point for small periods. The parameters are carefully chosen so that all possible midgap states are present. In particular, we have set \(v_i = 0\), which amounts to choosing the energy zero as the origin. These results show that midgap states are indeed the most prominent features at the end point. To understand how the midgap states arise, we first investigate the \(t_1\)-\(t_2\) model with \(v_1 = 0\) in details. In this case, since the lattice is bipartite, it is convenient to distinguish the amplitudes at the odd and the even sites by writing the wavefunction as \(\Psi = (\phi_o, \phi_e)\). The Hamiltonian then becomes

\[
H_2 = \begin{pmatrix} 0 & A \\ A^\dagger & 0 \end{pmatrix}. \tag{2}
\]

Here \(0\) is the null matrix and \(A\) is a non-Hermitian matrix

\[
A = \begin{pmatrix} t_1 & 0 & 0 & \cdots \\ t_2 & t_1 & 0 & \cdots \\ 0 & t_2 & t_1 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \tag{3}
\]

It is interesting to note that the adjoint of \(A\) satisfies

\[
A^\dagger = \varepsilon A \varepsilon \quad \text{with} \quad \varepsilon = \begin{pmatrix} 0 & 0 & \cdots & 1 \\ 0 & \cdots & 1 & 0 \\ \vdots & \vdots & \vdots & \ddots \\ 1 & 0 & \cdots & 0 \end{pmatrix}. \tag{4}
\]
Here the operator $\varepsilon$ effectively reflects the wavefunction with respect to the mid point of the lattice.

In the case of infinite chains, it is not hard to check that the corresponding matrices $\mathbf{A}$ and $\mathbf{A}^\dagger$ commute with each other and hence can be diagonalized simultaneously in Fourier space. For semi-infinite chains, however, $\mathbf{A}$ and $\mathbf{A}^\dagger$ do not commute and the spectrum of the $t_1$-$t_2$ model can be best understood in terms of the supersymmetric quantum mechanics. For this purpose, we first identify $H_2$ as the supercharge $Q_2$, which connects even and odd sites. The block-diagonal matrix $(H_2)^2 \equiv (H^S)$ is then identified as (up to a factor of two) the corresponding supersymmetric Hamiltonian, whose diagonal blocks $H_0^S \equiv \mathbf{A}\mathbf{A}^\dagger$ and $H_e^S \equiv \mathbf{A}^\dagger\mathbf{A}$ are, respectively, the effective Hamiltonians for the odd and the even sites. Note that because $\mathbf{A}$ and $\mathbf{A}^\dagger$ do not commute, $H_0^S \neq H_e^S$.

We will show below that the difference between $H_0^S$ and $H_e^S$ is the origin of the midgap states. Obviously, $H^S$ is positive definite with the possibility when its spectrum touches zero. When the later happens, the ground state $\phi_e$ of $H_e^S$ vanishes, the ground state wavefunctions $\phi_o$ and $\phi_e \equiv (\phi_o, \phi_e)$ have to be the zero-energy eigenfunction of $\mathbf{A}$ and $\mathbf{A}^\dagger$, i.e. $\mathbf{A}\phi_o = 0$ and $\mathbf{A}^\dagger\phi_e = 0$. In other words, the supercharge annihilates the ground state wavefunction $\Psi_0$

$$Q_2\Psi_0 = H_2\Psi_0 = 0.$$  \hspace{1cm} (5)

Clearly, in this case, the system has good supersymmetry because the ground state is invariant under “rotation” between even and odd sites:

$$e^{i\theta Q_2}\Psi_0 = \Psi_0, \hspace{1cm} \text{where } \theta \text{ is any real number.}$$  \hspace{1cm} (6)

where $\theta$ is any real number. The non-Hermiticity of $\mathbf{A}$ and $\mathbf{A}^\dagger$ implies that forward and backward hopping amplitudes between two sites are different, and hence the eigenfunctions have to either grow or decay from the end point. Obviously, because of the relation $\mathbf{A}^\dagger = e^{i\mathbf{A}\varepsilon}$, any non-trivial eigenfunctions satisfy $\phi_e = e^{i\varepsilon}\phi_o$. Therefore, if $\phi_o$ decays from the edge, $\phi_e$ must grow from the edge (vice versa). For semi-infinite chains, only the even sites are connected with the hard-wall boundary point. Thus $\phi_e$ is forced to vanish while $\phi_o$ decays into the bulk, so that $\Psi_0 = (\phi_o, 0)$. Note that the other possible state $\Psi_0 = (0, \phi_e)$ resides on the other end of the chain and is pushed to infinity. Therefore, overall speaking, there is only half a chance for the existence of the ground state $(\phi_o, 0)$. This also reflects in the hopping strength difference. Indeed, we find that $\phi_o$ decays only when $t_1 < t_2$. In this case, $H_0^S$ has a non-trivial zero energy eigenfunction, while $H_e^S$ does not. Therefore, the system has good supersymmetry with the ground state $\Psi_0$ being a localized state. For finite energies, however, $\phi_o$ and $\phi_e$ need not be eigenfunctions of $\mathbf{A}$ and $\mathbf{A}^\dagger$. Nevertheless, the supersymmetry allows a simple and elegant way to find the whole spectrum for the case $p = 2$. This is because $H_0^S$ has the exact form as $H_1$ ($p = 1$) with $t_1 = t_1t_2$ and $v_i = (t_1^2 + t_2^2)$. Since this is just the ordinary uniform hopping model, one can easily write down the eigenstate: $\phi_e(n) = \sin 2nk$. The wavefunction at odd site can be then found by using the supercharge operator. We find that $\phi_o = \mathbf{A}\phi_e/E$ with $E$ being the spectrum of $H_2$ which satisfies $E^2 = t_1^2 + t_2^2 + 2t_1t_2\cos 2k$. Since $E^2 \geq (t_1 - t_2)^2$, an energy gap opens up around $E = 0$ when $t_1 \neq t_2$. In the case of $t_1 < t_2$, the ground state $\Psi_0$ then arises as a midgap state. Note that $H_o^S$ is almost identical to $H_e^S$ except for the potential energy $v_1 = t_1^2$ at the end point; the deficit energy $t_2^2$ is entirely due to the missing bond cut off by the boundary. We will elaborate on this in Sec. IV.

We now address the effects of the potential $v_i$. For $p = 2$, it is convenient to denote the potentials over the even sites $v_o$ and the odd sites $v_o$. This decomposition, however, renders the particle-hole symmetry invalid at the level of the supercharge $H_2$. Nonetheless, the spectrum $(E)$ of $H_2$ can be mapped to the original spectrum of $H^S$ with $v_i = 0$ ($E^S_0$). For $E^S_0 \neq 0$ this mapping is given by $E^S_0 = (E - v_o)(E - v_o)$, while for $E^S_0 = 0$, since $v_o = 0$ still holds, one has $E = v_o$. Hence even though the physical spectrum $E$ may have no particle-hole symmetry, after appropriate transformations, the symmetric structure can be restored in $E^S_0$; in particular, the midgap state survives as clearly demonstrated in Fig. 6. For higher periods, the same manipulations as above can lead to similar conclusions. Therefore, unless explicitly needed, we shall ignore $v_i$ in the following.

Let us now apply the supersymmetric method to semi-infinite superconductors. After partial Fourier transformation along the interface, the problem becomes 1D superconductors with an end point. In this case, it is convenient to write the wavefunction by $\Psi = (u, v)$ with $u = (u_1, u_2, u_3, \cdots)$ being particle-like and $v = (v_1, v_2, v_3, \cdots)$ being hole-like wavefunctions. The reduced mean-field

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig3.png}
\caption{The effect of the potential is to break the particle-hole symmetry so that two side bands are distorted. However, the midgap state is not changed if $v_o = 0$. The parameters are: $t_1 = 0.7$ and $t_2 = 2.0$. For solid line, $v_o = 0, v_e = 0$, while for dash line $v_o = 0, v_e = 0.5$.}
\end{figure}
(BCS) Hamiltonian is Dirac-like\(^2\) and can be generally written as
\[
H_{BCS} = \begin{pmatrix} M & Q \\ Q & -M \end{pmatrix},
\]
where \(M\) corresponds to the reduced 1D Hamiltonian for particles and \(Q\) is essentially the pairing potential. One can also rewrite \(H_{BCS} = M \otimes \sigma_x + Q \otimes \sigma_z\), and treat this problem as a spin in the “magnetic field” \((Q, 0, M)\) pointing in the \(x - z\) plane. This analogy suggests that it is possible to rotate the magnetic field to the \(x - y\) plane. Indeed, this can be achieved by a rotation of \(2\pi/3\) with respect to the axis \((1, 1, 1)\). The transformation matrix\(^2\)
is
\[
U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix},
\]
where \(i\) and \(1\) are semi-infinite matrices. The rotated Hamiltonian then takes the form of a supercharge like \(H_2\)
\[
H'_{BCS} = U^\dagger H_{BCS} U = \begin{pmatrix} 0 & M - iQ \\ M + iQ & 0 \end{pmatrix}.
\]
The wavefunction is rotated accordingly: \(\Psi' = U^\dagger \Psi\). Therefore, in the supersymmetric form, particles and holes are mixed. As an illustration, we consider the mean-field Hamiltonian for \(d\)-wave superconductors
\[
H_R = -\sum_{\langle ij \rangle, \sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + \Delta_{ij}(c_{i\uparrow}^\dagger c_{j\downarrow} - c_{i\downarrow} c_{j\uparrow}) + h.c.
\]
where \(\langle ij \rangle\) denotes the nearest-neighbor bonds, \(t_{ij}\) and \(\Delta_{ij}\) are, respectively, the corresponding hopping and \(d\)-wave pairing amplitudes. For the \((1,1,0)\) interface, after Fourier transformation along the interface (which is taken to be the \(y\) direction), we obtain\(^2\)
\[
A = M - iQ = \begin{pmatrix} -\mu & -t + d & 0 & \cdots \\ -t - d & -\mu & -t + d & \cdots \\ -t & t & \mu & \cdots \\ 0 & -t & t & \mu & \cdots \end{pmatrix},
\]
where \(\mu\) is the chemical potential, \(t = 2t_0 \cos(k_y a/\sqrt{2})\) and \(d = 2\Delta_0 \sin(k_y a/\sqrt{2})\). The model for tight-binding \(d\)-wave superconductors is unique in the sense that the non-Hermiticity of \(A\) and \(A^\dagger\) can be removed by a gauge transformation. For this purpose, we write \(t - d = i e^{-g}\) and \(t + d = i e^{+g}\) with \(g = \sqrt{t^2 - d^2}\) and \(e^{2g} = (t - d)/(t + d)\). The eigenfunction \(\Psi_E\) of \(A\) is thus the gauge transformation of the eigenfunction \(\phi_E\) of
\[
A_0 = \begin{pmatrix} -\mu & -i & 0 & \cdots \\ -i & -\mu & -i & \cdots \\ 0 & -i & -\mu & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{pmatrix}.
\]
Specifically, we obtain \(\Psi_E(n) = e^{-ng} \phi_E\) (for \(A^\dagger\), one obtains \(\Psi_E(n) = e^{ng} \phi_E\)). Furthermore, \(\Psi_E\) and \(\phi_E\) have the same eigenvalue \(E\). This implies that the calculation of the zero mode is related to the spectrum of \(A_0\). If we restrict our discussion to the propagating modes, the spectrum of \(A_0\) is simply the ordinary cosine band. We find that when \(-2\sqrt{t^2 - d^2} < \mu < 2\sqrt{t^2 - d^2}\) is satisfied, \(A\) and \(A^\dagger\) can, respectively, support zero-modes of the form \((0, e^{-ng} \phi_{E=0})\) and \((e^{ng} \phi_{E=0}, 0)\). In this case, the ground state of \(H^S\) is selected by the sign of \(g\), and thus the zero-energy midgap state is given by
\[
u(n) = \frac{1}{\sqrt{2}} \left( \frac{t - |d|}{t + |d|} \right)^{n/2} \sin(k_F n a),
\]
\[
u(n) = \text{sign}(d) \frac{i}{\sqrt{2}} \left( \frac{t - |d|}{t + |d|} \right)^{n/2} \sin(k_F n a).
\]
Here \(k_F\) is determined by \(-2\sqrt{t^2 - d^2} \cos(k_F a) = \mu\) and depends on \(k_y\); therefore, even though the midgap states for different \(k_y\)’s have the same zero energy, their wavefunctions have \(k_y\) dependence. Note that for demonstration, we have only considered the case when \(k_F\) is real. Complete solutions, however, require to include the situation when \(k_F\) is complex. In both cases, the supersymmetry structure enables one to write down the explicit form of the zero-energy mode near the interface \((1,1,0)\).

III. GENERALIZED SUPERCHARGE AND ITS CONSEQUENCES

We now generalize the above results to higher periods \(p \geq 3\). It is useful to decompose the wavefunction as \(\Psi = (\phi_1, \phi_2, \cdots, \phi_p)\), where \(\phi_i\) denotes the sub-wavefunction formed by \(\{\Psi(kp + n); k = 0, 1, 2, \ldots\}\). The Hamiltonian is then cast in the form
\[
H_p = \begin{pmatrix} 0 & A_{12} & 0 & \cdots & A_{1p} \\ A_{12}^\dagger & 0 & A_{23} & \cdots & 0 \\ 0 & A_{23}^\dagger & 0 & \cdots & \vdots \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ A_{1p} & 0 & \cdots & A_{p-1,p} & 0 \end{pmatrix}.
\]
Again, here \(0\) and \(A_{nm}\) are block matrices; for all \(n \neq p\), \(A_{nm} = t_n 1\) are diagonal, while for \((m, n) = (1, p)\)
\[
A_{1p} = \begin{pmatrix} 0 & 0 & 0 & \cdots \\ t_p & 0 & 0 & \cdots \\ 0 & t_p & 0 & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{pmatrix}.
\]
To understand what happens for the semi-infinite chain, it is useful to start from the infinite chain with Hamiltonian \(H_p^\infty\). In this case, \(H_p^\infty\) also takes the same form except that \(A_{nm}\) are further extended to \(i = -\infty\). If we remove the hopping strength \(t_0\) and combine the remaining \(A_{nm}\) with \(A_{nm}^\dagger\) into \(Q_{nm}\) for all \(m\) and \(n\) pairs, \(Q_{nm}\) form a superalgebra if modulo \(p\) is performed (see Appendix A for mathematical details). The energy bands of \(H_p^\infty\) are determined by
where $E$ is the energy and $k$ is the Fourier mode. In general, there have at most $p$ energy bands. However, since in the polynomial $P(E, k)$, $(-1)^p + 1 t_1 t_2 t_3 \cdots t_p \cos (pk)$ is the only term that depends on $k$, the function $P(E, k) - (-1)^p + 1 t_1 t_2 t_3 \cdots t_p \cos (pk)$ maps $p$ bands into one single band: $2 t_1 t_2 t_3 \cdots t_p \cos (pk)$. This important observation implies that when $H_p = H_p^\infty$, the operator $H_S = P(H_p, 0) - (-1)^p + 1 t_1 t_2 t_3 \cdots t_p$ is block-diagonal [there are $p$ blocks with one for each $\phi_i$, see Eqs. (8) and (12)] and folds the spectrum of $H_p^\infty$ into one single band. Therefore, $H_S$ is similar to the supersymmetry Hamiltonian $H_S$. Indeed, for $p = 2$, we find $H_S = H_2^2 - (t_1^2 + t_2^2)$ which is essentially $H_S^\infty$.

For infinite chains, $H_S$ is highly symmetric. In fact, it commutes with all $Q_{mn}$. This reflects that it is symmetric under the permutation of $n$ and $m$ but it is more than that because any linear combination of $\sum m_n Q_{mn}$ also commutes with $H_S$. For semi-infinite chains, however, the above symmetry is broken: Not all $Q_{mn}$ commute with $H_S$. Physically, this is obvious because now $\phi_p$ is special and is the only component that connects with the boundary point $i = 0$ directly. As a result, $H_S$ is not completely block-diagonalized. In fact, because even for the infinite chains, $\phi_p(n) = \sin (k n a_p)$ is a solution for the $p$th block and it satisfies the hard-wall boundary condition at $i = 0$, the $p$th block is not affected. Therefore, there are only two blocks: one for the space formed by $\phi_p$; the other mixes $\phi_1, \phi_2, \ldots$ and $\phi_{p-1}$. This is demonstrated in Eq. (18) where we denote the block Hamiltonians by $H_-^+$ and $H_-^-$.

Clearly, the $t_1$-$t_2$ model is special because $H_+^+$ and $H_-^-$ are of the same size so that $H_S$ is completely block-diagonal. This is where the usual SUSY quantum mechanics applies. For $p \geq 3$, $H_+^+$ and $H_-^-$ are not of the same size, a generalization of SUSY quantum mechanics is needed. First, it is important to see if one can find an operator, similar to the supercharge $Q_2$, that commutes with $H_S$, $H_p$ is obviously a solution because $H_2 = Q_2$. However, in analogy to the case of $p = 2$, a second supercharge by collecting all block matrices in $H_p$ that connects $\phi_p$ to other components can be formed:

$$Q_p = \begin{pmatrix} 0 & 0 & \cdots & A_{1p} \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \cdots \\ A_{1p} & 0 & \cdots & A_{p-1p} \end{pmatrix} \text{ for } p \geq 3. \quad (18)$$

Note that the above definition can also include $p = 2$. In that case, one squeezes the block $A_{1p}$ into $A_{12}$ to obtain the form of $H_2$ in Eq. (6). Because $A_{12} = t_1 1$ and $A_{1p}$ is given by Eq. (10) with $t_p$ being replaced by $t_2$, adding $A_{12}$ and $A_{1p}$ reproduces $A$ defined in Eq. (6) precisely. Hence Eq. (18) can be regarded as an "analytical continuation" of $Q_2$ to $p \geq 3$. Furthermore, as shown in Appendix B, $[H_S, Q_p] = 0$ is satisfied, thus $Q_p$ provides a faithful generalization of $Q_2$. It coincides with $H_p$ only when $p = 2$. Note that from Appendix B, one can actually see that out of $Q_{mn}$ contained in $H_p, Q_p$ and $H_p$ (and their linear combinations) are the only two generators that commute with $H_S$ for general $p$.

Applying the condition that the supercharge annihilates midgap states $\Psi_0$, one finds that

$$\phi_p = 0 \quad \text{and} \quad A_{1p}^\dagger \phi_1 + A_{p-1p}^\dagger \phi_{p-1} = 0. \quad (19)$$

$\phi_p = 0$ implies that the wavefunction has the form $\Psi_0 \approx (\cdots, 0, \cdots)$ as pointed out earlier, while the second condition relates $\phi_{p-1}$ to $\phi_1$. It is important to realize that because $Q_p$ no longer coincides with $H_p$ for $p \geq 3$, $Q_p$ alone does not determine the energies and wavefunctions of the midgap states. Instead, because $Q_p \Psi_0 = 0$, the operator $H_p - Q_p$ determines the energies and further provides relations between $\phi_2, \cdots, \phi_{p-1}$ and $\phi_1$. This analysis shows that the energies $E_m$ of midgap states can be different from zero and must satisfy

$$\det \begin{pmatrix} -E_m & t_1 & 0 & \cdots & 0 \\ t_1 & -E_m & t_2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & -t_{p-2} & -E_m \end{pmatrix} = 0. \quad (20)$$

Therefore, there are at most $p - 1$ midgap states. To stabilize the midgap states, one further requires $\Psi_0$ to decay away from the edge. In the case of $p = 2$, this results in the condition $t_1 < t_2$. For $p = 3$, one first obtains from Eq. (20) $E_m = t_1$ and $\phi_1 = \pm \phi_2$, which, when combined with Eq. (19), results in $\Psi(3k + n) = \pm t_3/t_2 \Psi(3k - 3 + n)$. Thus midgap states exit only when $t_2 < t_3$. In general, one needs to relate $\phi_{p-1}$ to $\phi_1$. This further reduces the matrix in Eq. (20) and by defining the $(p - 2) \times (p - 2)$ matrix

$$h = \begin{pmatrix} -E_m & t_1 & 0 & \cdots & 0 \\ t_1 & -E_m & t_2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & -t_{p-3} & -E_m \end{pmatrix}, \quad (21)$$
we find that $\psi_1 = - t_{p-2} \psi_{p-1}$. When combined with Eq. (19), we obtain $\psi_1 = t_{p-2} t_p/\psi_{p-1} \psi_{p+1}$. Hence the midgap state with energy $E_m$ exists only when $t_{p-2} t_p > t_p$. Note that for higher periods, commensurate structures may appear in sublattices. These structures resemble the SUSY structures in lower periods. For example, when $p = 4$, there are at most three midgap states at $E_m = 0, \pm \sqrt{t_1^2 + t_2^2}$. In this case, the Hamiltonian $H_1^2$ is already block diagonal in even and odd sites. For even sites, $H_1^2$ is period of two and belongs to $H_2$ with $t_1' = t_1 t_4, t_2' = t_2 t_3, \mu_1' = t_1^2 + t_2^2$, and $\mu_2' = t_1^2 + t_2^2$ with the midgap energy given by $E_m = \mu_1' = t_1^2 + t_2^2$. It is clear that $E_m$ is precisely the square of the ground state wavefunction discussed above. First, because the boundary breaks the translational invariance, if one decomposes the wavefunction as $\Psi = (\phi_o, \phi_e)$, it is still true that only the even sites are connected to the hard-wall boundary point. In this case, for any set of $\{t_i\}$, the non-Hermitian matrix $A$ that enters Eq. (2) is given by

$$A = \begin{pmatrix} t_1 & 0 & 0 & \cdots \\ t_2 & t_3 & 0 & \cdots \\ 0 & t_4 & t_5 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \quad (22)$$

For the zero-energy state, because $A\phi_e = 0$, it is easy to see that $\phi_e = 0$: while the wavefunction at odd sites is determined by $A^\dagger \phi_o = 0$. If we set $\psi_1^2 = 1$, the wavefunction at site $2N + 1$ is given by $\Psi_0^{2N+1} = (t_1 t_3 t_5 \cdots t_{2N-1})/(t_2 t_4 t_6 \cdots t_{2N})$. Let $x_i \equiv [t_{2i-1}/t_{2i}]$, then $\ln \left| \Psi_0^{2N+1} \right| \approx \sum_{i=1}^{N} \ln x_i$. Clearly, because $\ln \left| \Psi_0^{2N+1} \right| \approx N \ln x$, the logarithm of the wavefunction at odd sites behaves effectively as a random walker. Since a random walker has high probability to go to $\pm \infty$, $\psi_0$ has high probability of decaying to zero far from the edge and becomes a localized zero-energy mode. This analogy leads to $\langle (\ln |\Psi_0^{2N+1}|)^2 \rangle = \sqrt{N} \sigma$ with $\sigma$ being the standard deviation of $\ln x$. In other words, $|\Psi_0^{2N+1}| \sim e^{\pm \sigma \sqrt{N}}$ where $\pm$ corresponds to states localized at either ends, respectively. We emphasize that this analysis indicates that only the standard deviation of $\ln x$ is relevant and there is no need for the assumption of Gaussian-type randomness, which is often invoked in previous works. Furthermore, the random-walk nature makes the zero-energy peak much more easily formed. This is illustrated in Fig. 4 where we show that even slight disorders near the edge may induce features resembling zero-bias peaks in tunneling measurements. In this case, the zero-energy state tends to decay from the edge but will not become

![Figure 4](image-url)
localized. Instead, after joining the non-disorder bulk region, it becomes a resonant state\(^ {20}\). Such phenomena may have already been seen in experiments\(^ {13}\).

### IV. IMPURITY STATES AS MIDGAP STATES

In this section, we demonstrate that in the supersymmetric approach the ordinarily recognized impurity states can be viewed as disguised midgap states. Let us consider the Goodwin model for the surface state\(^ {21}\). In this model, it was proposed that the surface state arises because the potential suddenly changes near the surface or the edge. In the tight binding limit, the Hamiltonian is given by\(^ {21}\)

\[
H_G = \sum_{i=1}^{\infty} t c_i^\dagger c_{i+1} + \text{h.c.} + U c_i^\dagger c_i. \tag{23}
\]

In other words, there is an impurity potential localized at the first site. It is commonly recognized that under appropriate condition, an impurity state (in this case, it is the Goodwin edge state) may arise and exhibit as an isolated line in the spectrum as illustrated in Fig.\( \text{fig:5} \)\( \text{a} \). Clearly, we see from Fig.\( \text{fig:5} \)\( \text{a} \) the spectrum with an impurity state is essentially the square of spectrum shown in Fig.\( \text{fig:5} \)\( \text{a} \), i.e., the spectrum with a midgap state.

To establish the relation described above, we go back to previous analysis on the \( t_1 - t_2 \) model. As is obvious, the spectrum of \( H^S \) (\( \equiv (H_G)^2 \)) is the square of that for \( H_G \), fulfilling the relation indicated in Fig.\( \text{fig:5} \)\( \text{a} \). It is hence useful and more transparent if we explicitly write down \( H^S \)

\[
H^S = (\begin{pmatrix} AA & 0 \\ 0 & A^\dagger A \end{pmatrix}). \tag{24}
\]

where

\[
H^S_o = AA\dagger = \begin{pmatrix} t_1^2 + t_2^2 & t_1 t_2 \\ t_1 t_2 & t_1^2 + t_2^2 \end{pmatrix}, \tag{25}
\]

is the effective Hamiltonian for the odd sites and

\[
H^S_e = A\dagger A = \begin{pmatrix} t_1^2 + t_2^2 & t_1 t_2 \\ t_1 t_2 & t_1^2 + t_2^2 \end{pmatrix}, \tag{26}
\]

is the effective Hamiltonian for the even sites. One sees that \( H^S_o \) and \( H^S_e \) differ by the potential at site \( 1 \). As mentioned, this is entirely due to the missing bond cut off by the boundary. On the other hand, even though \( H^S \) is block-diagonal, it does not imply even and odd sites are independently from each other. In fact, they are connected by the supercharge \( H_2 \). The point is that except for the zero energy which is an eigenvalue of \( H^S_o \), \( H^S_o \) and \( H^S_e \) share the same energy eigenvalue \( E^2 \) with \( E \) being the spectrum of \( H_2 \). The supersymmetric relation between even and odd sites enables one to solve the Goodwin model \( H_G \) as follows. One first rewrites

\[
H^S_o = \sum_{i=1}^{\infty} \left( t_1 t_2 c_i^\dagger c_{i+1} + \text{h.c.} + (t_1^2 + t_2^2) c_i^\dagger c_i \right) - t_2^2 c_1^\dagger c_1. \tag{27}
\]

Clearly, it shows that the effective Hamiltonian for the odd sites is equivalent to the Goodwin model with \( t = t_1 t_2, U = -t_2^2 \), and \( \mu = -(t_1^2 + t_2^2) \). The wavefunction of the midgap state on odd sites then become the wavefunction of the impurity state in the Goodwin model. Furthermore, the energy of the impurity state can be easily found to be \( E_{im} = -(t_1^2 + t_2^2) \). By solving \( t_1 \) and \( t_2 \) in terms of \( t \) and \( U \), we find \( E_{im} = U + t^2 / U \). Since the midgap states exist when \( |t_1| < |t_2| \), the impurity state appears only when \( |t| < |U| \) in consistent with the standard approach\(^ {21}\). The discussion above concerns with the case \( U < 0 \), hence the impurity energy resides on the left side (the solid line) in Fig.\( \text{fig:5} \)\( \text{b} \). For \( U > 0 \), the Goodwin model maps to \( -H^S_o \). One obtains the same expression for the impurity energy \( E_{im} = U + t^2 / U \) except that it resides on the right side (the dashed line) in Fig.\( \text{fig:5} \)\( \text{b} \).

In addition to the energy of the impurity states, the above analysis also implies that the entire spectrum is simply \( E_G = 2t \cos ka \). Furthermore, the supersymmetric relation between even and odd sites enables one to write down all wavefunctions for the Goodwin model explicitly. This is entirely due to the fact that the Hamiltonian of the supersymmetric partner to the Goodwin model is \( H^S \) which is a uniform hopping model. We obtain the wavefunction for the impurity state \( \Psi_G(n) = (t/U)^{n-1} \), while for the extended states, when \( U < 0 \),

\[
\Psi_G(n) = \frac{\sqrt{|U|} \sin nka + t/\sqrt{|U|} \sin(n - 1)ka}{E_k},
\]

with \( E_k = \pm \sqrt{|U| + t^2 / |U| + 2t \cos ka} \), and when \( U > 0 \),

\[
\Psi_G(n) = \frac{\sqrt{|U|} \sin nka - t/\sqrt{|U|} \sin(n - 1)ka}{E_k},
\]

with \( E_k = \pm \sqrt{|U| + t^2 / |U| - 2t \cos ka} \).
V. SUMMARY AND OUTLOOK

In summary, in this work we have shown that the properties of midgap states in semi-infinite 1D nanowires are dictated by a underlying discrete supersymmetry. This supersymmetric structure generalizes the ordinary supersymmetric quantum mechanics and offers a new point of view toward the origin of edge states. In the presence of hard-wall boundary condition (ψ = 0), the sublattice which directly connects to the hard-wall spans the null space of the supersymmetric ground state. As a consequence, the energies of the midgap states are determined by the eigenvalues of a reduced Hamiltonian, Eq. (20), whose size is much smaller than that of the original Hamiltonian. This reduction in matrix size significantly reduces the computation cost for determining the occurrence of the midgap states and offers a way to manipulate them. As an application, we investigate a structure with superlattice in hopping. In this case, the number of edge states is simply the period of the superlattice minus one. Therefore, changing the period offers a way to control the number of localized electronic states at the edge of the nanowires.

While so far in this work we have not considered electron-electron interactions, from adiabatic continuity, the results obtained here should still hold for cases when the electron-electron interactions are weak (so that quasi-particles are well defined). Moreover, if the “1D chain” results from the reduction of a higher dimensional structure where interactions are not important, then it is legitimate to ignore interactions in its effective 1D model. This is of course not correct in truly 1D atomic chains where it is known that interactions may dominate the physics and the quasi-particle pictures may fail. In this case, however, the states we obtain can be used as the basis to express the full Hamiltonian (with interactions) utilizing the relation \( c_{n}^{\dagger} = \psi_{0}(i)c_{0n}^{\dagger} + \sum_{E} \psi_{E}(i)c_{n}^{\dagger} \). When Coulomb interaction is included, it reduces to the Anderson model\(^{25}\) in which the edge state acts as an impurity state. The scattering of extended states by the edge states essentially causes the Kondo effect, resulting in the zero-bias peaks near the Fermi energies\(^{26}\). On the other hand, the interaction also correct the localized edge state. This is conventionally analyzed in the Fano-Anderson model\(^{25}\), in which it is known that as long as the new energy found remains inside the gap, the corresponding state is a localized state. In either of the above

\[ t_1t_2t_3t_4 \]
mentioned effects, our results will serve as useful inputs for attaining the final corrections.

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APPENDIX A: SUPERALGEBRA IN INFINITE $p$-PARTITE SYSTEMS

In this appendix, detailed superalgebra behind our generalized SUSY quantum mechanics is presented. For an infinite $p$-partite system, after modulo $p$, the system reduces to the set $\{1, 2, 3, \ldots, p\}$ with each number representing different sublattices. The reduced system is periodic with $p + 1$ being identified as $1$. In this periodic space, a set of generators $\{Q_{nm}; n, m = 1, 2, \ldots, p\}$ can be defined. Here $Q_{nm}$ are $p \times p$ Hermitian matrices whose only nonvanishing elements are in the $n$ th row and $m$ th column and the $m$ th row and $n$ th column. Note that $Q_{nn}$ has only one element, 1, in the $n$ th element along the diagonal. Obviously, when $n \neq m$, $Q_{nm}$ permutes the subwavefunctions $\phi_n$ and $\phi_m$; when combined with the hopping strength $t_{nm}$, in addition to permutation, it also rescales the wavefunctions. The Lie algebra formed by $Q_{nm}$ is a superalgebra because the anticommutator is necessary in order to be closed. The followings are nontrivial commutation relations: $\{Q_{ln}, Q_{nm}\} = Q_{ln}$ for $l \neq n$, $\{Q_{nm}, Q_{nm}\} = 2Q_{nn} + 2Q_{mm}$ for $n \neq m$, and $\{Q_{nn}, Q_{nm}\} = \delta_{nm}Q_n$; all the other commutators are zero. It is straightforward to check that for infinite systems, the SUSY Hamiltonian $H_S$ defined in Sec.III commutes with all $Q_{nm}$ even if the operation of modulo $p$ is not performed.

APPENDIX B: DERIVATION OF $[H_S, Q_p] = 0$

In this appendix, we outline the proof of $[H_S, Q_p] = 0$ for semi-infinite chains. We first write $Q_p = q_p + q_p^\dagger$ where $q_p$ is obtained by setting the last column in $Q_p$ to zero in Eq. (13). It is then suffice to prove $[H_S, q_p] = 0$. We note that $H_S$ has the following generic form

$$H_S = \begin{pmatrix} S_{11} & S_{12} & S_{13} & \cdots & 0 \\ S_{21} & S_{22} & S_{23} & \cdots & 0 \\ S_{31} & S_{32} & S_{33} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & S_{p-1,p-1} \end{pmatrix}.$$  

Here $H_S^0$ has the same form as that of the SUSY Hamiltonian for the corresponding infinite chain except that semi-infinite lattice points are removed, hence it is block-diagonal with the form: $(H_S^0)_{nm} = S_0\delta_{nm}$, where $n$ and $m$ are the block indices and

$$S_0 = \begin{pmatrix} 0 & 0 & 0 & \cdots & 0 \\ 0 & t & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \cdots & \vdots \\ 0 & 0 & \cdots & 0 \end{pmatrix}.$$  

and $t = t_1t_2t_3 \cdots t_p$. The block matrix $S_{nm}$ represents missing hopping amplitudes that goes between sublattices $m$ and $n$ due to the presence of the boundary point at $i = 0$. When computing $[H_S, q_p]$, one needs to compute $[S_0, A_{1p}^\dagger], A_{1p}^\dagger, S_{1m}$ and $A_{p-1,p}^\dagger, S_{p-1,m}$, thus only $S_{1m}$ and $S_{p-1,m}$ are needed. It is straightforward to show that $[S_0, A_{1p}^\dagger]$ has only one element $-t_p$, which is the 1st element along the diagonal ($\equiv \delta_{11}$). To obtain $S_{nm}$, one needs to multiply $H_p$ to itself by $n$ ($\leq p$) times because $H_S$ is a polynomial of $H_p$ containing at most $p$th power of $H_p$. Now the multiplication of $H_p$ to itself $n$ times effectively hops a particle $n$ times. Since $n \leq p$, only when the particle starts from the lattice points $1 \leq i \leq p - 1$, it will have chance to visit $i = 0$ and thus will have missing paths when $i = 0$ is removed. It implies that all $S_{nm}$ have only one element, which is also the 1st element along the diagonal. In addition, $S_{p-1,m} = 0$ for $m \geq 2$. As a result, by using Eq. (13), we obtain $A_{1p}^\dagger, S_{1m} = 0$ and hence we only need to compute $S_{p-1,1}$. Since the only missing path between the point 1 and the point $p - 1$ is $1 \rightarrow 0 \rightarrow 1 \rightarrow 2 \cdots \rightarrow p - 1$, we find that $S_{p-1,1} = -t_p^2t_1t_2 \cdots \delta_{11}$. This result, when combined with $[S_0, A_{1p}^\dagger] = -tt_p\delta_{11}$, we finally obtain $[H_S, Q_p] = 0$.

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19 This is equivalent to find the number of midgap states. Using $H^+$ and $H^-$, the number of midgap states can be formally counted. For instance, if one defines the index as $\text{ind}(z) \equiv \text{Tr} (\frac{H^+}{z-H^-} - \frac{H^-}{z-H^+}) + \text{Tr} (\frac{H^+}{z+H^-} - \frac{H^-}{z+H^+})$, $\text{ind}(0)$ gives the number of midgap states.

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