Evolution of quasiparticle edge states with Hubbard interaction in Rice-Mele chain

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We study the behavior of edge states in Rice-Mele model with Hubbard interaction, U, at half filling using density matrix renormalization group, exact diagonalization, and effective charge dynamics in Kumar representation. By increasing U for a fixed dimerization, δ, and staggered potential, V, we find the quasiparticle edge states in the charge gap to come down in energy from V in the absence of Hubbard interaction to zero energy at a critical interaction, $U_c \approx 2V$. This presents an uncommon situation where the competition between U and V leads to zero-energy edge states, although individually neither U nor V favors the edge states at zero energy. Upon increasing U further, the edge state energy starts increasing again until they are lost in the bulk. However, upon increasing U even further, these edge states reappear in the high-energy gap. So, with Hubbard interaction, the edge states in Rice-Mele chain transmigrate from the low- to high-energy charge gap.

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I. INTRODUCTION

The Rice-Mele model is an interesting problem of one-dimensional electrons, conceived as a generalization of the Su-Schrieffer-Heeger (SSH) model to diatomic polymers [1,2]. In its simplest form, it is a noninteracting tight-binding model with dimerized nearest-neighbor hopping (caused by static Peierls distortion [3]) and a staggered on-site potential. At half filling, the Rice-Mele model presents an example of a topological insulator with edge states. It has been quite fruitful in studying electric polarization and charge pumping [4–6], and also realized in optical lattices for its topological properties [7–10].

In the absence of staggered potential, i.e., in the SSH model, we recently investigated the behavior of edge states with interaction, and discovered that, by increasing the Hubbard interaction, the edge states transmigrate from the charge gap at low energies to the high-energy gap via an intermediate phase with no edge states [11]. How this transmigration of edge states would take effect in the presence of staggered potential is not clear and has not been investigated before. Previous works on Rice-Mele model with Hubbard interaction have explored different aspects of polarization [12–15] and Thouless pumping [16–19] for correlated electrons, but a basic understanding of the evolution of edge states with interaction is still found lacking. Therefore, in this paper, we study the half-filled Rice-Mele-Hubbard (RMH) model for its edge state behavior, as we did for the interacting SSH chain in Ref. [11].

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We perform this study by employing a combination of numerical and analytical methods involving density matrix renormalization group (DMRG), exact diagonalization (ED), and effective charge dynamics in Kumar representation [11,20]. In Sec. II, we carry out a purely numerical investigation of the edge states (arising due to dimerization, δ) of the charge quasiparticles in the RMH chain using DMRG and ED methods [21]. For a fixed staggered potential, V, by increasing the Hubbard interaction, U, we find the edge state energy to vary nonmonotonously from its noninteracting value, V. First, it decreases with U upto a critical value, $U_c \approx 2V$, where the edge state energy actually becomes zero. Thereafter, it starts increasing with U, and the edge states undergo transmigration from the (low-energy) charge gap to the high-energy gap for strong correlations. Notably, for any strong enough δ, we always find a U_c, where the edge states invariably occur at zero energy. This is a remarkable happenstance of competition between V and U. Generally, for the nonzero values of V or U, the quasiparticle edge states are found to have nonzero energies. So, it is quite a surprise to find them at zero energy inspite of the interaction. However, on a careful reflection, the existence of these zero-energy edge states looks inevitable, as it marks the change from band to Mott insulator across U_c, driven by the competition between V and U. In Sec. III, we present a theory capable of describing the physics of quasiparticle edge states in the RMH chain. The results obtained from this theory are compared with those obtained from DMRG and ED. We find a good qualitative match between them, and a strong agreement of the edge energies for weak to moderate correlations. A phase diagram in the U-V plane is also worked out for a fixed dimerization ($\delta = 0.7$) from this theory to highlight the key features of the edge state behavior resulting from the competition between the staggered potential and the Hubbard interaction. We end this paper with a summary in Sec. IV.

II. EDGE STATES IN RICE-MELE-HUBBARD CHAIN

The Rice-Mele-Hubbard Hamiltonian on an open chain of L sites can be written as follows:

$$\hat{H} = -t\sum_{l=1}^{L-1}\sum_{s=\uparrow,\downarrow}[1+(-)^l\delta](\hat{c}^{\dagger}_{l,s}\hat{c}_{l+1,s}+\text{H.c.}) + V\sum_{l=1}^{L}\sum_{s=\uparrow,\downarrow}(-)^l\hat{n}_{l,s} + U\sum_{l=1}^{L}\left(\hat{n}_{l,\uparrow}-\frac{1}{2}\right)\left(\hat{n}_{l,\downarrow}-\frac{1}{2}\right), \tag{1}$$

where the first term is the SSH model with δ as the dimerization parameter and t as the nearest-neighbor hopping amplitude, V is the staggered local potential, and U is the Hubbard interaction.

We study the edge state behavior of RMH model by investigating Eq. (1) for different values of dimerization ($\delta = 0.5, 0.7$) and staggered potential ($V = 1, 2, 5$). We put $t = 1$ in the calculations and employ the DMRG method to compute the edge state energy (ε_1) and the bulk charge gap (Δ_c). The minimum energy required to add a particle to the half-filled ground state, i.e., $E_g(L+1) - E_g(L)$, on an open chain is ε_1 for $\delta > 0$ and Δ_c for $\delta < 0$. Here, $E_g(N_e)$ denotes the ground-state energy of the RMH chain for N_e electrons, and $N_e = L$ corresponds to half filling. The sign of δ on an open chain matters because the edge states occur only for $\delta > 0$, and for $\delta < 0$ only the bulk exists. The system size used to calculate ε_1 and Δ_c is 60 sites, with 200–400 and 500–1500 sweeps, respectively, while maintaining the maximum truncation error of $\approx 10^{-12}$. The edge state energy and the charge gap thus calculated from DMRG are presented in Fig. 1. Note that we get the same result also by computing the energy cost, $E_g(L-1) - E_g(L)$, for removing one particle from the half-filled case.

Let us check the limiting case, $U = 0$, first. The noninteracting Rice-Mele chain is known to have the bulk charge gap, $\sqrt{V^2 + 4\delta^2 t^2}$, and the edge state energy, V [1]. Indeed, we get their correct values numerically for $U = 0$, as shown in Fig. 1. For $U \neq 0$, i.e., in the RMH chain, we find the edge state energy to show a prominent conelike variation with respect to U. Notably, the tip of this cone touches the zero energy, and the critical value of the Hubbard interaction at this tip, U_c,

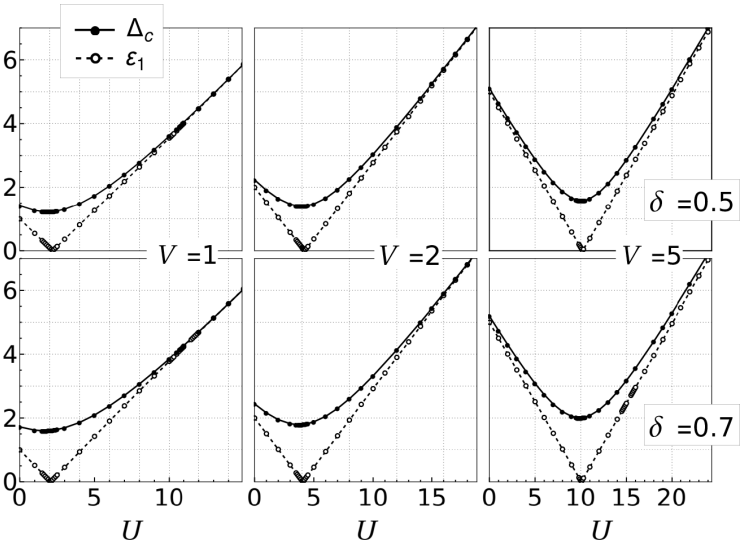


FIG. 1. Evolution of the bulk charge gap, Δ_c, and the edge state energy, ε_1, with Hubbard interaction, U, in units of hopping, t, for different values of staggered potential, V, and dimerization, δ, in the Rice-Mele-Hubbard chain for $L = 60$ at half filling. Notably, the cone-shaped ε_1 vs U touches zero energy on its tip at the critical interaction, $U_c \approx 2V$, and for a large enough U, the edge state merges with the bulk.

is directly proportional to the value of the staggered potential. We find that $U_c \approx 2V$, which does not seem to depend strongly on the degree of dimerization (here $\delta = 0.5$ and $\delta = 0.7$).

As the interaction crosses U_c, the edge state energy increases gradually and more rapidly with U than the bulk charge gap. So, the edge states merge into the bulk at some point, $U_{c,1}$. It means, the edge states disappear beyond $U_{c,1}$, like in the SSH-Hubbard chain [11]. From Fig. 1, it is clear that $U_{c,1}$ increases with increase in V for a fixed δ; i.e., strong interaction is required for the edge state energy to overcome the bulk gap in the presence of strong staggered potential. For example, $U_{c,1}$ at $\delta = 0.7$ is approximately 11 and 17 for $V = 1$ and 2, respectively.

Beyond $U_{c,1}$, the edge states stay lost upto a certain interaction strength $U_{c,2}$, after which they reappear in the high-energy band gap. To see this transmigration of edge states from the physical charge gap to high-energy gap [11], let us focus on Fig. 2, which for $\delta = 0.7$ and $V = 1$ shows the energies of the quasiparticle excitations above half filling. The minimum energy required to add Nth particle above the half-filled ground state is given by $\varepsilon_N = E_g(L + N) - E_g(L + N - 1)$. It is the excitation energy of incremental particle addition. For $\delta > 0$ and $N = 1$, it is the energy, ε_1, of the edge state when it exists in the (low-energy) charge gap. The thing to observe here is the quasiparticle state for $N = L/2$, i.e., ε_{10} in this plot for $L = 20$, separating off from the band into the high-energy gap. This transmigrating edge state is highlighted in Fig. 2 by thick black lines with empty circles.

We also calculate the electron number expectation values, $n_e(l) = \langle \hat{n}_{l\uparrow} + \hat{n}_{l\downarrow} \rangle$, on every site, l, in the ground state for seven different electronic fillings, $N_e = L$ (half filling), $L + 1$, $L + 2$, $L + L/2 - 1$, $L + L/2$ (three-quarter filling), $L + L/2 + 1$, $L + L/2 + 2$ for $V = 1$ and $U = 1, 4, 6, 10, 12$, and 15. The $n_e(l)$ versus l for these seven cases are plotted in Fig. 3 for $L = 20$. Of these, the two notable cases are for $N_e = L + 1$ and $L + L/2$, while the others are shown to provide an overall perspective. In the ground state of the half-filled case, $n_e(l)$ at the edges is 2 and 0 for $U = 1$, and 1 for other U's, as expected; see the first row from the top. In the ground state for $N_e = L + 1$ (the second row), the electronic occupancy for $U = 1$ is still 2 at one end, but at the other end, it changes to 1 (from 0 in the ground state of the half-filled case); note that for $U = 4$, 6, and 10, the occupancies at the two ends stay so. This is the edge state with energy ε_1 in the charge

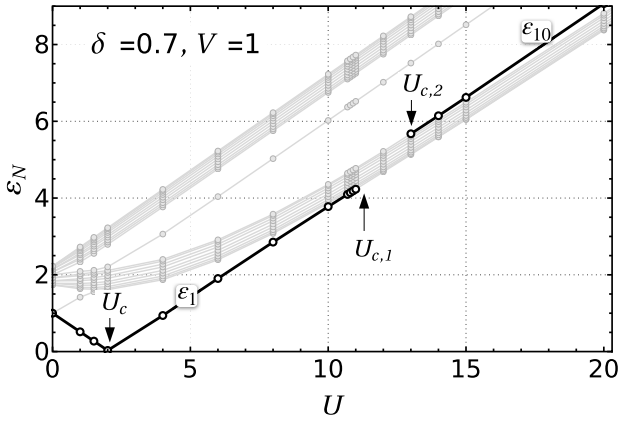


FIG. 2. Energies of the successive addition of electrons to the ground state of the half-filled RMH model, ε_N, calculated using DMRG on an open chain of length $L = 20$, for $\delta = 0.7$ and $V = 1$. See the text above for the definition of ε_N. The lowest cone-shaped black line touching zero at $U_c \approx 2$ corresponds to the edge state (marked as ε_1) in the charge gap; it is clearly seen to disappear into the bulk at $U_{c,1} \approx 11$ and reappear (as ε_{10}) in the high-energy gap around $U_{c,2} \approx 13$.

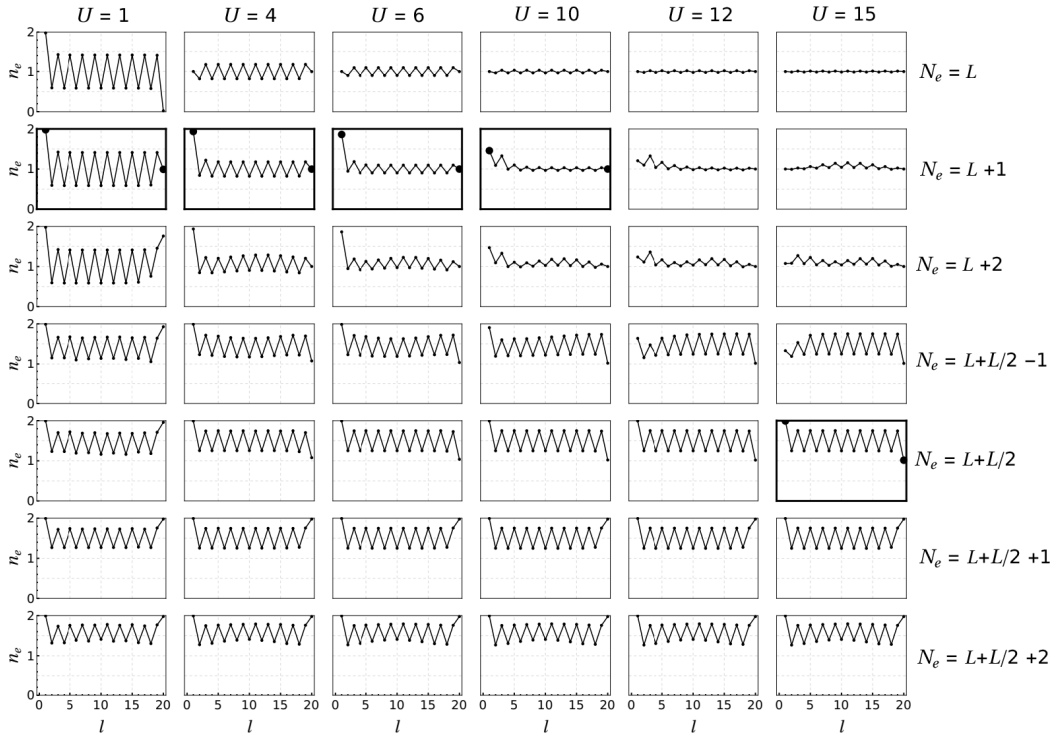


FIG. 3. Tracking the edge state transmigration by calculating the expectation value of electron number, $n_e(l)$, on site, l, using DMRG for $L = 20$, $\delta = 0.7$, and $V = 1$. In the second row (from the top), the plots for $U = 1, 4, 6$, and 10 are for the quasiparticle edge state in the charge gap. Notably, the same behavior is exhibited in the plot for $U = 15$ in the fifth row, which is for the edge state in the high-energy gap observed at three-quarter filling.

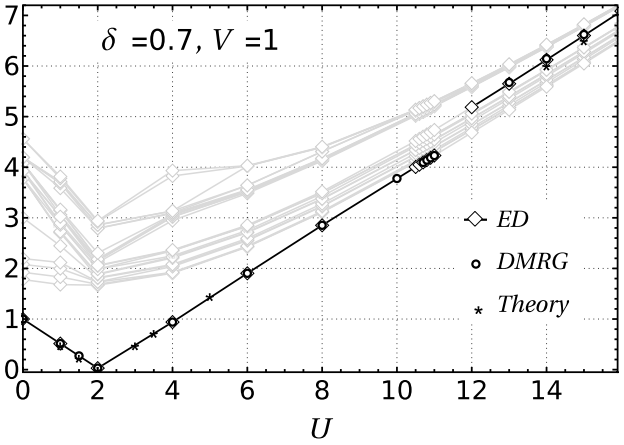


FIG. 4. The lowest few energy eigenvalues of the RMH model on an open chain of 10 sites with 11 electrons calculated using ED are plotted here after subtracting the ground-state energy at half filling (i.e., for 10 electrons). The edge state behavior from ED (black line with diamonds) compares very nicely with the data from DMRG on 20 sites (empty circles) and theory (star).

gap (see Fig. 2). For $U = 12$, however, this edge behavior for $N_e = L + 1$ is almost gone, and for $U = 15$, it does not exist at all. Notably, at $U = 15$, the same edge occupancies appear in the ground state for $N_e = L + L/2$, as described above for $N_e = L + 1$ when U was smaller; see the last plot in the third row from the bottom. From Fig. 2, we understand this to be the edge state with energy ε_{10} in the high-energy gap. This connection between the edge behavior of the $N_e = L + 1$ case for small U and that of the $N_e = L + L/2$ case for large U is highlighted in Fig. 3 by two big dots at the two edges in the respective plots with thick frames. Hence, for large U, the edge states indeed transmigrate from the charge gap to the high-energy gap.

This transmigration can also be seen by staying in the $N_e = L + 1$ sector itself. The edge state physics revealed above by changing the electronic filling is also reflected in the energy spectrum of a single particle added to half filling. We show this by calculating a reasonable number ($\approx$30) of low excitation energies in this sector using exact diagonalization for $L = 10$. After subtracting therefrom the ground-state energy of the half-filled case, we plot these energies in Fig. 4 for $\delta = 0.7$ and $V = 1$. Here, the lowest excitation indeed follows the edge state energy, ε_1, from DMRG. As we increase U, the edge state (black line) is clearly seen to transmigrate to the high-energy gap for strong correlations even on this small cluster. It compares reasonably with the edge state energies calculated from DMRG and the theory presented in the next section; since the edges behave as separate from the bulk, the system size does not quite affect the calculation of the edge state energy.

Another important feature revealed by these calculations, besides the transmigration, is that the edge state energy invariably becomes zero at $U_c(\approx 2V)$. We noted this feature earlier in the discussion. Let us now elaborate on it. For a nonzero U or V, the edge states are generally found to occur at nonzero energies, which is the general expectation for interacting electrons. But surprisingly, here we always find the edge state energy to become zero at a certain U_c. For a qualitative understanding of this property, consider the fully dimerized limit, i.e., $\delta = 1$, in which the two edges completely decoupled from the bulk are described purely by the local Hamiltonian, $-V(\hat{n}_{e,1} - \hat{n}_{e,L}) + U[1 - \hat{n}_{e,1}(2 - \hat{n}_{e,1}) - \hat{n}_{e,L}(2 - \hat{n}_{e,L})]/2$, where $\hat{n}_{e,l} = \hat{n}_{l,\uparrow} + \hat{n}_{l,\downarrow}$ is the total number of electrons on lth site. From this, we calculate the energies for different edge occupancies, $E(n_{e,1}, n_{e,L})$, and learn that, for $U < 2V$, the edge state energy, ε_1, is given by $E(2, 1) - E(2, 0) = V - U/2$, whereas for $U > 2V$, it is given by $E(2, 1) - E(1, 1) = -(V - U/2)$; the same is true if we remove an electron instead of adding one, i.e., replace $E(2, 1)$ by $E(1, 0)$. Note two features in this limiting case: (1) $\varepsilon_1 = |U - 2V|/2$ exhibits a cone-shaped variation with respect to U for a fixed V and touches zero

at $U = 2V$; and (2) the edge occupancies in the half-filled ground state change from (2, 0) to (1, 1) for $U > 2V$, which marks a qualitative change in the nature of ground state from the V dominated bandlike to the U dominated Mott-like. Interestingly, even when the two ends are coupled to the bulk for $\delta < 1$, the same qualitative behavior is exhibited by the edge states in our calculations.

Thus, in the RMH chain, we have a special situation where the "zero-energy edge states" arise due to interaction, contrary to the general expectation. For a given V, the half-filled RMH model in the ground state is a band insulator for small U and a Mott insulator for large U. The critical interaction, U_c, is where the change from band to Mott insulator happens. So, on both sides of U_c, the edge state energy is nonzero, but at U_c, it becomes zero. This is reminiscent of the interaction-driven transition from the band to Mott insulator via metallic phase in the ionic Hubbard model [22]. But here the bulk charge gap never goes to zero; instead, the edge state energy vanishes. Notably, the transmigration of edge states occurs only when $U > U_c$. Below we develop a theory that nicely describes these features.

III. THEORY OF CHARGE QUASIPARTICLES

To understand the numerically obtained edge state behavior presented above, we investigate the properties of charge quasiparticles in the RMH chain using Kumar representation. Here, we follow Ref. [11] to write the RMH Hamiltonian, Eq. (1), in Kumar representation [20] as

$$\hat{H} = -\frac{t}{2}\sum_{l=1}^{L-1}[1+(-)^l\delta]\{(\hat{f}_l^\dagger \hat{f}_{l+1} + \text{H.c.})(1+\vec{\sigma}_l\cdot\vec{\sigma}_{l+1}) + (-)^l(\hat{f}_l^\dagger \hat{f}_{l+1}^\dagger + \text{H.c.})(1-\vec{\sigma}_l\cdot\vec{\sigma}_{l+1})\}$$
$$-V\sum_{l=1}^{L}(-)^l\sigma_l^z\hat{f}_l^\dagger\hat{f}_l - \frac{U}{2}\sum_{l=1}^{L}\hat{f}_l^\dagger\hat{f}_l + V\sum_{l=1}^{L}(-)^l\sigma_l^z + \frac{U}{4}L, \tag{2}$$

where the spinless fermion operators, $\hat{f}_l$ and $\hat{f}_l^\dagger$, describe the charge excitations of the system and the Pauli operators, $\vec{\sigma}_l$, account effectively for the spin dynamics. Kumar representation, $\hat{c}_{l,\uparrow}^\dagger = [\hat{f}_l^\dagger + (-)^l\hat{f}_l]\sigma_l^+$ and $\hat{c}_{l,\downarrow}^\dagger = \frac{1}{2}\{[\hat{f}_l^\dagger - (-)^l\hat{f}_l] - [\hat{f}_l^\dagger + (-)^l\hat{f}_l]\sigma_l^z\}$, describes the electrons canonically in terms of these spinless fermions and Pauli operators [20].

From Eq. (2), we obtain a simpler effective model for the charge quasiparticles by replacing the spin-dependent operator, $\vec{\sigma}_l\cdot\vec{\sigma}_{l+1}$, by its average value in the bulk; this average value is denoted as ρ_{1-} over the odd bonds and ρ_{1+} for the even bonds (see Ref. [11]). Moreover, σ_l^z in the staggered potential term is replaced by the value m_l. For m_l, we take an idealized choice, $m_l = (-)^{l+1}$, motivated by the fact that the staggered potential tends the alternate sites to be doubly occupied or empty. We also tried involved estimations of m_l, but this simple choice works better qualitatively and also quantitatively. With these simplifications of Eq. (2), we get the following effective model for the charge quasiparticles:

$$\hat{H}_c = -\frac{t}{2}\sum_{l=1}^{L-1}[1+(-)^l\delta]\{[1+\rho_{1,(-)^l}]\hat{f}_l^\dagger\hat{f}_{l+1} + (-)^l[1-\rho_{1,(-)^l}]\hat{f}_l^\dagger\hat{f}_{l+1}^\dagger + \text{H.c.}\} + u\sum_{l=1}^{L}\hat{f}_l^\dagger\hat{f}_l, \tag{3}$$

whose energy dispersion in the bulk is given by

$$E_{k,\pm} = \sqrt{u^2 + |\alpha_k|^2 + |\beta_k|^2 \pm 2\sqrt{u^2|\beta_k|^2 + \{\Re(\alpha_k^*\beta_k)\}^2}} \tag{4}$$

for $\alpha_k = t[(1+\delta)(1-\rho_{1+}) + (1-\delta)(1-\rho_{1-})e^{i2k}]/2$ and $\beta_k = t[(1+\delta)(1+\rho_{1+}) + (1-\delta)(1+\rho_{1-})e^{i2k}]/2$ for $k \in [-\frac{\pi}{2}, \frac{\pi}{2}]$. Here, $u = V - U/2$. The dispersion, $E_{k,\pm}$, is derived by applying Fourier and Bogoliubov transformations successively on $\hat{H}_c$, assuming periodic boundary

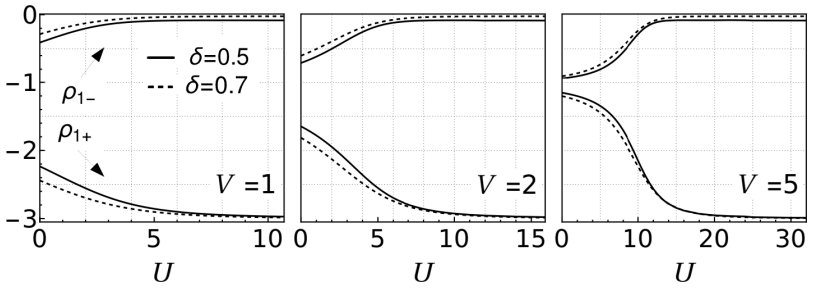


FIG. 5. Parameters $\rho_{1\pm}$ required for $\hat{H}_c$, Eq. (3), calculated as a function of U in the ground state of the half-filled RMH model, Eq. (1), using DMRG.

condition [23]. Minimum value of $E_{k,-}$ gives the bulk charge gap, Δ_c. For the edge states, we do Bogoliubov diagonalization of $\hat{H}_c$ numerically on open chain.

As in Ref. [11], we calculate $\rho_{1\pm}$ in the ground state of the half-filled RMH model, Eq. (1), using the DMRG method. We calculated $\rho_{1\pm}$ for $L = 60$, 100, and 200, and found practically the same values, with insignificant dependence on system size. Figure 5 shows the behavior of $\rho_{1\pm}$ with U for a few different values of V and δ. Note that a strong staggered potential needs a proportionately strong Hubbard interaction for ρ_{1+} and ρ_{1-} to get closer to the limiting values of -3 and 0, respectively. We put in Eq. (3) the $\rho_{1\pm}$ thus obtained and study the behavior of charge quasiparticles for the RMH chain.

In Fig. 6, the dashed lines represent the edge state energy obtained from our theory by solving Eq. (3) on open chain. Its quantitative match with the numerical data from DMRG (empty circles) is very good and the conelike feature of ε_1 versus U around U_c is correctly produced by the theory. But the charge gap is underestimated by the theory (solid lines), although Δ_c versus U looks qualitatively similar to that from DMRG (filled circles). Consequently, we see a difference in the value of $U_{c,1}$

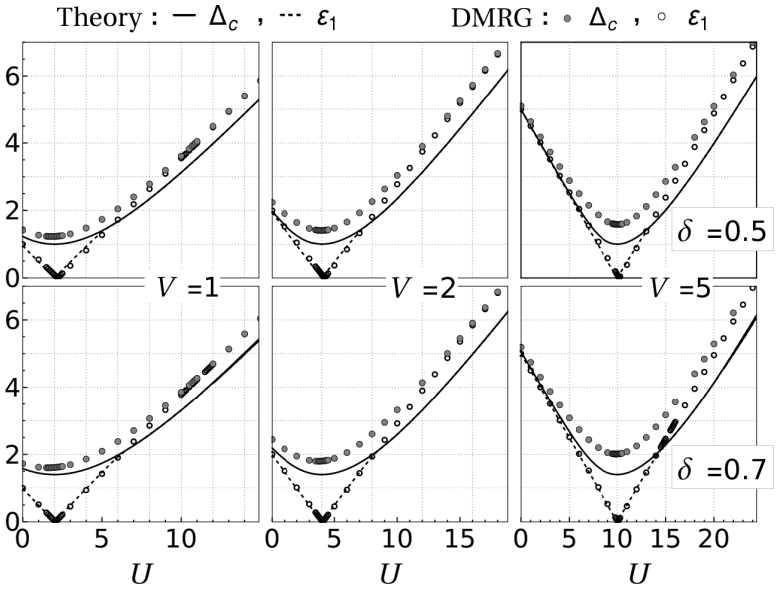


FIG. 6. Comparing the bulk charge gap (Δ_c) and the edge state energy (ε_1) vs U from theory (solid and dashed lines) and DMRG (filled and empty circles) for a few fixed values of V and δ. Notably, the theory captures the cone-shaped variation of ε_1 with U perfectly, but it underestimates Δ_c.

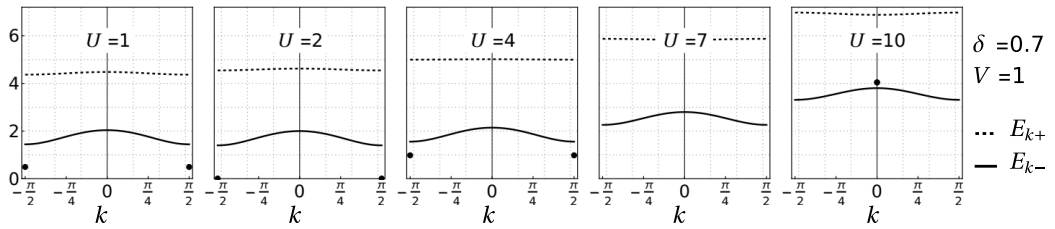


FIG. 7. Evolution of the quasiparticle energy dispersion, Eq. (4), with increasing U for a fixed δ and V. Thick black dots represent the edge states. For $U = 1$ and 2, which are $< U_{c,1}$, the edge states occur in the charge gap at $k = \pm\pi/2$. For $U = 10$, which is $> U_{c,2}$, the edge states are found at $k = 0$ in the high-energy gap. There is no edge state for $U = 7$, which is in between $U_{c,1}$ and $U_{c,2}$. Notice the edge states at zero energy for $U = 2$, i.e., U_c.

(where ε_1 touches Δ_c) from theory and numerics. For example, for $\delta = 0.7$ and $V = 1$, we get $U_c \approx 2.06$ (2), $U_{c,1} \approx 11$ (6.51), and $U_{c,2} \approx 13$ (7.76) from the DMRG (theory). Inspite of these quantitative differences, there is a qualitative consistency in the physical behavior seen from the numerics and this rather simple theory.

In Fig. 7, we show the evolution of quasiparticle energy dispersion with U for $\delta = 0.7$ and $V = 1$. Here, the bulk dispersion, Eq. (4), is presented together with the edge states (marked by thick dots). We see different edge state behavior in different regions across U_c, $U_{c,1}$, and $U_{c,2}$. For $U = 1$, which is $< U_c$, the edge states in the charge gap lie at the zone boundary ($k = \pm\pi/2$) with a nonzero energy. At $U = 2$, which is U_c, the edge states attain zero energy; the bulk always remains gapped. For $U = 4$, which is $> U_c$, the edge state energy again becomes nonzero. After it merges into the bulk at $U_{c,1}$, no edge states are found; see here the plot for $U = 7$. For $U > U_{c,2}$, i.e., $U = 10$ in this figure, the edge states reappear in the high-energy gap at the zone center ($k = 0$). The transmigration of edge states from the charge gap to high-energy gap, after having passed through zero energy, is quite evident here.

This theory lets us look into the quasiparticle edge states through their wavefunctions found by Bogoliubov diagonalization of $\hat{H}_c$ on open chain. Following Ref. [11], we define the quasiparticle operator $\hat{\eta}$ in terms of the spinless fermion $\hat{f}_l$ as $\hat{\eta} = \sum_{l=1}^{L}(v_l \hat{f}_l + w_l \hat{f}_l^\dagger)$; the coefficients v_l and w_l can be viewed as the components of vectors $\mathbf{v}$ and $\mathbf{w}$, respectively. In Fig. 8, we show the edge states computed in three different regions of U for $\delta = 0.7$ and $V = 1$; here we have shown the wavefunction of the quasiparticle edge state localized at $l = 1$, but the other edge state localized at $l = L$ behaves similarly. The plot for $U = 1$ corresponds to the region $U < U_c$; here, $\mathbf{v}$ is peaked at $l = 1$ and it rapidly dies off in the bulk. The plot for $U = 4$ represents the region: $U_c < U < U_{c,1}$, wherein $\mathbf{w}$ is peaked at $l = 1$. Note that U_c is acting here like a chemical potential below which the wavefunction is particlelike (with dominant $\mathbf{v}$) and above holelike (with dominant $\mathbf{w}$). In both

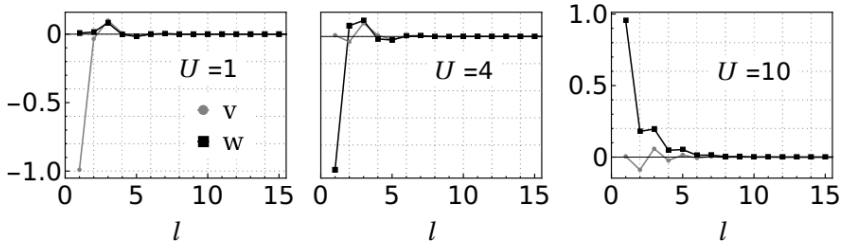


FIG. 8. Edge state wavefunction in three cases, $U = 1 < U_c$, $U_c < U = 4 < U_{c,1}$, and $U = 10 > U_{c,2}$, for $\delta = 0.7$ and $V = 1$.

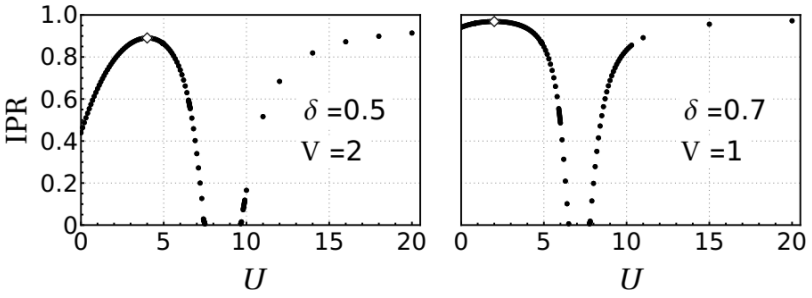


FIG. 9. IPR vs U. Here, a nonzero value of IPR represents the presence of two edge states. The white diamonds mark the maxima of IPR at $U_c \approx 2V$, corresponding to the zero-energy edge state.

these cases, the edge states lie in the physical charge gap at $k = \pi/2$. In the region $U_{c,1} < U < U_{c,2}$, we do not get any edge state. The plot for $U = 10$ belongs to the case $U > U_{c,2}$, where the edge state occurs in the high-energy gap and corresponds to $k = 0$ or π. The inverse participation ratio, $\text{IPR} = \sum_{l=1}^{L}(|v_l|^4 + |w_l|^4)$, is a good identifier of the edge states. In Fig. 9, we plot IPR as a function of U for $\delta = 0.5$, $V = 2$ and $\delta = 0.7$, $V = 1$. These plots clearly identify the region, $U_{c,1} < U < U_{c,2}$, with no edge state. Curiously, for $U < U_{c,1}$, the maxima of IPR is found to correspond to the zero-energy edge state at U_c.

Figure 10 sums up the edge state behavior of the RMH chain in the U-V plane for a fixed δ. Here, there are three phases categorized according to the position of the edge states in the energy spectrum. In the first phase (light gray region), ranging from $U = 0$ to $U_{c,1}$ (continuous line), the edge states are found in the low-energy charge gap. In the second phase (white region) from $U_{c,1}$ to $U_{c,2}$ (dotted line), the edge states do not exist; the width of this phase remains approximately the same for different values of the staggered potential for a given δ. From $U_{c,2}$ onward, the third phase (gray region) starts in which the edge states appear in the high-energy gap. In addition, there

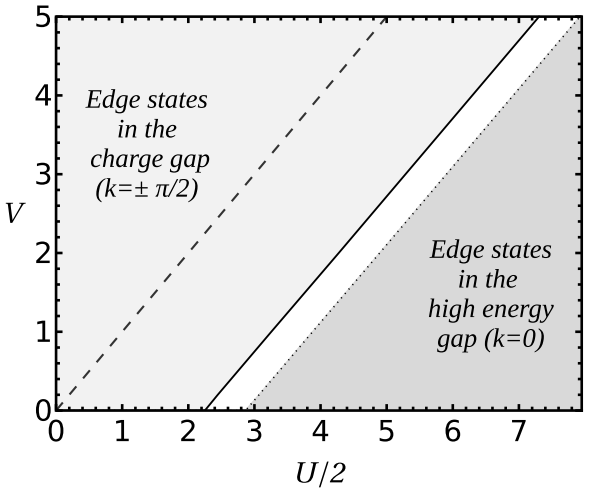


FIG. 10. Phase diagram of the half-filled Rice-Mele-Hubbard chain for $\delta = 0.7$, obtained from the theory of charge quasiparticles. The white region bounded by $U_{c,1}$ (solid line) and $U_{c,2}$ (dotted line) is the region where no edge state exists. In the light gray region for $U < U_{c,1}$, the edge states occur in the charge gap and the dashed line corresponds to U_c where the edge states attain zero energy. In the gray region for $U > U_{c,2}$, the edge states occur in the high-energy gap.

is another very important feature in the first phase, which is that the zero-energy edge states exist at U_c (dashed line).

IV. SUMMARY

We investigate the effect of Hubbard interaction on the edge states in the Rice-Mele chain at half filling and present some important results. The key findings of this study are as follows. For a fixed dimerization, δ, and staggered potential, V, the edge states invariably transmigrate from the low- to high-energy charge gap by increasing the Hubbard interaction, U, via an intermediate phase devoid of the edge states. It is consistent with the interaction-driven transmigration discovered in Ref. [11]. In addition, we also find the edge state energy to always become zero at a critical interaction, $U_c \approx 2V$, preceding the transmigration. It marks the transition from band to Mott insulator, not by closing the bulk charge gap, but by making the edge state energy zero. It is important to note that the competition between V and U realizes zero-energy edge states, but individually neither of them do so. This finding is significant because it points toward an interesting general possibility for interacting topological insulators where different competing interactions, which individually may be detrimental to the zero-energy edge states (more generally, the conducting surface states), but in competition with each other, may still help in realizing the conducting surface states.

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DATA AVAILABILITY

The data that support the findings of this article are available from the authors upon reasonable request.

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