Universality of Boundary Charge Fluctuations: Supplemental Material

Clara S. Weber,[1] Kiryl Piasotski,[1] Mikhail Pletyukhov,[1] Jelena Klinovaja,[2] Daniel Loss,[2] Herbert Schoeller,[1] and Dante M. Kennes[1,3,*]

[1] *Institut für Theorie der Statistischen Physik, RWTH Aachen, 52056 Aachen, Germany and JARA - Fundamentals of Future Information Technology*
[2] *Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland*
[3] *Max Planck Institute for the Structure and Dynamics of Matter, Center for Free Electron Laser Science, 22761 Hamburg, Germany*

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I. NUMERICAL RESULTS OF FIG.4B

U	0.0	0.4	0.8	1.2	1.6	2.0	2.4
C	1.0	0.92	0.88	0.96	0.89	0.96	1.18

TABLE I. Constants C used in the collapse of Fig. 4 (b) of the main text.

To achieve the universal collapse shown in Fig. 4 (b) of the main text we have numerically determined the constants C listed in Table I.

II. BOUNDARY CHARGE FLUCTUATIONS

Here we present a general analysis of the boundary charge fluctuations without assuming that the gap is small compared to the band width. This means that the length scale $\xi_g = v_F/E_g$ is not assumed to be much larger than the lattice spacing a. As in the main part of the letter we assume fixed particle number N (i.e., a canonical ensemble) and zero temperature here (other cases are discussed in Section II C). We take an effectively one-dimensional system with N_s lattice sites and N_B channels per site, labeled by $m = 1, \dots, N_s$ and $\sigma = 1, \dots, N_B$, respectively. Besides different spins, orbitals and other flavors, the channel indizes include also the degrees of freedom in transverse direction, i.e., parallel to the surface. The size of the one-dimensional unit cell is denoted by Za. For the real space position of a lattice site we write $x = ma$, and $L = N_s a$ defines the system size perpendicular to the boundary. Finally, we take the thermodynamic limit $N_s, N \to \infty$ such that the average charge per site $\bar{\rho} = N/N_s$ is kept constant. We use units $\hbar = e = 1$.

In Section II A we analyse the relation of the boundary charge fluctuations to the second moment of the longitudinal density-density correlation function. In Section II C we discuss the case of a grandcanonical ensemble and finite temperature.

A. Relation to the density-density correlation function

Our aim is to calculate the fluctuations of the boundary charge operator at one end of the system defined by

$$\hat{Q}_B = \sum_{m=1}^{N_s} f_m (\hat{\rho}_m - \bar{\rho}) \, , \tag{1}$$

where $\hat{\rho}_m = \sum_\sigma a^\dagger_{m\sigma} a_{m\sigma}$ is the charge operator at site m, and $a^\dagger_{m\sigma}$ creates a fermion on site m in channel σ. The macroscopic average is described by an envelope function $f_m \equiv f(x) = 1 - \theta_{l_p}(x - L_p)$, with $L \gtrsim L_p + l_p/2 \gtrsim l_p \gg \xi_g$, where $\theta_{\delta x}(x)$ is some representation of the θ-function broadened with δx. The scale L_p describes the length of a charge measurement probe and l_p is the scale on which the probe smoothly looses the contact to the sample. By convention, we define the scale l_p by the integral

$$l_p^{-1} = \int dx [f'(x)]^2 \, . \tag{2}$$

The envelope function is assumed to be smooth on the microscopic length scales ξ_g and a, i.e., $l_p \gg \xi_g, a$. As shown below the length scales L, L_p, and l_p can even be of the same order of magnitude, provided that $|L - L_p - l_p/2| \gtrsim O(\xi_g)$ and $|L_p - l_p/2| \gtrsim O(\xi_g)$. This condition means that the fall-off of the envelope function fits into the system size (up to $O(\xi_g)$). Otherwise, as we will see below, the length scale L_p does not enter the final solution for the boundary charge fluctuations.

Defining the correlation function

$$C_{mm'} = \langle \hat{\rho}_m \hat{\rho}_{m'} \rangle - \langle \hat{\rho}_m \rangle \langle \hat{\rho}_{m'} \rangle \, , \tag{3}$$

we can express the fluctuations $\Delta Q_B^2 = \langle \hat{Q}_B^2 \rangle - \langle \hat{Q}_B \rangle^2$ as

$$\Delta Q_B^2 = \sum_{m,m'=1}^{N_s} f_m f_{m'} C_{mm'} \, . \tag{4}$$

In the following we call $C_{mm'}$ the density-density correlation function of the effectively one-dimensional system but it should be kept in mind that it is the correlation between the charges ρ_m and $\rho_{m'}$ including the sum over *all* channel indizes. In particular, this includes also the sum over all transverse quasimomenta. Therefore, for higher-dimensional systems, it describes rather the correlation between the total charge of two stripes and not the correlation between the densities at two points in real space.

Using the sum rule (which is exact at fixed particle number)

$$\sum_{m'=1}^{N_s} C_{mm'} = 0\,, \tag{5}$$

together with $C_{mm'} = C_{m'm}$, we can replace $f_m f_{m'} \to -(1/2)(f_m - f_{m'})^2$ in (4) and obtain the very useful form

$$\Delta Q_B^2 = -\frac{1}{2}\sum_{m,m'=1}^{N_s}(f_m - f_{m'})^2 C_{mm'}\,. \tag{6}$$

This formula is very helpful since the correlation function $C_{mm'}$ is exponentially small for an insulator for $|x-x'| \gg \xi_g$, with $x = ma$ and $x' = m'a$. Therefore, only the part $|x-x'| \lesssim \xi_g$ is relevant. Since $f_m \equiv f(x)$ varies slowly on the scale ξ_g due to $\xi_g \ll l_p$, we can expand $f_m - f_{m'} \approx f'(\frac{x+x'}{2})(x-x')$ in (6). Using in addition that the derivative $f'(x) \sim 1/l_p$ is only non-zero for $x = L_p + O(l_p/2)$, we find that both $x, x' \sim L_p + O(l_p/2) \gg \xi_g$ are located away from the boundary far beyond the length scale ξ_g. This holds even in the case when L_p and $l_p/2$ have the same order of magnitude (up to $O(\xi_g)$) since the contribution from all $x, x' \sim \xi_g$ gives a contribution $\lesssim \left(\frac{\xi_g}{l_p}\right)^2$ to the fluctuations. Therefore, we can replace the correlation function $C_{mm'}$ by its bulk value

$$C^{\rm bulk}_{mm'} = a^2 C_{\rm bulk}(x,x')\,, \tag{7}$$

and obtain for $l_p \gg \xi_g$

$$\Delta Q_B^2 = -\frac{1}{2}a^2\sum_{m,m'=1}^{N_s}\left[f'(\frac{x+x'}{2})\right]^2 \times (x-x')^2 C_{\rm bulk}(x,x') + O(\frac{\xi_g}{l_p})^2\,. \tag{8}$$

As a result, the double sum scales as $a^2\sum_{m,m'} \lesssim \xi_g l_p$ and one can see that the fluctuations are finite in the thermodynamic limit. In this formula the bulk correlation function can be calculated in the thermodynamic limit for any ensemble and for any boundary condition. Note that this is not possible in the form (4) since the sum rule (5) does no longer hold exactly in a grandcanonical ensemble at finite temperature (see the discussion in Section II C).

Using $m = Z(n-1)+j$, where $j = 1,\ldots,Z$ denotes the site index within a unit cell and $n = 1,2,\ldots$ labels the unit cells, we can write $C_{\rm bulk}(x,x') = C^{\rm bulk}_{jj'}(Zna, Zn'a)$. Due to translational invariance on the size Za of a unit cell (which holds on average also in the presence of random disorder) the bulk correlation function depends only on the difference $n-n'$ and we can write

$$C_{\rm bulk}(x,x') = C^{\rm bulk}_{jj'}\big(Z(n-n')a\big)\,. \tag{9}$$

Using $f'(\frac{x+x'}{2}) = f'(Zn_s a)(1 + O(a/l_p))$, with $n_s = \frac{n+n'}{2}$, we find that the sum over n_s in (8) gives $\sum_{n_s} f'(Zn_s a)^2 = \frac{1}{Zal_p}\big(1 + O(Za/l_p)\big)$ according to (2). Again neglecting boundary effects $\sim O(\frac{\xi_g}{l_p})^2$, we obtain

$$l_p\,\Delta Q_B^2 = -\frac{a}{2Z}\sum_n\sum_{jj'} \times \big(Zna + (j-j')a\big)^2 C^{\rm bulk}_{jj'}(Zna)\,. \tag{10}$$

We note that this result is exact when performing the limits $L, L_p, l_p \to \infty$ with $L \gtrsim L_p + l_p/2 \gtrsim l_p$. Eq. (10) establishes a universal relation of the boundary charge fluctuations to the density-density correlation function of the bulk, including all microscopic details of the unit cell. As one can see only the product $l_p\,\Delta Q_B^2$ is related in a universal way to the bulk correlation function $C^{\rm bulk}_{jj'}(Zna)$, where l_p is defined by Eq. (2) in terms of the envelope function. Since the bulk correlation function can be calculated in any ensemble and with any boundary condition this equation is the most convenient starting point to calculate the boundary charge fluctuations very efficiently from bulk quantities without any need to determine the complicated eigenfunctions of finite or half-infinite systems.

As one can see from the proof only the condition $l_p \gg \xi_g$ enters together with the property that the support of the function $f'(x)$ fits into the system size such that

$$-\int_0^L dx f'(x) = 1 + O(\xi_g/l_p)\,, \tag{11}$$

$$\int_0^L dx\Big[f'(x)\Big]^2 = l_p^{-1}\Big(1 + O(\xi_g/l_p)\Big)\,. \tag{12}$$

This is the reason why the length scales L, L_p, l_p can all be of the same order of magnitude (in the sense defined above) without changing the leading order contribution of the fluctuations. This is very helpful for numerical calculations and the experimental observability since only the condition $l_p \gg \xi_g \gg a$ has to be fulfilled to find universal properties of the boundary charge fluctuations.

To proceed we note at this point that all universal properties of ΔQ_B^2 derived in this section follow from two fundamental properties of $C^{\rm bulk}_{jj'}(x)$ which have to be checked for the concrete model under consideration

$$C^{\rm bulk}_{jj'}(x) = \sum_\sigma \frac{1}{\xi_\sigma^2}\, g^{(\sigma)}_{jj'}(x/\xi_\sigma)e^{-x/\xi_\sigma}\,, \tag{13}$$

$$s^2 g^{(\sigma)}_{jj'}(s) \sim O(1) \quad \text{for} \quad |s| < 1\,. \tag{14}$$

The first condition (13) states exponential decay and indicates that the correlation function is in general a linear combination of many terms, each with its own decay length $\xi_\sigma < \xi_g$. This occurs generically in the presence of channel indizes describing flavor degrees of freedom (spin, orbital, etc.) or the transverse quasimomentum (see Section V). Due to the second condition (14) the pre-exponential function should scale as $g^{(\sigma)}_{jj'}(s) \sim 1/s^2$ for $|s| < 1$. We find this scaling independent of the microscopic details of the model. For $\xi_g \sim a$ this property is obvious since there is only a single length scale. In the low-energy regime $\xi_g \gg a$, we show in Section III C explicitly that the two properties are fulfilled for single-channel and noninteracting models. The physical reason for the general case is obvious. For $|x| \sim a \ll \xi_\sigma < \xi_g$ one probes high-energy scales where the gap is unimportant. Therefore, the correlation function will scale $\sim 1/a^2$. For $|x| \sim \xi_\sigma \gg a$, the lattice spacing does not play any role and a low-energy continuum theory is possible to describe the corresponding term of the correlation function. This theory is expected to depend mainly on a single length scale ξ_σ, such that the corresponding term of the correlation function will scale $\sim 1/\xi_\sigma^2$. In contrast, for $|x| \gg \xi_\sigma$ or $|s| \gg 1$, the scaling depends crucially on the low-energy properties of the model and a pre-exponential power-law with an interaction dependent exponent is expected. The latter is difficult to determine for interacting systems. For clean single-channel systems one obtains $1/|s|$ in the noninteracting case, see Section III. However, this regime is of no relevance for the fluctuations since the corresponding term of the correlation function is exponentially small for $|x| \gg \xi_\sigma$. We note that the exponential decay property (13) is also valid for the correlation function $C_{mm'}$ with a boundary but the scaling of the pre-exponential function for n, n' close to the boundary might be more subtle.

Using (13) and (14) one can estimate the order of magnitude of the fluctuations (10) as

$$l_p\,\Delta Q_B^2 = \sum_\sigma c_\sigma \xi_\sigma \equiv N_B \bar{\xi} \lesssim N_B \xi_g\,, \tag{15}$$

with $c_\sigma \sim O(1)$, and $\bar{\xi} = \frac{1}{N_B}\sum_\sigma c_\sigma \xi_\sigma \le \xi_g$ defining some average exponential decay length. This result shows that the boundary charge fluctuations $\Delta Q_B \lesssim \sqrt{N_B \xi_g / l_p} \ll \sqrt{N_B}$ are always much smaller than the boundary charge $Q_B \sim N_B$, even for $N_B \sim O(1)$, showing that the boundary charge is a well-defined observable for $l_p \gg \xi_g$[1], in analogy to interface charges studied in Refs. [2–7].

In the low-energy regime when $\xi_g \gg Za$, one can neglect all terms in (15) with $\xi_\sigma \sim Za \ll \xi_g$. For the terms with $\xi_\sigma \gg Za$, we can neglect the part $(j-j')a \sim Za \ll \xi_\sigma \sim Zna$ in (8) and the sum can be replaced by an integral. This leads to the compact formula

$$l_p\,\Delta Q_B^2 = -\frac{1}{2}\int dx\, x^2 \bar{C}_{\rm bulk}(x)\,, \tag{16}$$

where $\bar{C}_{\rm bulk}(x)$ is the correlation function averaged over j and j'

$$\bar{C}_{\rm bulk}(x) = \frac{1}{Z^2}\sum_{jj'} C^{\rm bulk}_{jj'}(x)\,. \tag{17}$$

B. Numerics in the infinite system size limit $N_s \to \infty$

One of the many important implications of the previous subsection is that the boundary charge fluctuations $l_p\,\Delta Q_B^2$ can be extracted either directly or equivalently (in the $L_p, l_p \to \infty$ limit) from the right hand side of Eq. (10) via the bulk correlation functions. In the translationally invariant case this can be utilized to significantly speed up the numerical determination of $l_p\,\Delta Q_B^2$ as one can work directly in the desired limit of $N_s \to \infty$, which is often more convenient. We use this in Fig. 1 of the main text to determine the non-zero U, but $d = 0$ data from a highly efficient infinite system size density matrix renormalization group approach. With this the problem is directly phrased in the correct limit of $N_s, L_p, l_p \to \infty$, with $N_s a \gtrsim L_p + l_p/2 \gtrsim l_p \gg \xi_g$, but the evaluation of Eq. (10) requires the evaluation of an infinite sum $\sum_n$. As usual in numerical approaches we truncate this infinite sum at finite, but large index by $\sum_{n=-\infty}^{\infty} \to \sum_{n=-n_c}^{n_c}$, where n_c needs to be converged to $n_c a \gg \xi_g$ (akin, but not exactly equal to keeping a finite l_p) . We choose $n_c = 499$ for the data shown in Fig. 1 of the main text.

C. Finite temperature and grandcanonical ensemble

For a canonical ensemble at fixed particle number, all our results are also valid at finite temperature T, provided that $T \ll \Delta$ is much smaller than the gap $E_g = 2\Delta$. In this case the finite temperature corrections to ΔQ_B^2 can be shown to be exponentially small of relative order $\sim \sqrt{T/\Delta}\, e^{-\Delta/T}$, see Section III B 1. This changes for a grandcanonical ensemble where the sum rule (5) is no longer fulfilled exactly. For an estimation we consider a non-interacting system and find after a straightforward calculation using Wick's theorem

$$\begin{aligned}\sum_{m'=1}^{N_s} C_{mm'} &= \\ &= \sum_s n_F(\epsilon_s)[1-n_F(\epsilon_s)] \sum_\sigma |\psi_s(m\sigma)|^2 \\ &\sim N_B \frac{T}{W}\, e^{-\Delta/T}\,,\end{aligned} \tag{18}$$

where $\psi_s(m\sigma)$ are the single-particle eigenstates with energy ϵ_s, $n_F(\epsilon_s)$ denotes the Fermi function, and W is the band width. As a result we find that in the steps to get Eq. (6) from (4), the contributions from f_m^2 and $f_{m'}^2$ lead to corrections of order

$$\Delta Q_B^2(T) - \Delta Q_B^2(T=0) \sim N_B \frac{L_p}{a}\frac{T}{W} e^{-\Delta/T}\,. \tag{19}$$

With $\Delta Q_B^2(T=0) \sim N_B \frac{\bar{\xi}}{l_p}$, and the thermal length $L_T \sim v_F/T \sim aW/T$ we conclude that the temperature dependent correction is of relative order

$$\frac{\Delta Q_B^2(T) - \Delta Q_B^2(T=0)}{\Delta Q_B^2(T=0)} \sim \frac{L_p l_p}{\bar{\xi}^2} \frac{\bar{\xi}}{L_T} e^{-\Delta/T} \,. \qquad (20)$$

However, even though $L_p l_p \gg \xi_g^2 > \bar{\xi}^2$, we expect these corrections to be very small at low temperatures $\bar{\xi} < \xi_g \ll L_T$ due to the exponentially small factor $e^{-\Delta/T}$. As a consequence we conclude that all our central results remain valid for a grandcanonical ensemble as well.

III. NONINTERACTING AND CLEAN MODELS

In this section we analyse the special case of noninteracting and clean systems. In Section III A we provide general reasons for the properties (13) and (14) by expressing the correlation function via the propagator. For the special case of the Rice-Mele model we present the exact solution for the fluctuations of the boundary charge in Section III B. Finally, in Section III C we present the generic low-energy theory for all single channel models in the low-energy regime in terms of a noninteracting Dirac model following the ideas of Ref. 8.

A. Properties of the density-density correlation function and the propagator

Here we provide qualitative reasons why the properties (13) and (14) are fulfilled. Due to translational invariance perpendicular to the effectively one-dimensional system (i.e., parallel to the boundary), we consider in the following a fixed value for the transverse quasimomentum, restricting the sum over the channels only to a finite and small number N_c of other flavor degree of freedom.

For any noninteracting and clean lattice model in a grandcanonical ensemble one can use Wick's theorem and obtains for the density-density correlation function

$$C_{mm'}^{\text{bulk}} = \delta_{mm'} \rho_m - \sum_{\sigma,\sigma'=1}^{N_c} |\langle a_{m\sigma}^\dagger a_{m'\sigma'} \rangle|^2 \,. \qquad (21)$$

The propagator $\langle a_{m\sigma}^\dagger a_{m'\sigma'} \rangle$ can be expressed via the single-particle Bloch eigenfunctions

$$\psi_k^{(\alpha)}(m,\sigma) = \frac{1}{\sqrt{2\pi}} \chi_k^{(\alpha)}(j,\sigma) e^{ikn} \,, \qquad (22)$$

with energy $\epsilon_k^{(\alpha)}$, where α is the band index and $-\pi < k < \pi$ denotes the quasimomentum in units of the inverse lattice spacing. With $a_{m\sigma}^\dagger = \sum_\alpha \int_{-\pi}^{\pi} dk \, c_{k\alpha}^\dagger \psi_k^{(\alpha)}(m,\sigma)$ and $\langle c_{k\alpha}^\dagger c_{k'\alpha'} \rangle = \delta_{\alpha\alpha'} \delta(k-k') n_F(\epsilon_k^{(\alpha)})$, we obtain

$$\langle a_{m\sigma}^\dagger a_{m'\sigma'} \rangle = \sum_\alpha \int_{-\pi}^{\pi} dk \times \psi_k^{(\alpha)}(m,\sigma)^* \psi_k^{(\alpha)}(m',\sigma') n_F(\epsilon_k^{(\alpha)}) \,, \qquad (23)$$

which, for the case of small temperatures $T \ll \Delta$ and by inserting (22), can be written as

$$\langle a_{m\sigma}^\dagger a_{m'\sigma'} \rangle = \sum_{\alpha=1}^{\nu} \int_{-\pi}^{\pi} \frac{dk}{2\pi} \times \chi_k^{(\alpha)}(j,\sigma)^* \chi_k^{(\alpha)}(j',\sigma') e^{-ik(n-n')} \,. \qquad (24)$$

Here $\sum_{\alpha=1}^{\nu}$ denotes the sum over the occupied bands. The Bloch vectors $\chi_k^{(\alpha)}$ depend parametrically on e^{ik} and on the dispersion $\epsilon_k^{(\alpha)}$. The latter has a branching point in the complex plane with an imaginary part $\text{Im}(k) \sim a/\xi_c$[9–12], where ξ_c is some length scale averaged over all channel indizes. Closing the integration contour in the complex plane this gives the exponential decay of the propagator $\sim e^{-Z|n-n'|a/\xi_c}$, leading via (21) to the corresponding exponential decay (13) of the correlation function. For scales $|n-n'|a \sim \xi_c$ and $\xi_c \gg a$ we get $k \sim |n-n'|^{-1} \sim a/\xi_c \ll 1$ such that all $e^{ik} \approx 1$ and $\epsilon_k^{(\alpha)} \sim \Delta$. Therefore, the integral $\int dk \sim a/\xi_c$ and the propagator scales in the same way. For very short scales $|n-n'| \sim O(1)$ and $\xi_c \gg a$, the gap is not relevant and the propagator is of $O(1)$. The same occurs if $|n-n'| \sim O(1)$ and $\xi_c \sim a$. This proves (14).

Finally we note that it is quite useful to express the propagator (24) and the fluctuations via the density matrix introduced in Ref. [11]. For the propagator we get

$$\langle a_{m\sigma}^\dagger a_{m'\sigma'} \rangle = \frac{Z}{2\pi} \int_{-\pi/Z}^{\pi/Z} d\bar{k} \; \hat{n}_{j'\sigma',j\sigma}(\bar{k}) \; e^{-i\bar{k}(m-m')} , \qquad (25)$$

where $\bar{k} = k/Z$,

$$\bar{\chi}_{\bar{k}}^{(\alpha)}(j,\sigma) = e^{i\frac{k}{Z}(Z-j)} \chi_k^{(\alpha)}(j,\sigma) \,, \qquad (26)$$

and the density matrix (written as an operator in unit cell space)

$$\hat{n}(\bar{k}) = \sum_{\alpha=1}^{\nu} |\bar{\chi}_{\bar{k}}^{(\alpha)}\rangle \langle \bar{\chi}_{\bar{k}}^{(\alpha)}| = \hat{n}(\bar{k})^\dagger \,. \qquad (27)$$

We note the properties

$$\hat{n}(\bar{k})^2 = \hat{n}(\bar{k}) \,, \qquad (28)$$

$$\text{tr}\, \hat{n}_(\bar{k}) = \nu \,, \qquad (29)$$

which follow immediately from the orthogonality relation $\langle \bar{\chi}_{\bar{k}}^{(\alpha)} | \bar{\chi}_{\bar{k}}^{(\alpha')} \rangle = \delta_{\alpha\alpha'}$.

Using (25) one finds after integration by parts

$$(m-m') \langle a_{m\sigma}^\dagger a_{m'\sigma'} \rangle = -i \frac{Z}{2\pi} \int_{-\pi/Z}^{\pi/Z} d\bar{k} \times \left[\partial_{\bar{k}} \hat{n}_{j'\sigma',j\sigma}(\bar{k}) \right] e^{-i\bar{k}(m-m')} \,. \qquad (30)$$

Therefore, from (10) and (21) one can write the fluctuations in terms of the density matrix as

$$l_p\,\Delta Q_B^2 = \frac{a}{2}\int_{-\pi/Z}^{\pi/Z}\frac{d\bar{k}}{2\pi}\mathrm{tr}\{[\partial_{\bar{k}}\hat{n}(\bar{k})]^2\}\,. \tag{31}$$

The formula (31) can be equivalently rewritten in terms of the Bloch momentum k (instead of $\bar{k}$):

$$l_p\,\Delta Q_B^2 = \frac{Za}{2}\int_{-\pi}^{\pi}\frac{dk}{2\pi}\mathrm{tr}\{[\partial_k\hat{n}(k)]^2\}. \tag{32}$$

At finite temperature we have to use the following form of the density matrix

$$\hat{n}(\bar{k}) \to \tilde{n}(\bar{k}) = \sum_\alpha |\bar{\chi}_{\bar{k}}^{(\alpha)}\rangle\langle\bar{\chi}_{\bar{k}}^{(\alpha)}|\, n_F(\epsilon_{\bar{k}}^{(\alpha)})\,. \tag{33}$$

B. Example: Rice-Mele model

The Rice-Mele model is defined by $Z = 2$ with two hoppings $t_{1/2} > 0$ and staggered on-site potentials $v = v_1 = -v_2$. The Bloch Hamiltonian h_k in the two-dimensional unit cell reads

$$h_k = \begin{pmatrix} v & -t_1 - t_2e^{-ik} \\ -t_1 - t_2e^{ik} & -v \end{pmatrix} \tag{34}$$

and has eigenvalues

$$\epsilon_k^{(\pm)} = \pm\epsilon_k = \pm\sqrt{\Delta^2 + 4t_1t_2\cos^2\frac{k}{2}}, \tag{35}$$

where $\Delta = \sqrt{v^2 + (t_1 - t_2)^2}$ is half the energy gap $E_g = 2\Delta$ between the valence $\epsilon_k^{(-)}$ and the conduction $\epsilon_k^{(+)}$ bands. The corresponding eigenstates read

$$\chi_k^{(\pm)} = \frac{1}{\sqrt{2\epsilon_k(\epsilon_k \mp v)}}\begin{pmatrix} t_1 + t_2e^{-ik} \\ v \mp \epsilon_k \end{pmatrix}. \tag{36}$$

The expectation value for the boundary charge has been analysed in all detail in Ref. [13]. To calculate the fluctuations of the boundary charge we first insert the eigenstates (36) in (26), and find from (27) for the density matrix of the valence band

$$\hat{n}(k) = \frac{1}{2\epsilon_k}\begin{pmatrix} \epsilon_k - v & t_1e^{\frac{i}{2}k} + t_2e^{-\frac{i}{2}k} \\ t_1e^{-\frac{i}{2}k} + t_2e^{\frac{i}{2}k} & \epsilon_k + v \end{pmatrix}. \tag{37}$$

Computing the k-derivative we obtain

$$\begin{aligned}&\partial_k\hat{n}(k) \\ =&\partial_k(\frac{1}{2\epsilon_k})\begin{pmatrix} -v & t_1e^{\frac{i}{2}k} + t_2e^{-\frac{i}{2}k} \\ t_1e^{-\frac{i}{2}k} + t_2e^{\frac{i}{2}k} & v \end{pmatrix} \\ &+\frac{i}{4\epsilon_k}\begin{pmatrix} 0 & t_1e^{\frac{i}{2}k} - t_2e^{-\frac{i}{2}k} \\ -t_1e^{-\frac{i}{2}k} + t_2e^{\frac{i}{2}k} & 0 \end{pmatrix}.\end{aligned} \tag{38}$$

Using $\partial_k(\frac{1}{\epsilon_k}) = \frac{t_1t_2\sin k}{\epsilon_k^3}$, we evaluate

$$\begin{aligned}&\frac{1}{2}\int_{-\pi}^{\pi}\frac{dk}{2\pi}\mathrm{tr}\{[\partial_k\hat{n}(k)]^2\} = \int_{-\pi}^{\pi}\frac{dk}{2\pi}\frac{1}{16\epsilon_k^6} \\ &\times[(\Delta^2 + 4t_1t_2)^2(t_1 - t_2)^2\cos^2\frac{k}{2} \\ &+\Delta^4(t_1 + t_2)^2\sin^2\frac{k}{2} + 4v^2t_1^2t_2^2\sin^2 k].\end{aligned} \tag{39}$$

Performing this integral, we obtain from (32)

$$l_p\,\Delta Q_B^2 = a\frac{t_1^2 + t_2^2}{8\Delta}\frac{1}{\sqrt{\Delta^2 + 4t_1t_2}}. \tag{40}$$

In the wide-band limit $\frac{t_1+t_2}{2} \equiv t \gg \Delta$ we estimate

$$l_p\,\Delta Q_B^2 \approx \frac{ta}{8\Delta} = \frac{v_F}{16\Delta}\,, \tag{41}$$

with $v_F = 2ta$.

1. Finite temperature

At finite temperature (but still at fixed particle number) we replace $\hat{n}(k)$ by $\tilde{n}(k)$ defined in (33) (here we use k instead of $\bar{k} = k/2$). For a two-band model ($\alpha = \pm$) with the particle-hole symmetry $\epsilon_k^{(-)} = -\epsilon_k^{(+)} \equiv -\epsilon_k$, we use the completeness relation $\sum_{\alpha=\pm}|\bar{\chi}_k^{(\alpha)}\rangle\langle\bar{\chi}_k^{(\alpha)}| = \hat{1}$ in order to simplify (33)

$$\tilde{n}(k) = n_F(-\epsilon_k)\,\hat{n}(k) + n_F(\epsilon_k)\,(\hat{1} - \hat{n}(k)). \tag{42}$$

Hence

$$\begin{aligned}&\partial_k\tilde{n}(k) = [n_F(-\epsilon_k) - n_F(\epsilon_k)]\partial_k\hat{n}(k) \\ &+\{[\hat{1} - \hat{n}(k)]n_F'(\epsilon_k) - \hat{n}(k)n_F'(-\epsilon_k)\}\frac{d\epsilon_k}{dk}.\end{aligned} \tag{43}$$

Squaring this expression and using the properties (28), (29) as well as $\mathrm{tr}[\hat{n}(k)\partial_k\hat{n}(k)] = \mathrm{tr}[(\hat{1} - \hat{n}(k))\partial_k\hat{n}(k)] = 0$, we find the wide-band limit expression

$$\begin{aligned}&l_p\,\Delta Q_B^2 \approx \\ &\approx Za\int_{-\infty}^{\infty}\frac{dk}{2\pi}\left\{\frac{v_F^2\Delta^2}{4a^2\epsilon_k^4}[n_F(-\epsilon_k) - n_F(\epsilon_k)]^2\right. \\ &\left.+\frac{1}{2}[(n_F'(-\epsilon_k))^2 + (n_F'(\epsilon_k))^2]\left(\frac{d\epsilon_k}{dk}\right)^2\right\}.\end{aligned} \tag{44}$$

Note that the first term in the integrand follows from its finite-band counterpart in (39) in the limit under consideration.

Choosing $\mu = 0$, we evaluate (44)

$$\begin{aligned}&l_p\,\Delta Q_B^2 \approx \\ &\approx 2\frac{v_F}{\Delta}\int_0^{\infty}\frac{dx}{2\pi}\left\{\frac{\tanh^2(\frac{\Delta}{2T}\sqrt{x^2+1})}{2(1+x^2)^2}\right. \\ &\left.+\frac{(\Delta/T)^2}{8\cosh^4(\frac{\Delta}{2T}\sqrt{x^2+1})}\frac{x^2}{x^2+1}\right\},\end{aligned}$$

with the rescaled integration variable $x = \frac{v_F k}{a\Delta}$. This function decays monotonically in T, and at $T \gtrsim \Delta$ it behaves like $\sim \frac{v_F}{12\pi T}$. At zero T we recover (41), finding additionally the low-temperature correction

$$\approx -\frac{2v_F}{\Delta\sqrt{2\pi\Delta/T}} e^{-\Delta/T}. \tag{45}$$

C. Low-energy theory for single channel models

For the case of a noninteracting and clean single channel lattice model in the limit of small gap $E_g \ll W$, where $\xi_g \gg a$, one can describe the low-energy physics by an effective Dirac Hamiltonian in $1+1$ dimensions[8]

$$H_{\rm bulk} = \int dx\, \underline{\psi}^\dagger(x) \{-iv_F\partial_x\sigma_z + \Delta\cos\gamma\,\sigma_x - \Delta\sin\gamma\,\sigma_y\}\, \underline{\psi}(x)\,, \tag{46}$$

where $E_g = 2\Delta$ is the gap size, $k_F = \pi\nu/(Za)$ is the Fermi momentum at which the gap opens, $v_F = 2ta\sin(k_F a)$ denotes the Fermi velocity ($t \sim W$ is the average hopping), and $\underline{\psi}(x)$ is a two-component field consisting of slowly varying right- and left-moving fields $\psi_\pm(x)$ such that the physical field operator can be expressed as

$$\psi(x) = \sum_{p=\pm} \psi_p(x) e^{ipk_F x}\,. \tag{47}$$

The variable γ describes the phase of the order parameter such that $\Delta e^{i\gamma}$ describes the transition matrix element from $-k_F$ to k_F, see Ref. 8.

The Dirac model has two bands with dispersion $\pm\epsilon_k = \pm\sqrt{v_F^2 k^2 + \Delta^2}$. For a chemical potential in the gap and $T \ll \Delta$ all states of the valence band are filled. The eigenstates of the valence band states are given by

$$\underline{\psi}_k(x) = \frac{1}{\sqrt{2\pi N_k}} \begin{pmatrix} -\Delta e^{i\gamma} \\ v_F k + \epsilon_k \end{pmatrix} e^{ikx}\,, \tag{48}$$

with normalization factor $N_k = \Delta^2 + (v_F k + \epsilon_k)^2 = 2\epsilon_k(\epsilon_k + v_F k)$. Using this result one can straightforwardly calculate the propagators

$$\begin{aligned}\langle\psi_p^\dagger(x)\psi_{p'}(x')\rangle &= \int dk \langle\psi_{k,p}^\dagger(x)\psi_{k,p'}(x')\rangle \\ &= \frac{1}{2}\delta(x-x')\delta_{pp'} + \frac{1}{4\pi\xi_g}\Big[i\sigma_z K_1\left(\frac{x-x'}{2\xi_g}\right) \\ &\quad - (\cos\gamma\,\sigma_x + \sin\gamma\,\sigma_y) K_0\left(\frac{x-x'}{2\xi_g}\right)\Big]_{pp'}\,,\end{aligned} \tag{49}$$

where K_ν denotes the modified Bessel function of the second kind, σ_i are the Pauli matrices, and $\xi_g = \frac{v_F}{2\Delta} = \frac{v_F}{E_g}$ is the exponential decay length. Using (47) and omitting the divergent contribution at $x = x'$ (which can not be determined from a low-energy model) we find for the density-density correlation function the form

$$\begin{aligned}C_{\rm bulk}(x,x') &= -|\langle\psi^\dagger(x)\psi(x')\rangle|^2 \\ &= -\frac{1}{4\pi^2\xi_g^2}\Big\{K_1\left(\frac{x-x'}{2\xi_g}\right)\sin[k_F(x-x')] \\ &\quad - K_0\left(\frac{x-x'}{2\xi_g}\right)\cos[k_F(x+x')+\gamma]\Big\}^2\,.\end{aligned} \tag{50}$$

To calculate $C^{\rm bulk}_{jj'}\big(Z(n-n')a\big)$ of the original lattice model, we insert $x = ma$ and $x' = m'a$ into this equation. Using $m = Z(n-1)+j$ and $m' = Z(n'-1)+j'$ together with $k_F = \pi\nu/(Za)$, one finds (except for $n = 0$ and $j = j'$) the final result

$$\begin{aligned}C^{\rm bulk}_{jj'}(Zn) &= -\frac{1}{4\pi^2\xi_g^2} \\ &\times\Big\{K_1\left(\frac{Zn+j-j'}{2\xi_g}\right)\sin[\pi\frac{\nu}{Z}(j-j')] \\ &- K_0\left(\frac{Zn+j-j'}{2\xi_g}\right)\cos[\pi\frac{\nu}{Z}(j+j')+\gamma]\Big\}^2\,.\end{aligned} \tag{51}$$

Comparing this analytical result in the low-energy limit with exact numerical ones for the original lattice model we find for small gaps a surprisingly perfect agreement even for small values of n. Using the asymptotic forms

$$K_0(s) \to \begin{cases}\sqrt{\frac{\pi}{2|s|}}\, e^{-|s|} & \text{for } |s| \gg 1 \\ -\ln|s| & \text{for } |s| \ll 1\end{cases} \tag{52}$$

$$K_1(s) \to \begin{cases}\text{sign}(s)\sqrt{\frac{\pi}{2|s|}}\, e^{-|s|} & \text{for } |s| \gg 1 \\ \frac{1}{s} & \text{for } |s| \ll 1\end{cases}\,, \tag{53}$$

we find that the properties (13) and (14) are fulfilled. Averaging the correlation function over j and j' according to (17) we find for $|n| \gg 1$ (where we can neglect $j - j'$ in the argument of the Bessel functions in (51)) the compact form

$$\bar{C}_{\rm bulk}(x) \approx -\frac{1}{8\pi^2\xi_g^2}\left\{\left[K_0\left(\frac{x}{2\xi_g}\right)\right]^2 + \left[K_1\left(\frac{x}{2\xi_g}\right)\right]^2\right\}\,, \tag{54}$$

with the following asymptotics for small and large $|x|$

$$\bar{C}_{\rm bulk}(x) \to -\frac{1}{2\pi}\begin{cases}\frac{1}{2\xi_g|x|} e^{-|x|/\xi_g} & \text{for } |x| \gg \xi_g \\ \frac{1}{\pi x^2} & \text{for } |x| \ll \xi_g\end{cases}\,. \tag{55}$$

Inserting the result (54) in (16) gives the following result for the boundary charge fluctuations close to the phase transition point

$$l_p\,\Delta Q_B^2 = \frac{\xi_g}{8} = \frac{v_F}{16\Delta}\,. \tag{56}$$

This result generalizes the result (41) obtained for the Rice-Mele model to any single channel model.

IV. SSH MODEL WITH DISORDER

Here we treat the disordered Su-Schrieffer-Heeger (SSH) model in Born approximation to calculate the gap at moderate disorder strength. The infinite bulk model is defined by the single-particle Hamiltonian

$$h = h_0 + V \,, \tag{57}$$

$$h_0 = -\sum_m t_m |m+1\rangle\langle m| + \text{h.c.} \,, \tag{58}$$

$$V = -\sum_m w_m |m+1\rangle\langle m| + \text{h.c.} \,, \tag{59}$$

where $t_m = t_{m+2}$ are alternating hoppings with $t_{1/2} > 0$, and w_m describes random bond disorder taken from a uniform distribution $w_m \in [-d_m/2, d_m/2)$, with $d_m = d_{m+2} > 0$ describing the strength of disorder on site m. The disorder-averaged progagator can be written in terms of the self-energy as

$$\begin{aligned}\bar{G}(E) &= \left(\prod_m \frac{1}{d_m}\int_{-d_m/2}^{d_m/2} dw_m\right)\frac{1}{E-h} \\ &= \frac{1}{E - h_0 - \Sigma(E)} \,.\end{aligned} \tag{60}$$

From the definition we get the useful properties (for any E in the complex plane)

$$\bar{G}(E)^\dagger = \bar{G}(E^*) \quad , \quad \Sigma(E)^\dagger = \Sigma(E^*) \,, \tag{61}$$

or

$$\bar{G}(E)^T = \bar{G}^*(E) \quad , \quad \Sigma(E)^T = \Sigma^*(E) \,, \tag{62}$$

where $A(E)^T$ is the transposed matrix and $A^*(E)$ denotes the conjugate complex of the matrix (without taking the conjugate complex of E). Due to translational invariance we can write the SSH Hamiltonian h_0 and the self-energy $\Sigma(E)$ in diagonal form with respect to the quasimomentum k

$$h_0 = \int_{-\pi}^{\pi} dk |k\rangle\langle k| \otimes h_k^{(0)} \,, \tag{63}$$

$$\Sigma(E) = \int_{-\pi}^{\pi} dk |k\rangle\langle k| \otimes \Sigma_k(E) \,, \tag{64}$$

where

$$\langle n|k\rangle = \frac{1}{\sqrt{2\pi}} e^{ikn} \tag{65}$$

are plane waves with respect to the unit cell index n, and $h_k^{(0)}$ and $\Sigma_k(E)$ are 2×2-matrices within the 2-dimensional unit cell space. For the SSH model we get the form

$$h_k^{(0)} = \begin{pmatrix} 0 & -t_1 - t_2 e^{-ik} \\ -t_1 - t_2 e^{ik} & 0 \end{pmatrix} . \tag{66}$$

In this notation matrix elements of the free propagator $g(E) = 1/(E - h_0)$ can be written as

$$g(E)_{mm'} = \hat{g}(E, n-n')_{jj'} \,, \tag{67}$$

where $m = 2(n-1) + j$, $m' = 2(n'-1) + j'$ and

$$\begin{aligned}\hat{g}(E,n) &= \int_{-\pi}^{\pi} \frac{dk}{2\pi}\, e^{ikn}\, \frac{1}{E - h_k^{(0)}} \\ &= \int_{-\pi}^{\pi} \frac{dk}{2\pi}\, e^{ikn}\, \frac{E - (t_1 + t_2\cos k)\sigma_x - (t_2 \sin k)\sigma_y}{E^2 - t_1^2 - t_2^2 - 2t_1 t_2 \cos k}\end{aligned} \tag{68}$$

is a 2×2-matrix with $\sigma_{x,y,z}$ denoting the Pauli matrices.

In standard Born approximation (see, e.g., Ref. 14) we find for the nonvanishing matrix elements

$$\Sigma(E)_{m,m+1} = \frac{d_m^2}{12}\, g(E)_{m+1,m} \,, \tag{69}$$

$$\Sigma(E)_{m+1,m} = \frac{d_m^2}{12}\, g(E)_{m,m+1} \,, \tag{70}$$

$$\Sigma(E)_{m,m} = \frac{d_m^2}{12}\, g(E)_{m+1,m+1} + \frac{d_{m-1}^2}{12}\, g(E)_{m-1,m-1} \,. \tag{71}$$

Since, according to (67) and (68), the diagonal elements $g(E)_{mm}$ of the propagator are independent of m, (71) describes only a constant shift of the energy leading to the renormalized energy

$$\tilde{E} = E\left(1 - \frac{d_1^2 + d_2^2}{12}\int_{-\pi}^{\pi}\frac{dk}{2\pi}\frac{1}{E^2 - t_1^2 - t_2^2 - 2t_1 t_2\cos k}\right) , \tag{72}$$

such that the averaged propagator in Born approximation can be written as

$$\bar{G}(E) = \frac{1}{\tilde{E} - h(E)} \,, \tag{73}$$

with $h(E) = h_0 + \Sigma(E)$. Using the matrix elements of the self-energy in Born approximation we can write

$$h(E) = -\sum_m \left\{ t_m(E)|m+1\rangle\langle m| + t_m^*(E)|m\rangle\langle m+1| \right\} , \tag{74}$$

where $t_m(E) = t_{m+2}(E)$ and

$$t_1(E) = t_1 - \Sigma(E)_{21} = t_1 - \frac{d_1^2}{12}\, g(E)_{12} \,, \tag{75}$$

$$t_2(E) = t_2 - \Sigma(E)_{32} = t_2 - \frac{d_2^2}{12}\, g(E)_{23} \,, \tag{76}$$

and $t_j^*(E)$ follows from the conjugate complex (but leaving E invariant). Using (67) we get $g(E)_{12} = \hat{g}(E,0)_{12}$ and $g(E)_{23} = \hat{g}(E,-1)_{21}$ which, together with (68), leads to

$$g(E)_{12} = \int_{-\pi}^{\pi}\frac{dk}{2\pi}\frac{t_1 + t_2 e^{ik}}{|t_1 + t_2 e^{ik}|^2 - E^2} \,, \tag{77}$$

$$g(E)_{23} = \int_{-\pi}^{\pi}\frac{dk}{2\pi}\frac{t_2 + t_1 e^{ik}}{|t_2 + t_1 e^{ik}|^2 - E^2} \,. \tag{78}$$

At zero energy we get

$$g(0)_{12} = \frac{1}{t_1}\theta(t_1 - t_2)\,, \tag{79}$$

$$g(0)_{23} = \frac{1}{t_2}\theta(t_2 - t_1)\,, \tag{80}$$

leading to the following final result for the gap in the presence of disorder

$$\begin{aligned} E_g &= 2|t_1(0) - t_2(0)| \\ &= |2(t_1 - t_2) - \frac{d_1^2}{6\,t_1}\theta(t_1 - t_2) + \frac{d_2^2}{6\,t_2}\theta(t_2 - t_1)|\,. \end{aligned} \tag{81}$$

For $t_1 > t_2$ this leads to the gap closing condition

$$r = \frac{t_1}{t_2} = \frac{1}{2}\left\{1 + \sqrt{1 + \frac{d_1^2}{3t_2^2}}\right\}\,, \tag{82}$$

which agrees rather well with the numerical result up to $d_1 \sim 2-3$. For $t_1 < t_2$, Born approximation turns out to be insufficient, which will be studied in a future work[15].

V. HIGHER DIMENSIONS

In this section we calculate the fluctuations for noninteracting and clean models in higher dimensions $D = 2, 3$. We start with $D = 2$ and combine a standard 2D quantum Hall insulator[16] with an additional modulation of the on-site potentials and nearest-neighbor hoppings in x-direction. Such models were studied extensively in Refs. [1, 8, 12, 13, 17, and 18] to study the expectation value of the boundary charge. We start from a 2D tight-binding model with sites labeled by (m, σ) with $m = 1, \ldots, N_s$ in x-direction and $\sigma = 1, \ldots, N_\perp$ in y-direction. The lattice spacing $a = a_x = a_y$ is assumed to be the same in both directions. We take open boundary conditions in x-direction and periodic ones in y-direction. We consider a constant magnetic field B perpendicular to the sample in Landau gauge $\underline{A}(m, \sigma) = (0, Bm, 0)$. As a result, the hopping in y-direction from $(m, \sigma) \to (m, \sigma + s)$ aquires a phase factor $e^{i2\pi sm/Z}$, where $\lambda_B = Za$ is the magnetic length defined by $\lambda_B/a = Z = \Phi_0/(Ba^2)$, where $\Phi_0 = hc/e$ denotes the flux quantum. For simplicity we assume that Z is an integer. If an additional flux Φ is applied through the hole of the cylinder when the system is deformed to a ring in y-direction, an additional phase factor $e^{-is\theta/N_\perp}$ with $\theta = 2\pi\Phi/\Phi_0$ has to be considered for the hopping in y-direction by s sites.

Taking real and negative nearest-neighbor hoppings $-t_m = -t_{m+Z}$ in x-direction and $-t_y$ in y-direction, together with real on-site potentials $v_m = v_{m+Z}$, we arrive at the following 2D tight-binding model

$$\begin{aligned} H &= \sum_{m=1}^{N_s}\sum_{\sigma=1}^{N_\perp} v_m a^\dagger_{m\sigma} a_{m\sigma} \\ &- \sum_{m=1}^{N_s-1}\sum_{\sigma=1}^{N_\perp} t_m (a^\dagger_{m+1,\sigma} a_{m\sigma} + \text{h.c.}) \\ &- t_y \sum_{m=1}^{N_s}\sum_{\sigma=1}^{N_\perp}\left(e^{i(2\pi m/Z - \theta/N_\perp)} a^\dagger_{m,\sigma+1} a_{m\sigma} + \text{h.c.}\right)\,, \end{aligned} \tag{83}$$

with $a_{m\sigma} = a_{m,\sigma+N_\perp}$ due to periodic boundary conditions in y-direction. Using Fourier transform for the modes in this direction

$$a_{m\sigma} = \frac{1}{\sqrt{N_\perp}}\sum_{k_y} e^{ik_y a\sigma} c_{mk_y}\,, \tag{84}$$

with

$$k_y = \frac{2\pi}{N_\perp a}s \quad , \quad s = 1, \ldots, N_\perp\,, \tag{85}$$

we can write the Hamiltonian as an independent sum over all transverse quasimomenta

$$H = \sum_{k_y} H(k_y) \tag{86}$$

$$\begin{aligned} H(k_y) &= \sum_{m=1}^{N_s} \bar{v}_m(k_y a + \theta/N_\perp) c^\dagger_{mk_y} c_{mk_y} \\ &- \sum_{m=1}^{N_s-1} t_m (c^\dagger_{m+1,k_y} c_{mk_y} + \text{h.c.})\,, \end{aligned} \tag{87}$$

with

$$\bar{v}_m(\varphi) = v_m - 2t_y \cos\left(\frac{2\pi}{Z}m - \varphi\right)\,. \tag{88}$$

The charge operator summed over all transverse modes is given by

$$\hat{\rho}_m = \sum_{\sigma=1}^{N_\perp} a^\dagger_{m\sigma} a_{m\sigma} = \sum_{k_y} c^\dagger_{mk_y} c_{mk_y}\,. \tag{89}$$

Since the Hamiltonian does not couple the transverse modes, the fluctuations of the boundary charge operator (1) can be written as an independent sum over the transverse modes

$$\Delta Q_B^2 = \sum_{k_y} \Delta Q_B^2(k_y)\,, \tag{90}$$

where $\Delta Q_B^2(k_y)$ describe the boundary charge fluctuations of the effectively 1-dimensional Hamiltonian $H(k_y)$ at fixed k_y. Denoting by $2\Delta(k_y)$ the gap of this Hamiltonian and by $v_F(k_y)$ the Fermi velocity, we can take in the low-energy limit of small gap compared to the band width the result (56), leading for $N_\perp \to \infty$ to the integral

$$l_p \Delta Q_B^2 = \sum_{k_y} \frac{v_F(k_y)}{16\Delta(k_y)} \to \frac{N_\perp a}{2\pi} \int_{-\pi/a}^{\pi/a} dk_y \frac{v_F(k_y)}{16\Delta(k_y)} . \quad (91)$$

To evaluate the result (91) explicitly, we consider an illustrative example in terms of the Rice-Mele model, with $Z = 2$ and $v_m = 0$. Using (88) we obtain

$$\bar{v}_m(\varphi) = (-1)^m v(\varphi) \ , \ v(\varphi) = -2t_y \cos(\varphi) . \quad (92)$$

The gap opens up at $k_F = \pi/(2a)$ which corresponds to half-filling. In the low-energy limit $t_y, |t_1 - t_2| \ll t = (t_1 + t_2)/2$, we obtain $v_F(k_y) = 2ta$ and

$$\Delta(k_y) = \sqrt{\left[v(k_y a + \theta/N_\perp)\right]^2 + |t_1 - t_2|^2} . \quad (93)$$

Inserting in (91) and calculating the integral leads to the final result

$$l_p \Delta Q_B^2 = \frac{N_\perp}{8\pi} \frac{v_F}{\sqrt{4t_y^2 + \Delta^2}} K\left(\frac{4t_y^2}{4t_y^2 + \Delta^2}\right) , \quad (94)$$

where $K(p) = \int_0^{\pi/2} dx \left[1 - p \sin^2(x)\right]^{-1/2}$ is the elliptic integral of first kind, and

$$E_g = 2\Delta = 2 \, \min_{k_y} \Delta(k_y) = 2|t_1 - t_2| \quad (95)$$

denotes the gap for the 2-dimensional system. As expected the fluctuations are independent of the phase θ.

For $\Delta \ll t_y$, we can use the asymptotics $K(p) \to \frac{1}{2} \ln\left(16/(1-p)\right)$ for $p \to 1$, and obtain a logarithmic scaling of the fluctuations as function of the gap close to the phase transition

$$l_p \, \Delta Q_B^2 \xrightarrow{\Delta \ll t_y} \frac{N_\perp}{16\pi} \frac{v_F}{t_y} \ln \frac{8t_y}{\Delta} . \quad (96)$$

For the Rice-Mele model, we can also use the exact result (40) to calculate the fluctuations at fixed k_y. Performing the integral over k_y this leads to the following result for the total fluctuations

$$l_p \, \Delta Q_B^2 = N_\perp a \frac{4t^2 + \Delta^2}{32\pi t_y^2} I(\frac{\Delta}{2t_y}, \frac{t}{t_y}) , \quad (97)$$

with

$$I(a, b) = \frac{1}{b\sqrt{1 + a^2}} K\left(\frac{b^2 - a^2}{b^2(1 + a^2)}\right) . \quad (98)$$

To compare with (94) we can rewrite this result as

$$l_p \Delta Q_B^2 = \frac{N_\perp}{8\pi} \frac{2ta(1 + \frac{\Delta^2}{4t^2})}{\sqrt{4t_y^2 + \Delta^2}} K\left(\frac{t_1 t_2}{t^2} \frac{4t_y^2}{4t_y^2 + \Delta^2}\right) , \quad (99)$$

and find that they agree for $\Delta = |t_1 - t_2| \ll t = (t_1 + t_2)/2$.

In the low-energy regime one can also analyse the boundary charge analytically. It is given as an independent sum over the boundary charges of the effective one-dimensional models

$$Q_B(\theta) = \sum_{k_y} Q_B^{1\text{D}}(k_y a + \frac{\theta}{N_\perp}) . \quad (100)$$

Using (85) and the periodicity $Q_B^{1\text{D}}(\varphi) = Q_B^{1\text{D}}(\varphi + 2\pi)$, this can also be written as

$$Q_B(\theta) = \frac{N_\perp}{2\pi} \sum_{l=-\infty}^{\infty} e^{il\theta} \int_0^{2\pi} d\varphi \, Q_B^{1\text{D}}(\varphi) e^{-ilN_\perp \varphi} . \quad (101)$$

At zero chemical potential the boundary charge of the one-dimensional model can be calculated from the low-energy analysis of Ref. [12] as

$$Q_B^{1\text{D}}(\varphi) = \frac{\gamma(\varphi)}{2\pi} + \frac{1}{4} - \theta_{\pi/2 < \gamma(\varphi) < \pi} , \quad (102)$$

where $-\pi < \gamma(\varphi) < \pi$ and

$$\Delta(\varphi) e^{i\gamma(\varphi)} = v(\varphi) + i(t_2 - t_1) . \quad (103)$$

Since $t_{1,2}$ are independent of the phase, $\gamma(\varphi) = \gamma(\varphi + 2\pi)$ is bounded to an interval smaller than 2π and the phase factor $e^{i\gamma(\varphi)}$ can not wind around the origin in the complex plane. As a consequence, $Q_B^{1\text{D}}(\varphi)$ is a smooth and periodic function of φ and the integral in (101) can only contribute for $l = 0$. Therefore, for this special model, the boundary charge is independent of θ and the Hall current is zero. This result holds not only in the low-energy regime but also at large gap.

Although the topology does not change at the phase transition point $r = t_1/t_2 = 1$, there is a discontinuous change of the appearance of edge states in the gap. For $r > 1$, there is no edge state for any k_y, whereas, for $r < 1$, an edge state appears for all k_y at energy $-v(k_y a + \theta/N_\perp) = 2t_y \cos(k_y a + \theta/N_\perp)$ which never touches the band edges. Therefore, the gap has to close at the transition, and the fluctuations show the same characteristic scaling as for topological phase transitions where the gap closing is induced by a change of the Chern number.

The above analysis can easily be generalized to a $3D$-system by choosing a nearest-neighbor hopping t_z in z-direction and adding a magnetic field of size B in y-direction. Omitting the additional flux Φ, we can write the Hamiltonian as an independent sum over all k_y and k_z

$$H = \sum_{k_y k_z} H(k_y, k_z) \quad (104)$$

$$H(k_y, k_z) = \sum_{m=1}^{N_s} \bar{v}_m(k_y, k_z) c^\dagger_{m k_y k_z} c_{m k_y k_z} - \sum_{m=1}^{N_s - 1} t_m (c^\dagger_{m+1, k_y k_z} c_{m k_y k_z} + \text{h.c.}) , \quad (105)$$

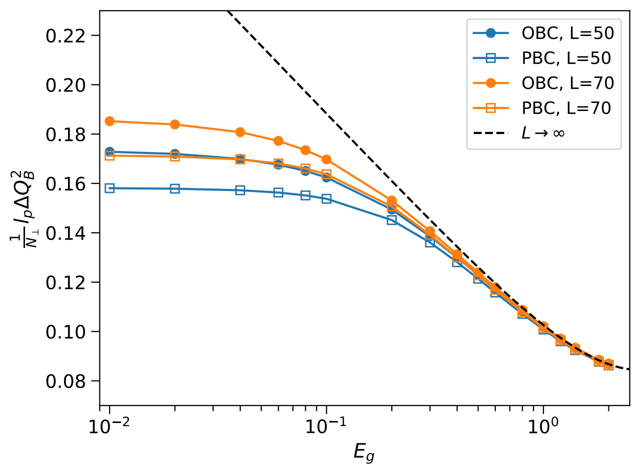

FIG. 1. Comparison of different system sizes $L = N_\perp a = N_s a$ and boundary conditions of the two dimensional model discussed in the text. The parameters are given by $Z = 2$, $v_m = 0$, $t_{1/2} = 1.0 \pm \Delta/2$, $t_y = 1.0$, $\theta = 0$, $L_p = L/2$ and $l_p = (24, 34)$ whereby Δ is varied in the interval $[0.005, 1.0]$.

with

$$\bar{v}_m(k_y, k_z) = v_m - 2t_y \cos\left(\frac{2\pi}{Z}m - k_y a\right) - 2t_z \cos\left(\frac{2\pi}{Z}m - k_z a\right). \tag{106}$$

Taking again the special case $Z = 2$ and $v_m = 0$, we obtain for each fixed (k_y, k_z) an effective Rice-Mele model with potential $v(k_y, k_z) = \bar{v}_1(k_y, k_z) = -\bar{v}_2(k_y, k_z)$, where

$$v(k_y, k_z) = 2t_y \cos(k_y a) + 2t_z \cos(k_z a)\,. \tag{107}$$

Using the exact result (40) for the calculation of the fluctuations at fixed (k_y, k_z) and integrating over the transverse momenta one arrives straightforwardly at the following result for the total fluctuations

$$l_p\,\Delta Q_B^2 = N_\perp^2 a^2 \frac{4t^2 + \Delta^2}{32\pi^2 t_y^2} \int_0^{\pi/a} dk_z I\left(g(k_z), h(k_z)\right)\,, \tag{108}$$

with

$$g(k_z) = \frac{1}{2t_y}\sqrt{t_z^2 \cos^2(k_z a) + \Delta^2}\,, \tag{109}$$

$$h(k_z) = \frac{1}{2t_y}\sqrt{t_z^2 \cos^2(k_z a) + 4t^2}\,, \tag{110}$$

and $I(a, b)$ is defined in (98). This leads to a convergent result for the fluctuations in the zero gap limit $\Delta \to 0$.

To access the influence of different boundary conditions at finite system size we consider the two-dimensional model described above on a square lattice with $L = N_\perp a = N_s a$. Figure 1 summarizes the finite size scaling (symbols) compared to the infinite limit (dashed line) for open (OPC) and periodic (PBC) boundary conditions. As the system size is increased the universal result is approached for increasingly smaller gaps E_g.

VI. SPECIAL PHASE TRANSITIONS

Sometimes an expansion of the Bloch Hamiltonian h_k around the quasimomentum where the gap opens does not contain linear terms due to special symmetry conditions. An exemplary model of this type has been discussed in Ref. [19]. It contains only constant and quadratic terms in k:

$$h_k = \begin{pmatrix} \Delta + \alpha k^2 & \Gamma k^2 \\ \Gamma k^2 & -\Delta - \beta k^2 \end{pmatrix}. \tag{111}$$

The gap between the two bands is $E_g = 2\Delta$. The Bloch eigenstates depend only on the combination $\frac{\Delta}{k^2}$. It follows immediately that the imaginary part κ of the branching point appears to be $\kappa \sim \sqrt{E_g}$. Thus, $l_p \Delta Q_B^2 \sim E_g^{-1/2}$.

This can be generalized to the case where the minimal nonvanishing order of k in the expansion of h_k is l. This gives straightforwardly the scaling $l_p \Delta Q_B^2 \sim \xi \sim E_g^{-1/l}$.

We note in passing that in quasi-two-dimensional models the band structure of the form (111) can be realized in the multilayer graphene with a special stacking[20]. However, as has been shown in Section V, for a $2D$-system the fluctuations follow from an integration over the transverse momentum k_y. Assuming close to the gap opening a general dispersion relation for the conduction band of the form

$$\epsilon(k_x, k_y) = (\Delta^{2/l} + ck^2)^{l/2}\,, \tag{112}$$

the solution of $\epsilon(k_x, k_y) = 0$ for fixed k_y gives in the complex plane the solution $k_x = 2i/\xi(k_y)$, with

$$\xi(k_y) = \frac{2\sqrt{c}}{\sqrt{\Delta^{2/l} + ck_y^2}}\,. \tag{113}$$

The gap at fixed k_y is given by $E_g(k_y) = 2\epsilon(0, k_y) = 2(\Delta^{2/l} + ck_y^2)^{l/2}$, leading to an exotic scaling for the fluctuations of Q_B at fixed k_y

$$l_p \Delta Q_B^2(k_y) \sim \xi(k_y) \sim E_g(k_y)^{-1/l}\,. \tag{114}$$

However, this does not change the logarithmic scaling of the total fluctuations in terms of the overall gap $E_g = 2\Delta$

$$l_p \Delta Q_B^2 \sim \int_{-\pi/a}^{\pi/a} dk_y\,\xi(k_y) \overset{E_g \to 0}{\sim} |\ln(E_g/W)|\,, \tag{115}$$

where W defines the high-energy cutoff in terms of the band width.

* Email: Dante.Kennes@rwth-aachen.de

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