# Entanglement scaling in critical two-dimensional fermionic and bosonic systems

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We relate the reduced density matrices of quadratic fermionic and bosonic models to their Green's function matrices in a unified way and calculate the scaling of the entanglement entropy of finite systems in an infinite universe exactly. For critical fermionic two-dimensional (2D) systems at $T=0$, two regimes of scaling are identified: generically, we find a logarithmic correction to the area law with a prefactor dependence on the chemical potential that confirms earlier predictions based on the Widom conjecture. If, however, the Fermi surface of the critical system is zero-dimensional, then we find an area law with a sublogarithmic correction. For a critical bosonic 2D array of coupled oscillators at $T=0$, our results show that the entanglement entropy follows the area law without corrections.

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## I. INTRODUCTION

Entanglement is a key feature of the nonclassical nature of quantum mechanics. It is a necessary resource for quantum computation and at the heart of interesting connections between quantum information theory and traditional quantum many-body theory, such as in quantum critical phenomena [1–3] or the quantum Hall effect [4,5].

One of the most widely used entanglement measures for pure states is the entropy of bipartite entanglement: For a pure state $|\Psi_{\mathcal{AB}}\rangle$ of a bipartite "universe" $\mathcal{AB}$ consisting of system $\mathcal{A}$ and environment $\mathcal{B}$, it is given by the von Neumann entropy $S_{\mathcal{A}}=-\mathrm{Tr}\,\rho_{\mathcal{A}}\log_2\rho_{\mathcal{A}}$, where $\rho_{\mathcal{A}}=\mathrm{Tr}_{\mathcal{B}}|\Psi_{\mathcal{AB}}\rangle\langle\Psi_{\mathcal{AB}}|$ is the reduced density matrix of system $\mathcal{A}$.

An important question is how the entanglement entropy scales at $T=0$ with the size of the system, assuming the universe to be in the thermodynamic limit. This was first studied by Beckenstein in the context of black hole entropy [6]. As opposed to thermodynamic entropy, which is extensive, entanglement entropy was found to be proportional to the area of the black hole's event horizon, its physical locus being essentially the hypersurface separating system and environment. Entanglement entropy scaling hence depends decisively on the dimension $d$ of the universe.

This observation has given rise to a long string of studies of this so-called area law. In one dimension $d=1$, scaling is well understood both for fermions [2,7–11] and bosons [12,13]. For one-dimensional spin chains at $T=0$, one finds that the entanglement entropy $S_{\mathcal{A}}(L)$ of a system $\mathcal{A}$ of linear size $L$ saturates away from criticality, but scales as $\log_2 L$ when the system becomes critical [2], i.e., when correlation lengths diverge. In the latter case, conformal field theory (CFT) yields [14,15] $S_{\mathcal{A}}(L)=\frac{c+\bar{c}}{6}\log_2 L+k$, where $c$ and $\bar{c}$ are the holomorphic and the antiholomorphic central charges of the field theory. Essentially, there is no physical limit to the boundary region between system and environment.

The situation is far less clear in higher dimensions $d>1$. The area law implies that, away from criticality, the entanglement entropy is essentially proportional to the surface area of system $\mathcal{A}$

$$S_{\mathcal{A}}\sim L^{d-1}, \tag{1}$$

as confirmed in analytical calculations for (bosonic) noncritical coupled oscillators [16].

At criticality, the correlation lengths diverge and one may expect corrections to the area law, as for $d=1$. For critical ground-states of fermionic tight-binding Hamiltonians, the entanglement entropy was indeed found to scale as

$$S_{\mathcal{A}}\sim L^{d-1}\log_2 L, \tag{2}$$

for both lattice models [17] and continuous fields [18]. The prefactor could only be derived [18] assuming (i) the validity of the Widom conjecture [19] and (ii) its applicability to the functional form of binary entropy. For bosons at criticality, numerical evidence for the area law (1) was found for a three-dimensional array of coupled oscillators [20]. Callan and Wilczek derived the area law in approximative field theoretical calculations [21].

Beyond the fundamental physical interest, entanglement scaling sets the scope of entanglement-based numerical methods, such as the density-matrix renormalization group (DMRG) [22,23], as the computation time required to simulate a quantum state using these methods on classical computers increases exponentially with its entanglement entropy.

In this paper, we study the bipartite entanglement entropy in a *unified* treatment for *exactly solvable* two-dimensional fermionic and bosonic models at $T=0$. To this purpose, we relate the reduced density matrix of a quadratic model to its Green's function matrices, generalizing work by Cheong and Henley [24] based on a coherent-state method developed by Chung and Peschel [25]. For the critical fermionic two-dimensional tight-binding model, we find as expected (2), but our exact calculation allows one to identify the dependence of the scaling law prefactor on the chemical potential $\mu$. We exactly verify the behavior predicted in [18], where the validity of the Widom conjecture and its applicability to the binary entropy were assumed. Interestingly, we observe a *sublogarithmic* correction to the area law if the gap of the model closes in a zero-dimensional region of momentum space (i.e., one or more points). For a critical bosonic two-dimensional model of coupled harmonic oscillators, we find the entanglement entropy to saturate to the area law (2), which confirms [20,21].

The generic quadratic Hamiltonians studied here are

 

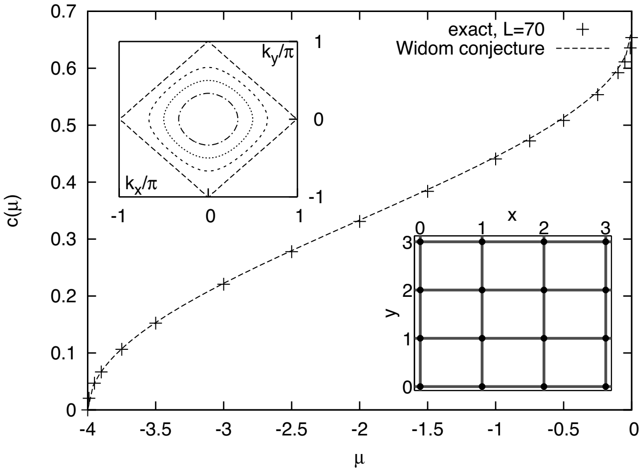


FIG. 1. The prefactor $c(\mu)$ in the entanglement entropy scaling law as a function of the chemical potential $\mu$ for the ground-state of the two-dimensional fermionic tight-binding model in comparison to the result of Gioev and Klich [18]. Insets show the hopping parameters and the Fermi surfaces for $\mu=-3,-2,-1,0$.

$$H_{F,B}=\sum_{ij}\left[a_i^\dagger V_{ij}a_j+\frac{1}{2}(a_i^\dagger W_{ij}a_j^\dagger+\text{H.c.})\right], \tag{3}$$

where $a_i\equiv c_i$ and $a_i\equiv b_i$ are fermionic and bosonic operators for $H_F$ and $H_B$, respectively. Previous field-theoretical work did not indicate any qualitative dependence of the entanglement entropy scaling on the presence or absence of interactions in the systems. For one-dimensional systems, it is known that the decisive difference is the presence or absence of criticality, in whatever way it comes about. This is why the free case is, for once, highly relevant.

## II. CALCULATING ENTROPY FROM GREEN'S MATRICES

We consider a bipartite universe $\mathcal{AB}$ of $N$ modes (or sites). System $\mathcal{A}$ consists of $n$ sites; in our calculations, we will eventually take the thermodynamic limit $N\to\infty$. The relation between the Green's function matrices of system $\mathcal{A}$ and its reduced density matrix $\rho_{\mathcal{A}}=\text{Tr}_{\mathcal{B}}\,\rho$ can be derived by determining the matrix elements of the full density matrix $\rho$ with respect to coherent states and integrating out the variables of the environment $\mathcal{B}$.

### A. Fermionic systems

The Green's function matrix for system $\mathcal{A}$ with respect to the operators $A_i\equiv c_i^\dagger+c_i$ and $B_i\equiv c_i^\dagger-c_i$, as defined by

$$[G_{BA}]_{ij}=\text{Tr}\rho B_iA_j \quad \text{with } i,j\in\mathcal{A}, \tag{4}$$

can be obtained *exactly* for the solvable Hamiltonian $H_F$, Eq. (3), following [26]. It can then be shown that $\rho_{\mathcal{A}}$ is given by

$$\langle\boldsymbol{\xi}|\rho_{\mathcal{A}}|\boldsymbol{\xi}'\rangle=\det\tfrac{1}{2}(\mathbb{1}-G_{BA})\times e^{-1/2(\boldsymbol{\xi}^\star-\boldsymbol{\xi}')^T(G_{BA}+\mathbb{1})(G_{BA}-\mathbb{1})^{-1}(\boldsymbol{\xi}^\star+\boldsymbol{\xi}')}, \tag{5}$$

where $\boldsymbol{\xi}=\{\xi_1,\ldots,\xi_n\}$ are the Grassmann variables associated with system $\mathcal{A}$, and $|\xi\rangle$ are the corresponding coherent states with $c_i|\boldsymbol{\xi}\rangle=\xi_i|\boldsymbol{\xi}\rangle$. Indeed, (5) reproduces all two-particle Green's functions correctly and is, due to Wick's theorem, thus the correct reduced density matrix.

To calculate the entropy of system $\mathcal{A}$, we diagonalize $\rho_{\mathcal{A}}$ by the Bogoliubov transformation

$$f_q=\sum_i\left(\frac{P_{qi}+Q_{qi}}{2}c_i+\frac{P_{qi}-Q_{qi}}{2}c_i^\dagger\right), \tag{6}$$

where $PP^T=QQ^T=\mathbb{1}$ (due to the anticommutation rules), $P_qG_{BA}^T=\nu_qQ_q$ and $Q_qG_{BA}=\nu_qP_q$. The diagonalized reduced density matrix reads

$$\rho_{\mathcal{A}}=\left(\prod_q\frac{1-\nu_q}{2}\right)e^{-\Sigma_q\varepsilon_qf_q^\dagger f_q}, \tag{7}$$

with pseudoenergies $\varepsilon_q=\ln\frac{1-\nu_q}{1+\nu_q}$, yielding the entropy

$$S_{\mathcal{A}}=\sum_{q=1}^n h\left(\frac{1+\nu_q}{2}\right), \tag{8}$$

with the so-called binary entropy

$$h(x)=-x\log_2x-(1-x)\log_2(1-x). \tag{9}$$

### B. Bosonic systems

For the quadratic Hamiltonian $H_B$, the Green's function matrices $G_{AA}$ and $G_{BB}$ with respect to the operators $A_i\equiv b_i^\dagger+b_i$ and $B_i\equiv b_i^\dagger-b_i$ can be obtained as in [27]. With respect to the bosonic coherent states $b_i|\boldsymbol{\phi}\rangle=\phi_i|\boldsymbol{\phi}\rangle$, the reduced density matrix then reads

$$\langle\boldsymbol{\phi}|\rho_{\mathcal{A}}|\boldsymbol{\phi}'\rangle=Ke^{(1/4)(\boldsymbol{\phi}^\star+\boldsymbol{\phi}')^T(G_{AA}-\mathbb{1})(G_{AA}+\mathbb{1})^{-1}(\boldsymbol{\phi}^\star+\boldsymbol{\phi}')}\times e^{-(1/4)(\boldsymbol{\phi}^\star-\boldsymbol{\phi}')^T(G_{BB}-\mathbb{1})^{-1}(G_{BB}+\mathbb{1})(\boldsymbol{\phi}^\star-\boldsymbol{\phi}')}, \tag{10}$$

where $K=\sqrt{\det(1+G_{AA})(1-G_{BB})}$ is determined by the normalization of $\rho_{\mathcal{A}}$.

The Bogoliubov transformation

$$g_q=\sum_i\left(\frac{P_{qi}+Q_{qi}}{2}b_i+\frac{P_{qi}-Q_{qi}}{2}b_i^\dagger\right), \tag{11}$$

with $P^TQ=Q^TP=\mathbb{1}$, $P_qG_{AA}=\mu_qQ_q$, and $Q_qG_{BB}=-\mu_qP_q$ diagonalizes $\rho_{\mathcal{A}}$, giving

$$\rho_{\mathcal{A}}=\left(\prod_q\frac{2}{\mu_q+1}\right)e^{-\Sigma_q\epsilon_qg_q^\dagger g_q}, \tag{12}$$

where $\epsilon_q=\ln\left(\frac{\mu_q+1}{\mu_q-1}\right)$ are pseudoenergies. The entropy $S_{\mathcal{A}}$ is the sum of the quasiparticle entropies

$$S_{\mathcal{A}}=\sum_{q=1}^n\left(\frac{\mu_q+1}{2}\log_2\frac{\mu_q+1}{2}-\frac{\mu_q-1}{2}\log_2\frac{\mu_q-1}{2}\right). \tag{13}$$

When we choose $T=0$, i.e., when $\rho$ is the ground-state density matrix, Eqs. (8) and (13) give the entanglement entropy.

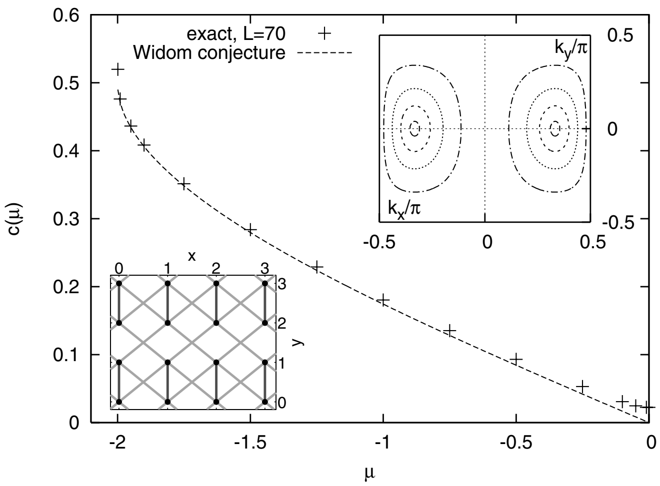


FIG. 2. The scaling prefactor $c(\mu)$ for the ground-state of a two-dimensional fermionic tight-binding model with next-nearest-neighbor hoppings in comparison to the result of [18]. Insets show the hopping parameters and the Fermi surfaces for $\mu \in [-0.25, -1.75]$ in the quartered Brillouin zone.

## III. CRITICAL FERMIONIC ENTANGLEMENT AND THE WIDOM CONJECTURE

The form of the logarithmic correction to the entanglement entropy in $(d>1)$-dimensional critical fermion models and bounds on it have been derived by Wolf [17] and Gioev and Klich [18]. Assuming that the Widom conjecture [19] holds also for $d>1$ and that the nonanalyticity of the binary entropy $h$ can be ignored at one point in the calculation, Gioev and Klich [18] arrive at

$$S_{\mathcal{A}} \equiv S_{\Omega}(L) = c(\mu) L \log_2 L + o(L \log_2 L), \tag{14}$$

$$c(\mu) = \frac{1}{2\pi}\frac{1}{12}\int_{\partial\Omega} \mathrm{d}S_x \int_{\partial\Gamma(\mu)} \mathrm{d}S_k |\mathbf{n_x n_k}|, \tag{15}$$

where $\Omega$ is the real-space region of $\mathcal{A}$, rescaled by $L$ such that $\mathrm{Vol}(\Omega)=1$. Vectors $\mathbf{n_x}$ and $\mathbf{n_k}$ denote the normal vectors on the real-space surface $\partial\Omega$ and the Fermi surface $\partial\Gamma(\mu)$. With the method introduced in Sec. II applied for $T=0$, one can calculate the entanglement entropy for finite $L$ *exactly* and thus check (14), also shedding some light on the validity of the assumptions leading to (15).

### A. Two-dimensional systems with a one-dimensional Fermi surface

The dispersion relation of the two-dimensional tight-binding model with periodic boundary conditions

$$H = -\sum_{x,y} (c_{x,y}^{\dagger} c_{x+1,y} + c_{x,y}^{\dagger} c_{x,y+1} + \mathrm{H.c.}) \tag{16}$$

is $E(\mathbf{k}) = -2(\cos k_x + \cos k_y)$. The ground-state Green's function matrix, from which we calculate the entanglement entropy, reads in the thermodynamic limit

$$G_{\mathbf{r},\mathbf{r}'} = \int_{\Gamma(\mu)} \frac{\mathrm{d}^2 k}{(2\pi)^2} e^{i\mathbf{k}(\mathbf{r}-\mathbf{r}')}, \tag{17}$$

with $\mathbf{r}=(x,y)$. Figure 1 shows the scaling prefactor $c(\mu)$ as fitted from the exact entanglement entropy of an $L\times L$ square with the rest of the universe, which was obtained from (8). It is in excellent agreement with (15) and thus also supports the Widom conjecture for $d=2$. The same agreement was found in the model

$$H = -\sum_{x,y} \{[1 + (-1)^y] c_{x,y}^{\dagger} c_{x,y+1} + c_{x,y}^{\dagger} c_{x+1,y+1} + c_{x,y}^{\dagger} c_{x-1,y+1} + \mathrm{H.c.}\} \tag{18}$$

which has a two-banded dispersion relation $E(\mathbf{k}) = \pm 2\sqrt{1 + 4\cos k_x \cos^2 k_y + 4\cos^2 k_x \cos^2 k_y}$ and a disconnected Fermi surface for $\mu \in [-2, 2]$, Fig. 2.

Recently, the correctness of (14) and (15) was in analogous manner also confirmed for a three-dimensional fermionic system [28].

### B. Two-dimensional systems with a zero-dimensional Fermi surface

Especially for a comparison to bosonic systems, it is interesting to investigate models with a zero-dimensional Fermi surface. In particular, we choose the two-dimensional model

$$H = -\sum_{x,y} \{h c_{x,y}^{\dagger} c_{x+1,y} + [1 + (-1)^{x+y}] c_{x,y}^{\dagger} c_{x,y+1} + \mathrm{H.c.}\}, \tag{19}$$

which has for $0 \le h \le 1$ the two-band dispersion relation $E(\mathbf{k}) = \pm 2\sqrt{1 + h^2\cos^2 k_x + 2h\cos k_x \cos k_y}$, i.e., a gap of size $4(1-h)$ at $\mathbf{k}=(\pi,0)$. Figure 3 shows for $\mu=0$ and $h\to 1$ how the entanglement entropy converges to the area law with a *sublogarithmic* correction, $S_{\Omega}(L) = Lo(\log_2 L)$, meaning $\lim_{L\to\infty} S_{\Omega}(L)/(L\log_2 L) = 0$. The curves $S_{\Omega}(L)/L$ for finite gaps were extrapolated to obtain $\lim_{L\to\infty} S_{\Omega}(L)/L$. Those values indicate, indeed, a divergence for $h\to 1$. This result is consistent with Eq. (14), as the scaling coefficient $c(\mu)$, Eq. (15), vanishes for systems in $d>1$ dimensions with a zero-dimensional Fermi surface. Further investigations have to determine the analytical form of the sublogarithmic correction and its universality.

## IV. CRITICAL BOSONIC ENTANGLEMENT

An important question is whether the logarithmic correction observed in the entanglement entropy scaling law for critical one-dimensional bosonic systems is also present in higher-dimensional systems. To investigate this, we examine a two-dimensional system of coupled oscillators

$$H = \frac{1}{2}\sum_{x,y} [\Pi_{x,y}^2 + \omega_0^2 \Phi_{x,y}^2 + (\Phi_{x,y} - \Phi_{x+1,y})^2 + (\Phi_{x,y} - \Phi_{x,y+1})^2], \tag{20}$$

where $\Phi_{x,y}$, $\Pi_{x,y}$, and $\omega_0$ are coordinate, momentum, and self-frequency of the oscillator at site $\mathbf{r}=(x,y)$, respec-

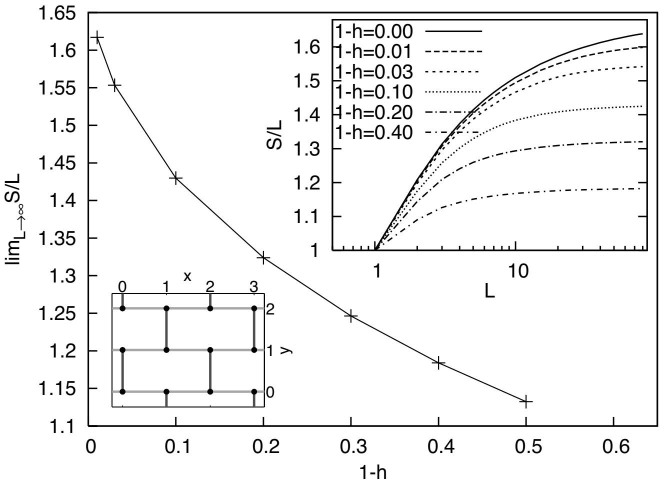


FIG. 3. The upper-right inset shows the entanglement entropy per surface unit $S_\Omega(L)/L$ (block of $n=L^2$ sites) for a two-dimensional fermionic tight-binding model with modulated vertical hopping (see the lower-left inset) at $T=0$. The energy gap $4(1-h)$ closes in the point $\mathbf{k}=(\pi,0)$. The extrapolation $\lim_{L\to\infty}S_\Omega(L)/L$ suggests a divergence for $h\to 1$.

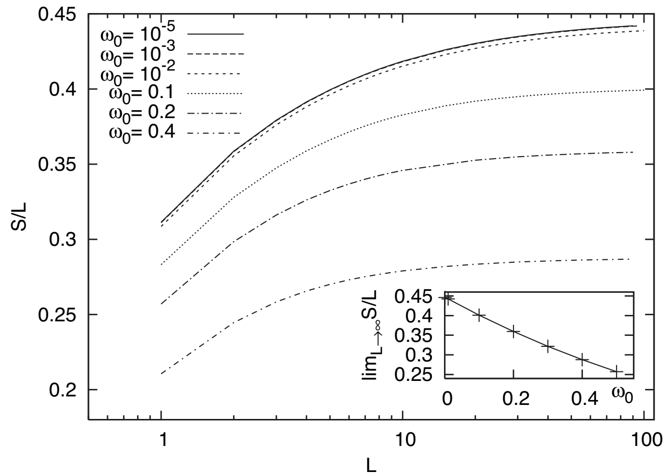


FIG. 4. The entanglement entropy per surface unit $S_\Omega(L)/L$ (block with $n=L^2$ sites) for the bosonic two-dimensional system of coupled harmonic oscillators at $T=0$. The curves converge for small energy gaps $\omega_0$. The extrapolation $\lim_{L\to\infty}S_\Omega(L)/L$ yields, for the critical limit, the area law $S_\Omega(L)\approx 0.45L$.

tively. The masses and coupling strengths are set to unity. The system has the dispersion relation $E(\mathbf{k}) =\sqrt{\omega_0^2+4\sin^2 k_x/2+4\sin^2 k_y/2}$, i.e., a gap of size $\omega_0$ at $\mathbf{k}=(0,0)$.

In the low-energy limit, the harmonic oscillators can be reduced to a field theory only containing $(\nabla\phi)^2$, which describes a massless free bosonic model. The scaling of entanglement entropy in this model has been studied by Srednicki [20] numerically in $d=3$ dimensions and by Callan and Wilczek [21] with approximate field theoretical methods for all $d>1$. Both provide evidence for the area law (1).

Applying the transformation $b_{\mathbf{i}}=\sqrt{\frac{\omega}{2}}(\Phi_{\mathbf{i}}+\frac{i}{\omega}\Pi_{\mathbf{i}})$ with $\omega=\sqrt{\omega_0^2+4}$, the Hamiltonian (20) is mapped to the canonical form (3) and is thus amenable to the method introduced in Sec. II. The translation invariant Green's function matrices $G_{AA}$ and $G_{BB}$ of system $\mathcal{A}$ are at $T=0$

$$G_{AA}(\mathbf{r},\mathbf{0})=\frac{1}{\pi^2}\int_0^\pi\int_0^\pi \mathrm{d}^2k\frac{\omega}{E(\mathbf{k})}\cos k_x x\cos k_y y$$

$$G_{BB}(\mathbf{r},\mathbf{0})=-\frac{1}{\pi^2}\int_0^\pi\int_0^\pi \mathrm{d}^2k\frac{E(\mathbf{k})}{\omega}\cos k_x x\cos k_y y,$$

and the entanglement entropy is obtained from Eq. (13). Special care has to be taken for the limit $\omega_0\to 0$, as this results in a singularity of the integrand for $G_{AA}$. We calculated the entropy for ever smaller but finite gaps $\omega_0$ and refined in each numerical integration the momentum space resolution until the integral converged. The limit $\omega_0\to 0$ was then investigated by extrapolation. Figure 4 displays the entanglement entropy as a function of the linear size $L$ of system $\mathcal{A}$ for several $\omega_0$. The curves converge for $\omega_0\to 0$, and a finite-size scaling analysis yields (see inset) $\lim_{\omega_0\to 0}\lim_{L\to\infty}S_\Omega(L)/L\approx 0.45$, i.e., the critical model obeys for $d=2$ the area law $S_\Omega(L)\approx 0.45L$. The fact that no logarithmic correction is observed although the system is critical may be attributed to the fact that the gap closes in a single point (or zero-dimensional region) of momentum space. This is very similar to the same situation for fermionic systems analyzed in Sec. III B.

## V. CONCLUSIONS

A relation between Green's function matrices of quadratic fermionic and bosonic Hamiltonians to reduced density matrices was used to study bipartite entanglement entropy in critical two-dimensional systems. We identified three different regimes for the scaling of the entropy and presented exact quantitative results: (i) For critical fermionic systems with a one-dimensional Fermi surface, it follows the area law with a logarithmic correction and the corresponding prefactor determined in [18] under assumption of the Widom conjecture is correct. This gives also support for the Widom conjecture in two dimensions. (ii) For critical fermionic systems with a zero-dimensional Fermi surface, it follows the area law with a sublogarithmic correction. (iii) For critical bosonic systems, it follows the area law without corrections. Those findings demonstrate the subtle nature of entanglement at criticality, the physical explanation of which remains a challenging topic for future research.

## ACKNOWLEDGMENTS

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