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On the Bisognano–Wichmann entanglement Hamiltonian of nonrelativistic fermions

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Abstract. We study the ground-state entanglement Hamiltonian of free nonrelativistic fermions for semi-infinite domains in one dimension. This is encoded in the two-point correlations projected onto the subsystem, an operator that commutes with the linear deformation of the physical Hamiltonian. The corresponding eigenfunctions are shown to possess the exact same structure both in the continuum as well as on the lattice. Namely, they are superpositions of the occupied single-particle modes of the total Hamiltonian, weighted by the inverse of their energy as measured from the Fermi level, and multiplied by an extra phase proportional to the integrated weight. Using this ansatz, we prove that the Bisognano–Wichmann form of the entanglement Hamiltonian becomes exact, up to a nonuniversal prefactor that depends on the dispersion for gapped chains.

Keywords: entanglement in extended quantum systems, solvable lattice models

Contents

1. Introduction

The study of entanglement properties plays a pivotal role in quantum many-body physics [1–4]. The central object of these investigations is the reduced density matrix (RDM), which encodes all the information on the entanglement between a subsystem and its remainder. The analogy with the standard setup of statistical mechanics suggests to write the RDM in an exponential form, and the associated entanglement Hamiltonian (EH) has been the topic of intensive research [5]. One of the key questions to address is the characterization of the EH for many-body ground states, with a particular focus on its locality properties and its relation to the physical Hamiltonian. Beside the pure theoretical interest, these properties also play a decisive role in novel tomographic protocols developed in quantum simulator experiments [6, 7].

Although extracting the EH for generic many-body systems is an immensely complicated task, one might hope to gain insight from the study of a related quantum field theory (QFT), that is expected to capture universal features of the model. In fact, the analog of the EH in algebraic QFT is known as the modular Hamiltonian, and it is associated with an observable algebra defined on a restricted spacetime region [8, 9]. In particular, considering a wedge region associated to a semi-infinite subsystem, the seminal result of Bisognano and Wichmann (BW) states, that for a relativistic QFT the modular Hamiltonian is given by the generator of Lorentz boosts [10, 11]. In one spatial dimension, the EH can thus be constructed as

$$\mathcal{H}_{\rm BW} = \frac{2\pi}{v} \int_0^{\infty} x\, T_{00}\,(x)\, \mathrm{d}x\,, \tag{1}$$

where $T_{00}(x)$ is the energy-density component of the stress tensor, and v is the velocity of excitations, which is required to make the expression dimensionless. In other words, the EH can be written as a deformation of the physical Hamiltonian by a linear weight function, which can alternatively be interpreted as a local inverse temperature. While the BW theorem holds for an arbitrary relativistic QFT, its generalizations to other subsystem geometries require conformal symmetry [12–15].

The structure of the EH described by the BW theorem, however, does not only emerge in QFT. Indeed, the discretized version of (1) was found to describe integrable quantum chains in their gapped phase [16]. This follows from the intimate connection between the RDM and the corner transfer matrix (CTM) of a corresponding two-dimensional statistical model, which was first introduced and studied by Baxter [17–19]. In fact, it was understood later on, that the generator of the CTM can be identified as a Lorentz boost operator on the lattice [20–23], which further clarifies the immediate analogy with the BW result.

The CTM method thus yields the EH of integrable chains in a form similar to the original Hamiltonian, but with couplings that increase linearly from the boundary. In particular, for models that can be mapped into free fermions, the eigenvalues and eigenvectors of the deformed Hamiltonian were studied in detail [24–28]. For gapped chains one obtains an equidistant spectrum, with a level spacing that goes towards zero at criticality. In CTM studies, one then usually regularizes the problem by considering a finite chain. However, for such a geometry, the actual EH is rather given by a sine-deformation of the couplings [29], as predicted by conformal field theory (CFT) [15]. Thus, in order to study the EH at criticality, one needs to work directly in the thermodynamic limit.

The goal of this paper is to show that the EH for semi-infinite domains can nevertheless be treated on a common footing for both critical and gapped nonrelativistic free-fermion systems, both in the continuum as well as on the lattice. We start by considering a one-dimensional Fermi gas in the continuum, and show that the eigenfunctions of the EH are given by weighted superpositions of the occupied plane wave modes of the physical Hamiltonian. The weight is given by the inverse of the energy measured from the Fermi surface, and each mode picks up an extra phase proportional to the integrated weight. The prefactor of this phase is related to the corresponding eigenvalue of the EH, and one recovers an *exact* BW form (1) with the parameter v given by the Fermi velocity. The EH can thus be obtained directly in the thermodynamic limit, despite the entanglement entropy being ill-defined due to the continuous spectrum.

In a next step, we extend our discussion to the lattice, considering homogeneous or dimerized hopping chains, and show that the very same construction holds for the eigenvectors of the EH. While at criticality one obtains a continuous spectrum, the presence of a gap in the dimerized case induces a quantization as in the CTM studies [16]. In turn, one finds a BW form with a nonuniversal (mass-dependent) prefactor, which can be related to the properties of the integrated weight. Finally, we show that the construction can also be applied for a hopping chain with a staggered chemical potential, yielding an equidistant spectrum which, however, differs from the CTM quantization.

The structure of the paper is as follows. In section 2 we consider the EH of the free Fermi gas on the line, which has a critical Fermi sea ground state. This is followed in section 3 by the study of the analogous lattice problem, the homogeneous hopping chain. The EH for the gapped case is studied for chains with dimerized hopping and staggered chemical potential in sections 4 and 5, respectively. The paper concludes with a discussion in section 6, followed by two appendices presenting some technical details of the calculations.

2. One-dimensional Fermi gas

We first consider the free Fermi gas on the infinite line, defined by the single-particle Hamiltonian

$$\hat{H} = -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \frac{q_F^2}{2}. \tag{2}$$

The ground state is a Fermi sea, with the plane-wave eigenstates filled up to the Fermi momentum q_F. The two-point correlations are then given by the sine kernel

$$K(x,x') = \int_{-q_F}^{q_F} \frac{\mathrm{d}q}{2\pi}\,\mathrm{e}^{\mathrm{i}q(x-x')} = \frac{\sin q_F(x-x')}{\pi(x-x')}, \tag{3}$$

which completely characterizes the ground state. We are interested in the entanglement properties of a semi-infinite bipartition $A = [0,\infty)$, with the RDM written in the form

$$\rho_A = \frac{1}{\mathcal{Z}}\mathrm{e}^{-\hat{\mathcal{H}}}, \tag{4}$$

where $\hat{\mathcal{H}}$ is the entanglement Hamiltonian and $\mathcal{Z}$ ensures normalization. Due to Wick's theorem, the EH is entirely determined by the reduced correlation kernel, which acts as the integral operator

$$\hat{K}\psi(x) = \int_0^\infty \mathrm{d}x' K(x,x')\,\psi(x'), \tag{5}$$

and is related to the EH as [30, 31]

$$\hat{K} = \frac{1}{\mathrm{e}^{\hat{\mathcal{H}}}+1}. \tag{6}$$

Hence, in order to find $\hat{\mathcal{H}}$, one needs to solve the eigenvalue problem of the integral operator $\hat{K}$. Similarly to the case of a finite interval [32], this task is made easier by observing that the differential operator

$$\hat{D} = -\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}x}x\frac{\mathrm{d}}{\mathrm{d}x} - x\frac{{q_F}^2}{2} \tag{7}$$

commutes exactly with the integral operator in (5). The calculation of the commutator $[\hat{K}, \hat{D}] = 0$ is given in appendix A. Note that the operator (7) has precisely the BW form, i.e. it is a simple linear deformation of the physical Hamiltonian in (2). In order to solve its eigenvalue problem $\hat{D}\psi(x) = \lambda\psi(x)$, we first rescale variables as $y = q_F x$ and $\chi = \lambda/q_F$, such that we arrive at

$$\left(\frac{\mathrm{d}}{\mathrm{d}y} y \frac{\mathrm{d}}{\mathrm{d}y} + y\right)\psi(y) = -2\chi\,\psi(y). \tag{8}$$

With a further change of variables $z = -2iy$, we look for a solution of the form $\psi(y) = \mathrm{e}^{-z/2}\Phi(z)$ such that the differential equation (8) becomes

$$z\frac{\mathrm{d}^2\Phi}{\mathrm{d}z^2} + (1-z)\frac{\mathrm{d}\Phi}{\mathrm{d}z} - \left(\frac{1}{2} - \mathrm{i}\chi\right)\Phi = 0. \tag{9}$$

This is nothing but the confluent hypergeometric equation with parameters $a = 1/2 - \mathrm{i}\chi$ and $b = 1$, and the solution that is regular at $z = 0$ is given by Kummer's function $\Phi(z) = M(a, b, z)$. It can be defined as a generalized hypergeometric series, however, for our purposes it is more useful to consider its integral representation [33]

$$M(a,b,z) = \frac{\Gamma(b)}{\Gamma(a)\Gamma(b-a)}\int_0^1 \mathrm{d}u\,\mathrm{e}^{zu}u^{a-1}(1-u)^{b-a-1}. \tag{10}$$

Substituting for the parameters a, b and changing back to the y variable, the solution for the eigenfunction reads

$$\psi_\chi(y) = \frac{1}{|\Gamma\left(\frac{1}{2}+\mathrm{i}\chi\right)|^2}\int_{-1}^1 \mathrm{d}p\,\frac{\mathrm{e}^{\mathrm{i}yp}\mathrm{e}^{\mathrm{i}\chi\ln\left(\frac{1+p}{1-p}\right)}}{\sqrt{1-p^2}}, \tag{11}$$

where we have symmetrized the integral by changing to the variable $p = 1 - 2u$.

Before continuing with our analysis, it is instructive to check that expression (11) satisfies the differential equation (8). Dropping the prefactor and applying the derivatives to the integrand one finds

$$\int_{-1}^1 \mathrm{d}p\left[y\left(1-p^2\right) + \mathrm{i}p\right]\frac{\mathrm{e}^{\mathrm{i}yp}\mathrm{e}^{\mathrm{i}\chi\ln\left(\frac{1+p}{1-p}\right)}}{\sqrt{1-p^2}}. \tag{12}$$

One can then integrate by parts in the first term using

$$y\,\mathrm{e}^{\mathrm{i}yp} = -\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}p}\mathrm{e}^{\mathrm{i}yp}, \qquad \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}p}\sqrt{1-p^2} = \frac{-\mathrm{i}p}{\sqrt{1-p^2}}, \tag{13}$$

such that the second term in the brackets in (12) is canceled. The remaining term is given by the derivative of the logarithmic phase factor, which yields

$$\frac{\mathrm{d}}{\mathrm{d}p}\ln\left(\frac{1+p}{1-p}\right) = \frac{2}{1-p^2} \tag{14}$$

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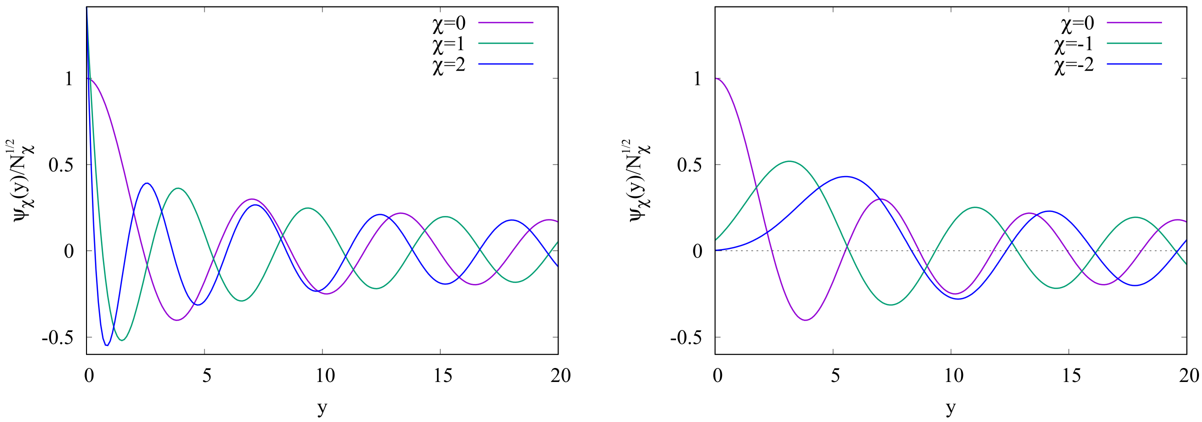

Figure 1. Eigenfunctions $\psi_\chi(y)$ of the differential equation (8) for various eigenvalues $\chi \geqslant 0$ (left) and $\chi \leqslant 0$ (right). The normalization N_χ is fixed by (26).

such that the $1-p^2$ factor is canceled and one indeed recovers $-2\chi\,\psi_\chi(y)$.

One can now find a simple interpretation of the result (11). In fact, the eigenfunction can be thought of as a wave packet constructed from the momenta within the Fermi sea, with a corresponding amplitude $1/\sqrt{1-p^2}$. This can be interpreted as a probability inversely proportional to the energy of the given mode, as measured from the Fermi level. Additionally, each mode acquires an extra phase which, according to (14), is given by the integral of the weight up to momentum p, and has a logarithmic divergence around the Fermi points. The eigenvalue χ appears as a factor multiplying this phase, and can assume arbitrary values, i.e. the operator $\hat{D}$ has a continuous spectrum.

The eigenfunctions are shown in figure 1 for various eigenvalues χ. Note that, due to the continuous spectrum, the $\psi_\chi(y)$ are not normalizable, and the factor in front of the integral in (11) sets $\psi_\chi(0)=1$. However, in figure 1 we adopt a different normalization, which comes from the requirement of orthonormality and will be derived later. One observes that, for $\chi>0$, the oscillations increase and $\psi_\chi(y)$ becomes more and more peaked around $y=0$, whereas for $\chi<0$ the eigenfunction is pushed away from the boundary.

To find the asymptotics for $y \gg 1$, it is useful to first introduce new variables $p=\tanh(z)$, in order to remove the divergent phase factor in (11). One then has

$$\psi_\chi(y) = \frac{\cosh(\pi\chi)}{\pi}\int_{-\infty}^{\infty} \mathrm{d}z\, \frac{\mathrm{e}^{\mathrm{i}y\tanh(z)}\mathrm{e}^{\mathrm{i}2\chi z}}{\cosh(z)}, \tag{15}$$

where we used the properties of the Γ function for imaginary arguments. One can now apply a stationary phase approximation, which yields the condition

$$\frac{y}{\cosh^2 z_0} + 2\chi = 0, \qquad \tanh(z_0) = \sqrt{1-\frac{2|\chi|}{y}}. \tag{16}$$

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Note that the stationary points $\pm z_0$ exist only for $\chi < 0$, and one finds, up to normalization, the approximation

$$\psi_\chi(y) \propto \sqrt{\frac{\pi}{y\sqrt{1-\frac{2|\chi|}{y}}}} \exp\left[\mathrm{i}y\sqrt{1-\frac{2|\chi|}{y}} + \mathrm{i}2\chi\,\mathrm{atanh}\sqrt{1-\frac{2|\chi|}{y}} - \mathrm{i}\pi/4\right] + \mathrm{c.c.} \tag{17}$$

In particular, for $y \gg 2|\chi|$ the second phase factor can be expanded and one finds $\chi\ln(2y/|\chi|)$, such that the frequency of the oscillations increases logarithmically.

The commutation property $[\hat{K},\hat{D}]=0$ ensures, that $\psi_\chi(y)$ are also the eigenfunctions of the sine kernel on the half-line, it thus remains to evaluate the corresponding eigenvalue. For this purpose, we apply the substitution used in (15) also in the sine kernel to find

$$K(y,y') = \int_{-\infty}^{\infty} \frac{\mathrm{d}z}{2\pi} \frac{\mathrm{e}^{\mathrm{i}(y-y')\tanh(z)}}{\cosh^2(z)}. \tag{18}$$

Applying the integral operator to $\psi_\chi(y')$, the y' integral has to be carried out on the half line, one thus simply obtains the Fourier transform of the step function $\Theta(y')$, which is given by

$$\int_{-\infty}^{\infty} \mathrm{d}y'\,\Theta(y')\,\mathrm{e}^{\mathrm{i}Qy'} = \lim_{\epsilon\to 0^+} \frac{\mathrm{i}}{Q+\mathrm{i}\epsilon}. \tag{19}$$

Ignoring the normalization factor, the function $\hat{K}\psi_\chi(y)$ thus has the integral representation

$$\int_{-\infty}^{\infty} \mathrm{d}z \frac{\mathrm{e}^{\mathrm{i}y\tanh(z)}}{\cosh^2(z)} \lim_{\epsilon\to 0^+} \oint_\gamma \frac{\mathrm{d}z'}{2\pi} \frac{\mathrm{i}}{\tanh(z')-\tanh(z)+\mathrm{i}\epsilon} \frac{\mathrm{e}^{\mathrm{i}2\chi z'}}{\cosh(z')}, \tag{20}$$

where we have extended the z' integration to a contour γ on the complex plane. For $\chi > 0$, the contour is chosen as an infinitely large semi-circle on the upper half-plane, whereas for $\chi < 0$ the contour must be closed on the lower half-plane. With this choice, the contribution of the integral on the arc vanishes, and one only needs to evaluate the residues at the poles, which lie at

$$z' = z + \mathrm{i}n\pi - \frac{\mathrm{i}\epsilon}{1-\tanh^2(z)}, \tag{21}$$

where n is an integer.

Let us first consider $\chi > 0$, such that the poles that lie within the contour correspond to $n = 1, 2, \ldots$, and their residue is given by $\cosh^2(z)$. At the same time, the factor in the denominator becomes $\cosh(z') = (-1)^n\cosh(z)$, such that we have for the contour integral

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$$-\lim_{\epsilon\to 0}\oint_\Gamma \frac{\mathrm{d}z'}{2\pi\,\mathrm{i}}\frac{1}{\tanh(z')-\tanh(z)+\mathrm{i}\epsilon}\frac{\mathrm{e}^{\mathrm{i}2\chi z'}}{\cosh(z')} = -\mathrm{e}^{\mathrm{i}2\chi z}\cosh(z)\sum_{n=1}^{\infty}(-1)^n\,\mathrm{e}^{-n2\pi\chi}. \qquad (22)$$

Plugging the result back into (20), it is easy to see that the z dependent terms reproduce the eigenfunction $\psi_\chi(y)$, while the corresponding eigenvalue is given by the sum. Using the formula for the geometric series, one arrives at

$$\hat{K}\psi_\chi(y) = \frac{1}{\mathrm{e}^{2\pi\chi}+1}\psi_\chi(y)\,. \qquad (23)$$

The case $\chi<0$ is very similar, but now the poles on the lower half plane with $n=0,-1,\ldots$ contribute in the sum in (22), while the sign factor is absorbed by changing the direction of the contour integration, such that the sum delivers the very same result (23). One thus finds, that the eigenvalue of the sine kernel is simply given by the Fermi function with an argument $2\pi\chi$. Comparing with (6) and restoring the length scales $y=xq_F$ and $\chi=\lambda/q_F$, one finds

$$\hat{\mathcal{H}} = \frac{2\pi}{q_F}\hat{D}, \qquad (24)$$

and thus the BW theorem (1) holds exactly. In fact, despite the infrared divergence of the entanglement entropy due to the continuum spectrum, the EH remains perfectly well defined.

To conclude this section, we check the orthonormality of the eigenfunctions. To this end we need to evaluate

$$\int_0^\infty \mathrm{d}y\,\psi^*_\chi(y)\,\psi_{\chi'}(y) = \frac{\cosh^2(\pi\chi)}{\pi^2}\int_{-\infty}^{\infty}\mathrm{d}z\,\frac{2\pi}{\mathrm{e}^{2\pi\chi}+1}\mathrm{e}^{\mathrm{i}2(\chi'-\chi)z}, \qquad (25)$$

where we have carried out the same contour integration as before. In turn, one arrives at

$$\int_0^\infty \mathrm{d}y\,\psi^*_\chi(y)\,\psi_{\chi'}(y) = N_\chi\,\delta(\chi-\chi'), \qquad N_\chi = \frac{1+\mathrm{e}^{-2\pi\chi}}{2}, \qquad (26)$$

and to ensure the correct delta function normalization between the eigenfunctions, $\psi_\chi(y)$ must be multiplied by a factor $N_\chi^{-1/2}$, which was adopted in figure 1.

3. Homogeneous hopping chain

We now move on to consider free fermions on an infinite chain, given by a hopping model of the form

$$\hat{H} = -\frac{1}{2}\sum_{n=-\infty}^{\infty}\left(c_n^\dagger c_{n+1}+c_{n+1}^\dagger c_n\right)+\cos q_{\mathrm{F}}\sum_{n=-\infty}^{\infty}c_n^\dagger c_n\,. \qquad (27)$$

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The chemical potential $\mu = -\cos q_{\mathrm{F}}$ is chosen such that the Fermi momentum is given by q_{F}. The reduced correlation matrix $C_{m,n} = \langle c_m^\dagger c_n \rangle$ with $m, n \geqslant 1$ is given by the discrete version of the sine kernel

$$C_{m,n} = \frac{\sin q_{\mathrm{F}}\,(m-n)}{\pi\,(m-n)}, \tag{28}$$

and encodes all the information on entanglement. In particular, the EH is given by the relation [30, 31]

$$\mathcal{H} = \sum_{m,n\geqslant 1} H_{m,n} c_m^\dagger c_n\,, \qquad C = \frac{1}{\mathrm{e}^{H}+1}. \tag{29}$$

We thus have to treat the eigenvalue problem of the discrete sine kernel (28) on the half-infinite chain. Similarly to the continuum case, this can be simplified by finding a commuting operator with a much simpler structure. Indeed, analogously to the case of an interval [34, 35], one can show (see appendix A) that the tridiagonal matrix

$$T_{m,n} = t_m\,\delta_{m+1,n} + t_{m-1}\,\delta_{m-1,n} + d_m \delta_{m,n} \tag{30}$$

with entries defined by

$$t_m = -\frac{1}{2}m, \qquad d_m = \cos q_{\mathrm{F}}\,(m-1/2)\,, \tag{31}$$

commutes exactly with the correlation matrix, $[C, T] = 0$. Just as in the continuum case, the commuting operator has precisely the BW form, with the linear deformation being slightly shifted for the on-site d_m and hopping terms t_m, respectively.

In analogy with the continuum case, we try the following ansatz for the eigenvector

$$\psi_\lambda(m) = \int_{-q_{\mathrm{F}}}^{q_{\mathrm{F}}} \frac{\mathrm{d}q}{2\pi} \frac{\mathrm{e}^{\mathrm{i}q(m-1/2)}\mathrm{e}^{\mathrm{i}\lambda\varphi_q}}{\sqrt{\cos q - \cos q_{\mathrm{F}}}}, \tag{32}$$

where the denominator contains again the square root of the energies measured from the Fermi level. The variable $m-1/2$ in the first phase factor is suggested by the reflection symmetry $m \to 1-m$ of the problem, which should translate to the eigenvalue $-\lambda$, whereas the phase φ_q is yet to be determined. Multiplying with the tridiagonal matrix, the integrand of the vector $-2T\psi_\lambda$ reads

$$[(2m-1)\,(\cos q - \cos q_{\mathrm{F}}) + \mathrm{i}\sin q]\, \frac{\mathrm{e}^{\mathrm{i}q(m-1/2)}\mathrm{e}^{\mathrm{i}\lambda\varphi_q}}{\sqrt{\cos q - \cos q_{\mathrm{F}}}}. \tag{33}$$

One can then integrate by parts in the first term using

$$(2m-1)\,\mathrm{e}^{\mathrm{i}q(m-1/2)} = -2\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}q}\mathrm{e}^{\mathrm{i}q(m-1/2)}, \qquad 2\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}q}\sqrt{\cos q - \cos q_{\mathrm{F}}} = \frac{-\mathrm{i}\sin q}{\sqrt{\cos q - \cos q_{\mathrm{F}}}}, \tag{34}$$

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such that the derivative of the square root cancels the second term in (33), while the boundary term vanishes automatically. One has thus the requirement

$$\frac{\mathrm{d}\varphi_q}{\mathrm{d}q} = \frac{1}{\cos q - \cos q_{\mathrm{F}}}, \tag{35}$$

which yields $-2T\psi_\lambda = -2\lambda\psi_\lambda$. Hence, in complete analogy to the continuum case (14), the extra phase is given by the integral of the inverse energy difference, which gives

$$\varphi_q = \frac{1}{\sin q_{\mathrm{F}}} \ln\left(\frac{\tan\frac{q_{\mathrm{F}}}{2} + \tan\frac{q}{2}}{\tan\frac{q_{\mathrm{F}}}{2} - \tan\frac{q}{2}}\right). \tag{36}$$

Note that the lower limit of the integral was set to $q = 0$, which ensures that the phase is odd, $\varphi_{-q} = \varphi_q$, and thus the eigenvector in (32) is real.

The next step is to substitute variables $\tanh(z) = \tan(q/2)/\tan(q_{\mathrm{F}}/2)$, to cure the divergence of the phase factor. Indeed, this gives $\varphi_q = 2z/\sin q_{\mathrm{F}}$, and the inverse transformation and its Jacobian read

$$q(z) = 2\mathrm{atan}\left[\tan(q_{\mathrm{F}}/2)\tanh(z)\right], \qquad \frac{\mathrm{d}q}{\mathrm{d}z} = \frac{2\sin q_{\mathrm{F}}}{\cos q_{\mathrm{F}} + \cosh(2z)}, \tag{37}$$

while the energy difference can be expressed as

$$\cos q - \cos q_{\mathrm{F}} = \frac{2\sin^2(q_{\mathrm{F}}/2)}{\cosh^2(z)\left[1 + \tan^2(q_{\mathrm{F}}/2)\tanh^2(z)\right]} = \frac{\sin^2 q_{\mathrm{F}}}{\cos q_{\mathrm{F}} + \cosh(2z)}. \tag{38}$$

Putting everything together, the eigenvector can be written as

$$\psi_\lambda(m) = \int_{-\infty}^{\infty} \frac{\mathrm{d}z}{\pi} \frac{\mathrm{e}^{\mathrm{i}q(z)(m-1/2)}\mathrm{e}^{\mathrm{i}2\lambda z/\sin q_{\mathrm{F}}}}{\sqrt{\cos q_{\mathrm{F}} + \cosh(2z)}}. \tag{39}$$

With the integral representation at hand, one could proceed to evaluate the corresponding eigenvalue of C. We first rewrite its matrix elements using the transformation (37) as

$$C_{m,n} = \int_{-\infty}^{\infty} \frac{\mathrm{d}z}{2\pi} \frac{\mathrm{d}q}{\mathrm{d}z} \mathrm{e}^{\mathrm{i}q(z)(m-n)}. \tag{40}$$

To evaluate the matrix multiplication $C\psi_\lambda$, we use the identity

$$\sum_{n=1}^{\infty} \mathrm{e}^{\mathrm{i}Q(n-1/2)} = \lim_{\epsilon\to 0^+} \frac{\mathrm{i}}{2\sin\left(\frac{Q}{2} + \mathrm{i}\epsilon\right)}, \tag{41}$$

which leads us to the contour integral

$$\int_{-\infty}^{\infty} \frac{\mathrm{d}z}{2\pi} \frac{\mathrm{d}q}{\mathrm{d}z} \mathrm{e}^{\mathrm{i}q(z)(m-1/2)} \lim_{\epsilon\to 0^+} \oint_\gamma \frac{\mathrm{d}z'}{2\pi} \frac{\mathrm{d}q}{\mathrm{d}z'} \frac{\mathrm{i}}{2\sin\left(\frac{q(z')-q(z)}{2} + \mathrm{i}\epsilon\right)} \frac{\mathrm{e}^{\mathrm{i}2\lambda z'/\sin q_{\mathrm{F}}}}{\sqrt{\cos q(z') - \cos q_{\mathrm{F}}}}. \tag{42}$$

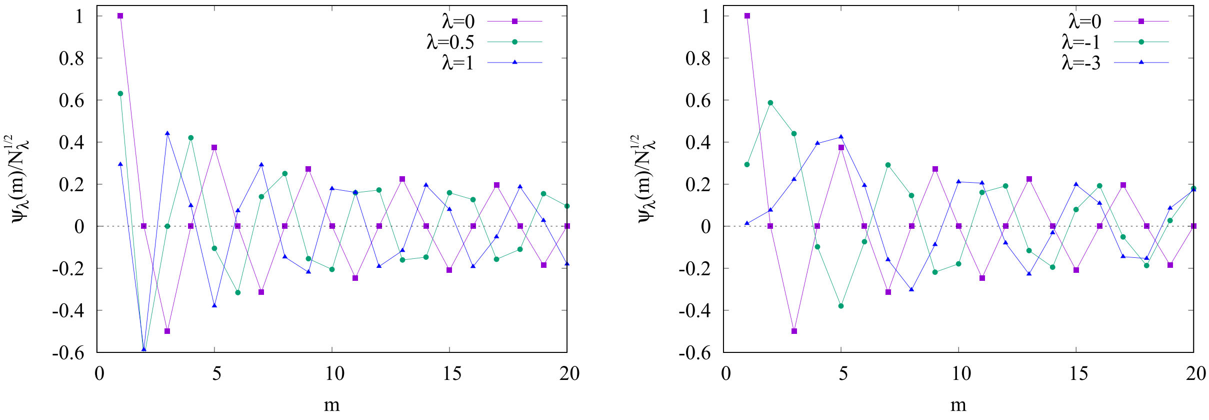

Figure 2. Eigenvectors $\psi_\lambda(m)$ of the tridiagonal matrix (30) for various eigenvalues $\lambda \geqslant 0$ (left) and $\lambda \leqslant 0$ (right). The normalization N_λ is fixed by (45).

The poles of the integrand are the same (21) as in the previous section, and for $\lambda > 0$ ($\lambda < 0$) we can close the contour on the upper (lower) half-plane. The residues are simply given by $(\frac{\mathrm{d}q}{\mathrm{d}z})^{-1}$ which cancels with the Jacobian. Due to the presence of the square root in the denominator, some care is needed when extending the weight factor to the complex plane, in order to avoid branch cuts. Indeed, here one should use the first expression in (38), which implies

$$\sqrt{\cos q\,(z') - \cos q_F} = (-1)^n \sqrt{\cos q\,(z) - \cos q_{\mathrm{F}}}\,. \tag{43}$$

The structure is thus exactly the same as in (20), and yields immediately the relations.

$$C\psi_\lambda = \frac{1}{\mathrm{e}^{\frac{2\pi\lambda}{\sin q_{\mathrm{F}}}} + 1}\psi_\lambda\,, \qquad H = \frac{2\pi}{\sin q_{\mathrm{F}}} T\,. \tag{44}$$

In other words, the BW form (1) is exact even on the lattice and at arbitrary fillings, setting $v = \sin q_{\mathrm{F}}$.

The normalization of the eigenvectors can be obtained analogously to the previous section

$$\sum_{m=1}^{\infty} \psi_\lambda^*(m)\,\psi_{\lambda'}(m) = N_\lambda \delta(\lambda - \lambda')\,, \qquad N_\lambda = \frac{1}{\mathrm{e}^{\frac{2\pi\lambda}{\sin q_{\mathrm{F}}}} + 1}\,. \tag{45}$$

Note that the difference with respect to (45) comes from the prefactor in (11), which is missing from the ansatz (32). The properly normalized eigenvectors are shown in figure 2, and follow the same pattern as observed in figure 1 for the continuous case. Namely, for $\lambda > 0$ the eigenvectors are attracted, while for $\lambda < 0$ they are repelled from the boundary. Note that for larger $\lambda > 0$ the structure becomes quickly rather irregular, which is due to the discrete sampling from an increasingly oscillatory function.

Finally, we point out a remarkable connection of our ansatz (32) to orthogonal polynomials. Indeed, it was already observed in earlier studies of CTM spectra [25, 27], that the eigenvectors of T are given by the Meixner–Pollaczek polynomials. It is rooted in the fact, that $\psi_\lambda(m)$ satisfy a three-term recurrence relation. In particular, the Meixner–Pollaczek polynomials are defined by the recurrence relation [36]

$$(n+1)\,P_{n+1}^{(\alpha)}(x;\phi)+(n+2\alpha-1)\,P_{n-1}^{(\alpha)}(x;\phi)=2\,(x\sin\phi+(n+\alpha)\cos\phi)\,P_{n}^{(\alpha)}(x;\phi)\,. \quad (46)$$

It is easy to see that setting $\alpha=1/2$, $\phi=q_{\rm F}$ and $x=-\lambda/\sin q_{\rm F}$, one obtains precisely the eigenvalue equation of the tridiagonal matrix with elements (31) under the identification $P_n^{(1/2)}(x;q_{\rm F})\sim\psi_\lambda(n+1)$ for $n=0,1,\ldots$. In fact, it turns out that there is a proportionality factor between them, which has to be fixed by comparing the orthogonality relations satisfied by the Meixner–Pollaczek polynomials, which is carried out in appendix B.

4. Dimerized chain

The dimerized (or SSH) chain is described by a hopping model with alternating amplitudes

$$\hat{H}=-\sum_n\left(\frac{1+\delta}{2}\,c^\dagger_{2n-1}c_{2n}+\frac{1-\delta}{2}\,c^\dagger_{2n}c_{2n+1}+\text{h.c.}\right) \quad (47)$$

Since the chain has only two-site shift invariance, a Fourier transformation in terms of the sublattice momentum must be followed by a rotation within the cell degrees of freedom in order to diagonalize the model. This is most easily expressed in terms of the halved sublattice momentum, which varies within the reduced Brillouin zone $q\in[-\pi/2,\pi/2]$. In particular, we introduce new fermion operators α_q and β_q via the transformation

$$c_{2n-1}=\frac{1}{\sqrt{2N}}\sum_q \mathrm{e}^{\mathrm{i}q(2n-1)}\mathrm{e}^{-\mathrm{i}\theta_q/2}\,(\alpha_q+\beta_q)\,, \qquad c_{2n}=\frac{1}{\sqrt{2N}}\sum_q \mathrm{e}^{\mathrm{i}q2n}\mathrm{e}^{\mathrm{i}\theta_q/2}\,(\alpha_q-\beta_q)\,. \quad (48)$$

It is then easy to see, that the phase factor must be chosen as

$$\mathrm{e}^{\mathrm{i}\theta_q}=\frac{\cos q-\mathrm{i}\delta\sin q}{\omega_q}, \qquad \omega_q=\sqrt{\cos^2 q+\delta^2\sin^2 q}\,, \quad (49)$$

in order to bring the Hamiltonian into the diagonal from

$$\hat{H}=-\sum_q\omega_q\left(\alpha^\dagger_q\alpha_q-\beta^\dagger_q\beta_q\right)\,. \quad (50)$$

Note that, for simplicity, we have formulated the transformations above on a periodic chain of $2N$ sites. However, we are interested in the limit $N\to\infty$ where the momentum variable q becomes continuous.

The Hamiltonian (50) is characterized by a band structure with a gap of size $2|\delta|$, and the ground state is given by filling only the lower band, i.e. $\langle\alpha^\dagger_q\alpha_q\rangle=1$ and $\langle\beta^\dagger_q\beta_q\rangle=0$.

The correlation matrix still has a checkerboard structure, with the nonvanishing entries given by

$$C_{2m-1,2n} = \int_{-\pi/2}^{\pi/2} \frac{\mathrm{d}q}{2\pi} \mathrm{e}^{\mathrm{i}qr} \mathrm{e}^{\mathrm{i}\theta_q}, \qquad C_{2m,2n+1} = \int_{-\pi/2}^{\pi/2} \frac{\mathrm{d}q}{2\pi} \mathrm{e}^{\mathrm{i}qr} \mathrm{e}^{-\mathrm{i}\theta_q}, \tag{51}$$

where $r = 2n - 2m + 1$, and $C_{2m-1,2n-1} = C_{2m,2n} = \delta_{m,n}/2$. It is a simple exercise to show (see appendix A), that one can again define a commuting tridiagonal matrix with the hopping amplitudes given by

$$t_{2m-1} = -\frac{1+\delta}{2}(2m-1), \qquad t_{2m} = -\frac{1-\delta}{2}2m, \tag{52}$$

while the diagonal terms are zero, $d_m = 0$.

Inspired by the results of the previous sections and the structure of the transformation (48), we propose the ansatz

$$\psi_\lambda(m) = \int_{-\pi/2}^{\pi/2} \frac{\mathrm{d}q}{2\pi} \frac{\mathrm{e}^{\mathrm{i}q(m-1/2)} \mathrm{e}^{\mathrm{i}\lambda\varphi_q} \mathrm{e}^{\mathrm{i}(-1)^m \theta_q/2}}{\sqrt{\omega_q}} = \int_{-\pi/2}^{\pi/2} \frac{\mathrm{d}q}{2\pi} \frac{\mathrm{e}^{\mathrm{i}q(m-1/2)} \mathrm{e}^{\mathrm{i}\lambda\varphi_q}}{\sqrt{\cos q + (-1)^m \mathrm{i}\delta \sin q}}, \tag{53}$$

where we incorporated the additional phase factors into the wavefunction. Multiplying by $-2T$ using (52) and assuming m odd, one obtains for the integrand

$$[(2m-1)(\cos q + \mathrm{i}\delta \sin q) + (\mathrm{i}\sin q + \delta \cos q)] \frac{\mathrm{e}^{\mathrm{i}q(m-1/2)} \mathrm{e}^{\mathrm{i}\lambda\varphi_q}}{\sqrt{\cos q + \mathrm{i}\delta \sin q}}. \tag{54}$$

Rewriting the factor $2m-1$ as a q-derivative and integrating by parts, one has for the derivative of the square root

$$2\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}q}\left[\sqrt{\cos q + \mathrm{i}\delta \sin q}\right] = \frac{-\mathrm{i}\sin q - \delta \cos q}{\sqrt{\cos q + \mathrm{i}\delta \sin q}}, \tag{55}$$

which again exactly cancels the second term in (54). To obtain the eigenvalue -2λ, the extra phase has to satisfy

$$\frac{\mathrm{d}\varphi_q}{\mathrm{d}q} = \frac{1}{\sqrt{\cos^2 q + \delta^2 \sin^2 q}}, \tag{56}$$

which can be integrated as

$$\varphi_q = F(q, \delta'), \qquad \delta' = \sqrt{1-\delta^2}, \tag{57}$$

in terms of the incomplete elliptic integral of the first kind, and we introduced the complementary modulus δ'.

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In sharp contrast to the critical case, however, the boundary contribution to the partial integral does not vanish automatically, due to the presence of the gap. It is easy to see that the vanishing of this term requires

$$\mathrm{e}^{\mathrm{i}\frac{\pi}{2}(m-1/2)}\sqrt{\mathrm{i}\delta}\mathrm{e}^{\mathrm{i}\lambda\varphi_{\pi/2}} = \mathrm{e}^{-\mathrm{i}\frac{\pi}{2}(m-1/2)}\sqrt{-\mathrm{i}\delta}\mathrm{e}^{-\mathrm{i}\lambda\varphi_{\pi/2}}, \tag{58}$$

and setting $m = 2\ell + 1$ this further implies

$$\lambda_\ell = \frac{\pi}{2K(\delta')}\begin{cases}2\ell+1 & \text{if } \delta > 0\\ 2\ell & \text{if } \delta < 0\end{cases}, \qquad \ell = 0, \pm 1, \pm 2, \ldots \tag{59}$$

where $K(\delta')$ denotes the complete elliptic integral. Hence, it is precisely this extra requirement that imposes the quantization of the eigenvalues in the gapped case. The levels are equidistant and their spacing decreases approaching the critical point $\delta \to 0$, where $K(\delta') \to \infty$, signaling the transition to a continuum spectrum. Note also that the spectrum is particle-hole symmetric, and one can easily verify that the eigenvectors satisfy the property $\psi_{-\lambda}(m) = (-1)^m \psi_\lambda(m)$. Furthermore, one can check that the derivation for m even yields the very same results.

We now move to the calculation of the corresponding eigenvalues of C. As in the previous cases, we introduce the phase $u = \varphi_q$ as a new variable, which allows us to extend the integral to the complex plane with vanishing contributions at infinity. The inverse transformation and its Jacobian read

$$q(u) = \mathrm{am}(u, \delta'), \qquad \frac{\mathrm{d}q}{\mathrm{d}u} = \mathrm{dn}(u, \delta'), \tag{60}$$

where am and dn denote the Jacobi and delta amplitude, respectively, and one obtains the contour integral

$$\psi_\lambda(m) = \oint_\gamma \frac{\mathrm{d}u}{2\pi}\mathrm{dn}(u,\delta')\frac{\mathrm{e}^{\mathrm{i}\,\mathrm{am}(u,\delta')(m-1/2)}\mathrm{e}^{\mathrm{i}\lambda u}}{\sqrt{\mathrm{cn}(u,\delta') + \mathrm{i}(-1)^m\delta\,\mathrm{sn}(u,\delta')}}, \tag{61}$$

where sn and cn are the elliptic sine and cosine, respectively. The contour γ has a rectangular shape as depicted in figure 3 for $\lambda > 0$. Indeed, the main difference w.r.t. the critical case is that the domain on the real axis is a finite interval $[-K(\delta'), K(\delta')]$. At its endpoints the integrand has the same value due to the quantization condition (58). One can show that this remains true along the vertical lines in figure 3, such that their contributions cancel, and one can close the contour at infinity. For $\lambda < 0$, the contour must be drawn on the lower half plane.

From this point, the calculation is completely analogous to the critical case. The poles will be given by the condition $\mathrm{am}(u', \delta') = \mathrm{am}(u, \delta')$ which, using the periodicity properties of the Jacobi amplitude along the imaginary direction, yields $u' = u + in4K(\delta)$. The square root in the denominator of (61) yields again a factor $(-1)^n$,

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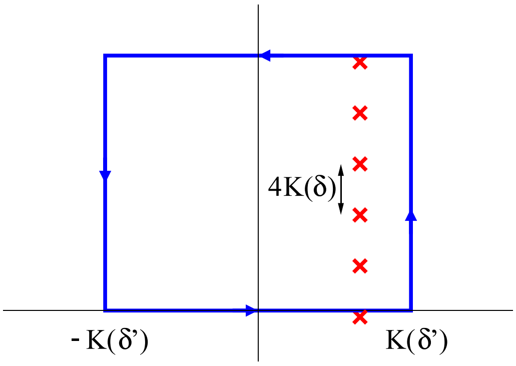

Figure 3. Rectangular integration contour (blue) for the eigenvector (61), with the upper side taken to infinity. The red crosses indicate the poles $u' = u + in4K(\delta) - \mathrm{i}\epsilon$ that appear when multiplying with the matrix C.

and the infinite sum over the poles reproduces the Fermi function. One thus obtains for the EH and its spectrum

$$H = 4K(\delta)\,T, \qquad \varepsilon_\ell = 2\pi \frac{K(\delta)}{K(\delta')} \begin{cases} 2\ell+1 & \text{if } \delta > 0 \\ 2\ell & \text{if } \delta < 0 \end{cases}. \tag{62}$$

One should note that the result seemingly differs from the one obtained via the duality with two interlaced transverse Ising chains [37], which gives $\pi K(k')/K(k)$ for the halved spacing of the spectrum with $k = \frac{1-|\delta|}{1+|\delta|}$. However, using elliptic integral identities, one can show that the two results are actually identical.

Finally, the normalization of the eigenvectors can also be obtained using the contour integral representation as

$$\sum_{m=1}^{\infty} \psi_\lambda^*(m)\,\psi_{\lambda'}(m) = N_\lambda \delta_{\lambda,\lambda'}, \qquad N_\lambda = \frac{1}{\mathrm{e}^{4K(\delta)\lambda}+1}\frac{K(\delta')}{\pi}. \tag{63}$$

The factor multiplying the Fermi function is simply the size of the integration domain on the real axis divided by 2π, and diverges as $\delta \to 0$. The eigenvectors for two different dimerizations are shown in figure 4. One can clearly see that their amplitude decays much faster as in the critical case, especially for larger values of the gap. Note that we have shown only eigenvalues with $\lambda < 0$, as those with $-\lambda$ are simply multiplied by a factor $(-1)^m$.

5. Hopping chain with staggered potential

As a final example, let us consider the hopping chain in a staggered chemical potential

$$\hat{H} = -\frac{1}{2}\sum_n \left(c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_n\right) + \mu \sum_n (-1)^n c_n^\dagger c_n. \tag{64}$$

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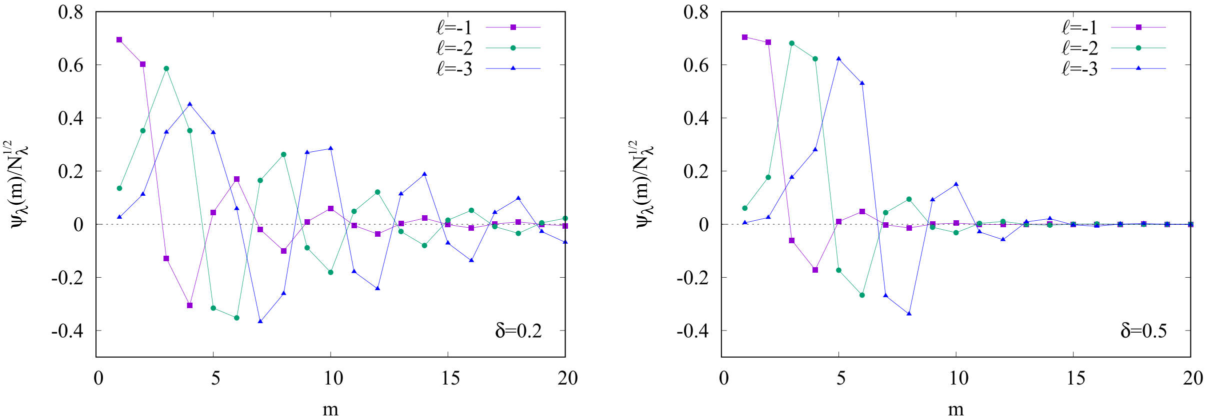

Figure 4. Eigenvectors $\psi_\lambda(m)$ of the tridiagonal matrix of the dimerized chain with elements (52), for various eigenvalues (59) and two different dimerizations $\delta = 0.2$ (left) and $\delta = 0.5$ (right). The normalization N_λ is fixed by (63).

The unit cell contains again two sites and one can proceed as in the previous section. Using the reduced sublattice momentum q and introducing new operators via

$$c_{2m-1} = \frac{1}{\sqrt{2N}} \sum_q \mathrm{e}^{\mathrm{i}q(2m-1)} \left(\sqrt{1+\frac{\mu}{\Omega_q}}\alpha_q + \sqrt{1-\frac{\mu}{\Omega_q}}\mathrm{e}^{\mathrm{i}q}\beta_q \right),$$

$$c_{2m} = \frac{1}{\sqrt{2N}} \sum_q \mathrm{e}^{\mathrm{i}q2m} \left(\sqrt{1-\frac{\mu}{\Omega_q}}\alpha_q - \sqrt{1+\frac{\mu}{\Omega_q}}\mathrm{e}^{\mathrm{i}q}\beta_q \right), \tag{65}$$

one arrives at the diagonal form of the Hamiltonian and corresponding dispersion relation

$$H = -\sum_q \Omega_q \left(\alpha_q^\dagger \alpha_q - \beta_q^\dagger \beta_q \right), \qquad \Omega_q = \sqrt{\cos^2 q + \mu^2}. \tag{66}$$

The ground state is again given by the filled band of α_q fermions, and in appendix A we show that the corresponding correlation matrix commutes with the tridiagonal matrix defined by

$$t_m = -\frac{1}{2}m, \qquad d_m = (-1)^m \mu (m - 1/2). \tag{67}$$

Compared with (48), we see that the transformation (65) now includes, instead of a phase, a different weight factor for even and odd sites. Incorporating this extra weight, we shall use the ansatz for the eigenvectors

$$\psi_\lambda(m) = \int_{-\pi/2}^{\pi/2} \frac{\mathrm{d}q}{2\pi} \mathrm{e}^{\mathrm{i}q(m-1/2)} \mathrm{e}^{\mathrm{i}\lambda\varphi_q} \frac{\sqrt{\Omega_q - (-1)^m \mu}}{\Omega_q}. \tag{68}$$

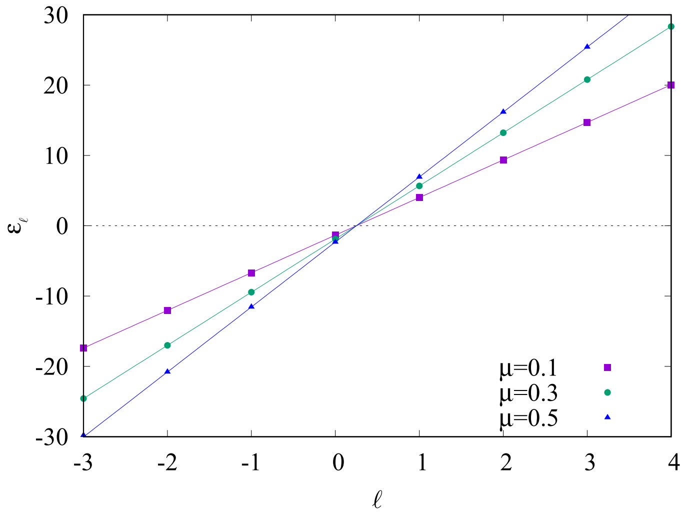

Figure 5. Single-particle spectra (symbols) of the EH of a hopping chain with a staggered field, for a finite half-chain of size $N=50$ and various μ. The lines show the $N\to\infty$ result in (72).

Multiplying with $-2T$ and using the expression of the dispersion (66), one obtains the integrand

$$\left[(2m-1)\sqrt{\Omega_q-(-1)^m\mu}+\mathrm{i}\sin q\frac{\sqrt{\Omega_q+(-1)^m\mu}}{\Omega_q}\right]\mathrm{e}^{\mathrm{i}q(m-1/2)}\mathrm{e}^{\mathrm{i}\lambda\varphi_q}. \tag{69}$$

Integrating by parts in the first term, one finds again a cancellation with the second term, and the phase must satisfy $\frac{\mathrm{d}\varphi_q}{\mathrm{d}q}=\Omega_q^{-1}$, which can be integrated as

$$\varphi_q=\kappa F(q,\kappa), \qquad \kappa=\frac{1}{\sqrt{1+\mu^2}}. \tag{70}$$

Furthermore, the boundary contribution can be assessed by noting that $\Omega_{\pm\pi/2}=|\mu|$, and thus for $\mu>0$ ($\mu<0$) one needs to consider only the case $m=2\ell+1$ ($m=2\ell$). The requirement is that the phase factor $\mathrm{e}^{\mathrm{i}\frac{\pi}{2}(m-1/2)}\mathrm{e}^{\mathrm{i}\lambda\varphi_{\pi/2}}$ be real, which yields

$$\lambda_\ell=\frac{\pi}{2\kappa K(\kappa)}\begin{cases}2\ell-\frac{1}{2} & \text{if } \mu>0\\ 2\ell+\frac{1}{2} & \text{if } \mu<0\end{cases}, \qquad \ell=0,\pm1,\pm2,\ldots \tag{71}$$

Note that the difference in the quantization w.r.t. (59) is due to the missing phase factor in the transformation (65). In particular, (71) breaks the particle-hole symmetry of the spectrum, which transforms as $\lambda_\ell\to-\lambda_{-\ell}$ under $\mu\to-\mu$.

Finally, we discuss the spectrum of C, which is obtained completely analogously to the previous section. The only difference is the extra factor κ in the phase φ_q, such that the EH and its spectrum read

$$H = 4\kappa K(\kappa')T, \qquad \varepsilon_\ell = 2\pi \frac{K(\kappa')}{K(\kappa)} \begin{cases} 2\ell - \frac{1}{2} & \text{if } \mu > 0 \\ 2\ell + \frac{1}{2} & \text{if } \mu < 0 \end{cases}. \tag{72}$$

We have checked this result against numerical calculations for a finite open chain of total size $2N$. The ε_ℓ are computed from the eigenvalues of the reduced correlation matrix of the half-chain with size $N = 50$, and shown in figure 5 for various μ. The comparison with the $N \to \infty$ result (lines) in (72) shows an excellent agreement, which is expected for a gapped system with $N \gg \xi$, i.e. when the size far exceeds the correlation length. The corresponding eigenvectors are very similar to the dimerized case in figure 4, and their normalization is analogous to (63), with the exchange $\delta' \to \kappa$ and an extra factor κ coming from the size of the integration domain on the real axis.

6. Discussion

We have studied the EH in nonrelativistic free-fermion systems for a semi-infinite domain, which is described by the deformed physical Hamiltonian with linearly increasing couplings. Its single-particle eigenstates have a remarkably simple and universal structure, which holds both for models defined in the continuum as well as on the lattice, and both for critical and gapped ground states. Indeed, in all the cases considered, these are obtained as a superposition of the modes of the total system, weighted with the inverse of their single-particle energy measured from the Fermi level. Additionally, each mode receives an extra phase that is proportional to the integrated weight, and the prefactor is related to the corresponding eigenvalue. The spectrum is continuous for critical systems, and becomes discrete with an equidistant spacing for the gapped chains under study. While for the dimerized chain this can also be obtained by duality with the transverse Ising chain and the corresponding CTM [37], the result for the staggered chain is different and features a slightly shifted level structure. In fact, it is unclear whether there exists a classical 2D integrable model whose CTM would reproduce the same spectrum.

A further important observation is that, despite the nonrelativistic form of the models considered, the BW form becomes exact, i.e. the EH is equal to the linearly deformed Hamiltonian up to a prefactor. While in the critical case one finds the expected form (1) of the BW theorem with v given by the Fermi velocity, for gapped systems the prefactor is nonuniversal. It is related to the behaviour of the inverse of the extra phase appearing in the eigenfunctions, in particular its periodicity along the imaginary direction on the complex plane. In contrast to the relativistic case, it carries a nontrivial dependence on the mass gap.

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There are various possible extensions of this work. First, one could ask if the ansatz found for a semi-infinite subsystem could be generalized to other geometries, such as the interval, where the entanglement entropy has been studied thoroughly [38–40]. The commuting operator/matrix corresponds to the parabolic deformation of the Hamiltonian both in the continuum as well as on the lattice [41], and their spectra and eigenfunctions were studied in detail [34, 42]. In turn, one finds that the EH is nontrivially related to the commuting operator. While in the continuum the corrections vanish in the limit of a large interval [43], on the lattice the structure of the EH is modified and involves longer range hopping [44], such that the CFT prediction can be recovered only after an appropriate continuum limit [45, 46]. It would be interesting to see, if the eigenvectors of the EH could be cast in a form analogous to the one obtained here. Finding such a representation could provide physical insight on the corrections observed in the EH beyond the CFT result. It could also help to attack the massive case [37], where no analytical QFT result is available so far and one has to rely on numerical approaches [47].

One could also address more general lattice models, e.g. when the dimerized hopping and staggered fields are simultaneously present. A non-Hermitian version of such an SSH model has recently been studied in the context of the EH, finding some nontrivial behaviour at the critical point [48]. Another interesting scenario where commuting operators play a crucial role is the one of inhomogeneous hopping chains related to orthogonal polynomials [49–51]. In the continuum limit, such inhomogeneous models can be described by a CFT in a curved background metric [52], and the EH can be derived by appropriate conformal mappings [53, 54], with a BW form shown to emerge in particular cases [55]. Generalizing our ansatz to the eigenvectors of the EH in these models could shed light on novel features.

Finally, it remains to understand how the ansatz could be adapted to interacting integrable systems, such as the XXZ chain, where the EH in the gapped phase can be obtained via the CTM method and is known to have the BW form [16]. The integrable generalization of the ansatz is further motivated by the fact, that the substitution applied in (37) is reminiscent of the rapidity parametrization. Finding the proper formulation could give a direct access to the EH also in the critical phase, which could so far only be probed indirectly via numerical simulations [56–58].

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Appendix A. Calculation of commutators

A.1. Fermi gas

We shall prove here that the differential operator (7) indeed commutes with the integral operator $\hat{K}$ involving the sine kernel (3) on the semi-infinite domain. One has

$$\begin{aligned}-2\hat{D}\hat{K}f &= \left(x\frac{\mathrm{d}^2}{\mathrm{d}x^2}+\frac{\mathrm{d}}{\mathrm{d}x}+q_\mathrm{F}^2 x\right)\int_0^\infty \mathrm{d}y\, K(x-y)\, f(y)\\ &= \int_0^\infty \mathrm{d}y\, f(y)\left(x\frac{\mathrm{d}^2}{\mathrm{d}y^2}-\frac{\mathrm{d}}{\mathrm{d}y}+q_\mathrm{F}^2 x\right)K(x-y)\end{aligned} \tag{A1}$$

as well as

$$\begin{aligned}-2\hat{K}\hat{D}f &= \int_0^\infty \mathrm{d}y\, K(x-y)\left(y\frac{\mathrm{d}^2}{\mathrm{d}y^2}+\frac{\mathrm{d}}{\mathrm{d}y}+q_\mathrm{F}^2 y\right)f(y)\\ &= \int_0^\infty \mathrm{d}y\, f(y)\left(\frac{\mathrm{d}^2}{\mathrm{d}y^2}y-\frac{\mathrm{d}}{\mathrm{d}y}+q_\mathrm{F}^2 y\right)K(x-y),\end{aligned} \tag{A2}$$

where in the last step we have integrated by parts. Note that there is a boundary contribution $-K(x)f(0)$ from the first order derivative. This, however, is cancelled by the boundary term of the second order derivative at the second partial integration, which gives $-f(y)\frac{\mathrm{d}}{\mathrm{d}y}[yK(x-y)]\Big|_0^\infty = K(x)f(0)$. Note that one also needs to require that the function $f(y)\to 0$ and its derivative $f'(y)\to 0$ as $y\to\infty$. One has further

$$\frac{\mathrm{d}^2}{\mathrm{d}y^2}yK(x-y) = -2K'(x-y)+yK''(x-y), \tag{A3}$$

such that the commutator reads

$$\begin{aligned}-2\left[\hat{D},\hat{K}\right]f = \int_0^\infty \mathrm{d}y\, f(y)\,&[(x-y)\,K''(x-y)+2K'(x-y)\\ &+q_\mathrm{F}^2(x-y)\,K(x-y)].\end{aligned} \tag{A4}$$

It is then easy to see that

$$\begin{aligned}K'(x-y) &= q_\mathrm{F}\frac{\cos q_\mathrm{F}(x-y)}{\pi(x-y)}-\frac{\sin q_\mathrm{F}(x-y)}{\pi(x-y)^2},\\ K''(x-y) &= -q_\mathrm{F}^2\frac{\sin q_\mathrm{F}(x-y)}{\pi(x-y)}-2q_\mathrm{F}\frac{\cos q_\mathrm{F}(x-y)}{\pi(x-y)^2}+2\frac{\sin q_\mathrm{F}(x-y)}{\pi(x-y)^3}\end{aligned} \tag{A5}$$

and thus substituting into (A4) the commutator vanishes.

A.2. Hopping chain

Next we show, that the tridiagonal matrix (30) with elements given by (31) commutes with the discrete sine kernel in (28). One has

$$-2(TC)_{m,n} = m\,C_{m+1,n}+(m-1)\,C_{m-1,n}-2\cos q_\mathrm{F}(m-1/2)\,C_{m,n}$$

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$$-2\,(CT)_{m,n} = n\,C_{m,n+1} + (n-1)\,C_{m,n-1} - 2\cos q_{\mathrm{F}}\,(n-1/2)\,C_{m,n} \tag{A6}$$

One can then introduce $r = m - n$ and rewrite

$$-2\,[T,C]_{m,n} = r\,(C_{m+1,n} + C_{m-1,n}) + C_{m+1,n} - C_{m-1,n} - 2r\cos q_{\mathrm{F}} C_{m,n} \tag{A7}$$

Furthermore one has

$$\begin{aligned} C_{m+1,n} + C_{m-1,n} &= \frac{\sin q_{\mathrm{F}}\,(r+1)}{\pi\,(r+1)} + \frac{\sin q_{\mathrm{F}}\,(r-1)}{\pi\,(r-1)} = \frac{2r\sin q_{\mathrm{F}} r\cos q_{\mathrm{F}} - 2\sin q_{\mathrm{F}}\cos q_{\mathrm{F}} r}{\pi\,(r^2-1)}, \\ C_{m+1,n} - C_{m-1,n} &= \frac{\sin q_{\mathrm{F}}\,(r+1)}{\pi\,(r+1)} - \frac{\sin q_{\mathrm{F}}\,(r-1)}{\pi\,(r-1)} = \frac{2r\sin q_{\mathrm{F}}\cos q_{\mathrm{F}} r - 2\sin q_{\mathrm{F}} r\cos q_{\mathrm{F}}}{\pi\,(r^2-1)}, \end{aligned} \tag{A8}$$

and substituting into (A7) one can easily recover $[T,C]=0$.

A.3. Dimerized chain

For the dimerized chain T and C have an alternating structure. However, they both couple only sites over odd distances, such that their product is nonvanishing only for even index distances. Assuming even indices one has

$$\begin{aligned} -2\,(TC)_{2m,2n} &= (1-\delta)\,2m\,C_{2m+1,2n} + (1+\delta)\,(2m-1)\,C_{2m-1,2n} \\ -2\,(CT)_{2m,2n} &= (1-\delta)\,2n\,C_{2m,2n+1} + (1+\delta)\,(2n-1)\,C_{2m,2n-1} \end{aligned} \tag{A9}$$

Furthermore, the correlation matrix elements have the structure

$$C_{2m-1,2n} = \mathcal{C}_r + \delta\,\mathcal{S}_r, \qquad C_{2m,2n+1} = \mathcal{C}_r - \delta\,\mathcal{S}_r, \tag{A10}$$

where $r = 2n+1-2m$ and we defined the integrals

$$\mathcal{C}_r = \int_{-\pi/2}^{\pi/2} \frac{\mathrm{d}q}{2\pi} \frac{\cos qr\cos q}{\sqrt{\cos^2 q + \delta^2\sin^2 q}}, \qquad \mathcal{S}_r = \int_{-\pi/2}^{\pi/2} \frac{\mathrm{d}q}{2\pi} \frac{\sin qr\sin q}{\sqrt{\cos^2 q + \delta^2\sin^2 q}}. \tag{A11}$$

Inserting these expressions, one obtains for the commutator matrix element

$$\begin{aligned} -2\,[C,T]_{2m,2n} = &(r-1)\left[\mathcal{C}_r + \mathcal{C}_{r-2} + \delta^2\,(\mathcal{S}_r - \mathcal{S}_{r-2})\right] + (\mathcal{C}_r - \mathcal{C}_{r-2}) + \delta^2\,(\mathcal{S}_r + \mathcal{S}_{r-2}) \\ &- (2m+2n-1)\,\delta\,(\mathcal{C}_r - \mathcal{C}_{r-2} + \mathcal{S}_r + \mathcal{S}_{r-2}) \end{aligned} \tag{A12}$$

The first of these terms can be evaluated using trigonometric identities as

$$\begin{aligned} (r-1)\left[\mathcal{C}_r + \mathcal{C}_{r-2} + \delta^2\,(\mathcal{S}_r - \mathcal{S}_{r-2})\right] &= \int_{-\pi/2}^{\pi/2} \frac{\mathrm{d}q}{2\pi}\,(r-1)\cos q\,(r-1)\sqrt{\cos^2 q + \delta^2\sin^2 q} \\ &= \int_{-\pi/2}^{\pi/2} \frac{\mathrm{d}q}{2\pi}\,(1-\delta^2)\,\frac{\sin q\,(r-1)\sin 2q}{\sqrt{\cos^2 q + \delta^2\sin^2 q}}, \end{aligned} \tag{A13}$$

where in the second line we have integrated by parts. For the rest of the terms we need the expressions

$$\mathcal{S}_r + \mathcal{S}_{r-2} = -(\mathcal{C}_r - \mathcal{C}_{r-2}) = \int_{-\pi/2}^{\pi/2} \frac{\mathrm{d}q}{2\pi} \frac{\sin q\,(r-1)\sin 2q}{\sqrt{\cos^2 q + \delta^2 \sin^2 q}}. \tag{A14}$$

One can then immediately verify, that the first term in (A12) cancels with the second and third one in the first line, while the second line also gives zero. The proof for the case of odd indices follows similarly.

A.4. Staggered potential

For the staggered potential the elements of the correlation matrix with $r = m-n$ read

$$C_{m,n} - \frac{1}{2}\delta_{m,n} = \begin{cases} -(-1)^m \mu \int_{-\pi/2}^{\pi/2} \frac{\mathrm{d}q}{2\pi} \frac{\cos qr}{\sqrt{\cos^2 q + \mu^2}} & m-n \text{ even} \\ \int_{-\pi/2}^{\pi/2} \frac{\mathrm{d}q}{2\pi} \frac{\cos qr \cos q}{\sqrt{\cos^2 q + \mu^2}} & m-n \text{ odd} \end{cases} \tag{A15}$$

The matrix products with the T have a similar form as for the homogeneous chain in (A6), except for the alternation of the potential. However, when calculating the commutator, one has now the property $C_{m-1,n} = \pm C_{m,n+1}$, where the plus/minus sign corresponds to $m-n$ being even or odd. This yields

$$\begin{aligned} &-2\,[T,C]_{m,n} \\ &= \begin{cases} (m-n)\left(C_{m+1,n} + C_{m-1,n} - (-1)^m 2\mu C_{m,n}\right) + C_{m+1,n} - C_{m-1,n} & m-n \text{ even} \\ (m+n-1)\left(C_{m+1,n} + C_{m-1,n} - (-1)^m 2\mu C_{m,n}\right) & m-n \text{ odd} \end{cases} \end{aligned} \tag{A16}$$

Considering the case $m-n$ even first, one finds from (A15)

$$r\left(C_{m+1,n} + C_{m-1,n} - (-1)^m 2\mu C_{m,n}\right) = \int_{-\pi/2}^{\pi/2} \frac{\mathrm{d}q}{2\pi} 2r \cos qr \sqrt{\cos^2 q + \mu^2}, \tag{A17}$$

$$C_{m+1,n} - C_{m-1,n} = -\int_{-\pi/2}^{\pi/2} \frac{\mathrm{d}q}{2\pi} \frac{\sin qr \sin 2q}{\sqrt{\cos^2 q + \mu^2}}. \tag{A18}$$

Integrating by parts in (A17), one finds exactly the negative of (A18), and thus the commutator (A16) vanishes. It is easy to check using (A15) that the same holds true for $m-n$ odd as well.

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Appendix B. Relation to orthogonal polynomials

Here we show that the eigenvectors (32) are related to the so-called Meixner–Pollaczek polynomials [36], and derive the proportionality factor between them. These hypergeometric orthogonal polynomials can be expressed as

$$P_n^{(\alpha)}(x;\phi) = \frac{(2\alpha)_n}{n!} \mathrm{e}^{\mathrm{i}n\phi} {}_2F_1\left(\begin{matrix} -n,\ \lambda + \mathrm{i}x \\ 2\lambda \end{matrix} ; 1 - \mathrm{e}^{-2\mathrm{i}\phi} \right) \tag{B1}$$

where $(2\alpha)_n$ is the Pochhammer symbol, and the first few polynomials are given by

$$\begin{aligned} P_0^{(\alpha)}(x;\phi) &= 1 \\ P_1^{(\alpha)}(x;\phi) &= 2(\alpha\cos\phi + x\sin\phi) \\ P_2^{(\alpha)}(x;\phi) &= x^2 + \alpha^2 + \left(\alpha^2 + \alpha - x^2\right)\cos(2\phi) + (1+2\lambda)x\sin(2\phi) \end{aligned} \tag{B2}$$

The Meixner–Pollaczek polynomials satisfy the orthogonality relation with respect to a weight function

$$\begin{aligned} \int_{-\infty}^{\infty} \mathrm{d}x\, w(x;\alpha,\phi)\, P_n^{(\alpha)}(x;\phi)\, P_m^{(\alpha)}(x;\phi) &= \frac{2\pi\,\Gamma(n+2\alpha)}{(2\sin\phi)^{2\alpha} n!}\delta_{m,n}, \\ w(x;\alpha,\phi) &= |\Gamma(\alpha + \mathrm{i}x)|^2 \mathrm{e}^{(2\phi-\pi)x}. \end{aligned} \tag{B3}$$

As pointed out in the main text, our eigenvectors correspond to $\alpha = 1/2$, $\phi = q_\mathrm{F}$, and $x = -\lambda/\sin q_\mathrm{F}$, there is, however, a proportionality factor to be fixed. A direct numerical comparison of the first few components of $\psi_\lambda(m)$ and (B2) for various values of λ and q_F suggests the relation

$$P_n^{(1/2)}(x;q_\mathrm{F}) = \sqrt{2}\mathrm{e}^{\frac{q_\mathrm{F}\lambda}{\sin q_\mathrm{F}}} \cosh\left(\frac{\pi\lambda}{\sin q_\mathrm{F}}\right) \psi_\lambda(n+1). \tag{B4}$$

We will now prove that the orthogonality relation (B3) is indeed satisfied with this choice. Plugging in one has

$$\begin{aligned} \pi \int_{-\infty}^{\infty} \mathrm{d}x \left(1 + \mathrm{e}^{-2\pi x}\right) \int_{-\infty}^{\infty} \frac{\mathrm{d}z}{\pi} \frac{\mathrm{e}^{\mathrm{i}q(z)(m+1/2)}}{\sqrt{\cos q_\mathrm{F} + \cosh(2z)}} \\ \times \int_{-\infty}^{\infty} \frac{\mathrm{d}z'}{\pi} \frac{\mathrm{e}^{-\mathrm{i}q(z')(n+1/2)}}{\sqrt{\cos q_\mathrm{F} + \cosh(2z')}} \mathrm{e}^{\mathrm{i}2x(z'-z)}. \end{aligned} \tag{B5}$$

The integral over x can be carried out and reads

$$\int_{-\infty}^{\infty} \mathrm{d}x \left(1 + \mathrm{e}^{-2\pi x}\right) \mathrm{e}^{\mathrm{i}2x(z'-z)} = \pi\left[\delta(z'-z) + \delta(z'-z+\mathrm{i}\pi)\right]. \tag{B6}$$

The first delta function simply reproduces $\frac{\pi}{\sin q_\mathrm{F}} C_{m,n}$. The second one requires an $\mathrm{i}\pi$ shift between the two variables. In order to understand its effect, let us shift the variables

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$z \to z + \mathrm{i}\pi/2$ and $z' \to z' - \mathrm{i}\pi/2$ to the upper and lower half-planes, respectively. The corresponding changes are

$$\cosh(2z) \to -\cosh(2z), \qquad \tanh(z) \to \coth(z), \tag{B7}$$

and similarly for z'. In turn, the function $q(z)$ and its Jacobian transforms into

$$\bar{q}(z) = 2\mathrm{atan}\left[\tan(q_{\mathrm{F}}/2)\coth(z)\right], \qquad \frac{\mathrm{d}\bar{q}}{\mathrm{d}z} = \frac{2\sin q_{\mathrm{F}}}{\cos q_{\mathrm{F}} - \cosh(2z)}, \tag{B8}$$

such that $\bar{q}(z)$ now maps the infinite line to the complement $\bar{F}$ of the Fermi sea. The second delta function in (B6) thus yields the following contribution

$$-\pi \int_{-\infty}^{\infty} \frac{\mathrm{d}z}{2\pi} \frac{2}{\cos q_{\mathrm{F}} - \cosh(2z)} \mathrm{e}^{\mathrm{i}\bar{q}(z)(m-n)}, \tag{B9}$$

where the extra sign appears because of the branch cut of the square root. The weight factor is thus proportional to the Jacobian of the transformation, and changing back to the $\bar{q}$ variable, one obtains the complementary sine kernel

$$\frac{\pi}{\sin q_{\mathrm{F}}} \bar{C}_{m,n} = \frac{\pi}{\sin q_{\mathrm{F}}} \left(\delta_{m,n} - C_{m,n}\right) \tag{B10}$$

Adding the two pieces, we obtain the relation (B3).

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