

Free-fermion entanglement and spheroidal functions

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We consider the entanglement properties of free fermions in one dimension and review an approach which relates the problem to the solution of a certain differential equation. The single-particle eigenfunctions of the entanglement Hamiltonian are then seen to be spheroidal functions or generalizations of them. The analytical results for the eigenvalue spectrum agree with those obtained by other methods. In the continuum case, there are close connections to random matrix theory.

I. INTRODUCTION

The entanglement properties of many-particle quantum states have been the topic of many studies in recent years [1]. This holds in particular for the ground state of free fermionic systems. These are Slater determinants, and in this case the reduced density matrix (RDM) for some portion of the total system has the form

$$\rho = \frac{1}{Z} e^{-\mathcal{H}} \quad (1)$$

where \mathcal{H} is again a free-particle Hamiltonian, see [2]. Its single-particle eigenfunctions φ_k and the corresponding eigenvalues ε_k can be determined either from the one-particle correlation functions [3–6] or from the overlap of the occupied states in the subsystem [7, 10–12]. Their properties for the most studied case, namely a segment in a chain of free fermions, are relatively well-known. Thus the low-lying $|\varepsilon_k|$ vary roughly linearly with k and the slope is proportional to $1/\ln L$ if the subsystem has length L and $\ln L$ is large. This leads to a logarithmic variation $S = 1/3 \ln L$ of the entanglement entropy S which is characteristic for critical systems and follows from conformal invariance, see [13]. The law was first obtained from an asymptotic analysis of the correlation matrix using the Fisher-Hartwig conjecture [14], and further subleading terms have been derived in the same way [15, 16]. The eigenfunctions φ_k are largest near the boundaries for small $|\varepsilon_k|$ and concentrated in the interior of the subsystem for large $|\varepsilon_k|$. This can be seen easily from numerical calculations. For a half-filled system, there are also analytical expressions in the continuum limit [9]. Altogether, a picture emerges, where the (entanglement) Hamiltonian \mathcal{H} has both bulk and

boundary-like states with the latter dominating the entanglement.

Given the relatively simple form of the correlations (or the overlap), one wonders whether a complete analytical treatment of the problem is possible. This is, in fact, the case and it turns out that it was done a long time ago by Slepian in the analysis of time and band limited signals [17, 18]. A good account of the background can be found in his 1982 John von Neumann lecture [19]. The work has received a large number of citations in very different areas. The analogy to the entanglement problem, where one deals with limited regions in momentum space (the Fermi sea) and in real space (the subsystem), was pointed out already by Gioev and Klich [8]. However, while they derived a formula for S in higher dimensions, we focus here on the eigenvalue problem.

It turns out that the eigenfunctions φ_k , or their Fourier transforms, are the (prolate) spheroidal functions which appear if one separates the Helmholtz equation in elliptical coordinates, or generalizations of them. They enter in the continuum case because the integral kernel of the entanglement problem commutes with the corresponding differential operator. Those concentrated in the interior of the subsystem are quite familiar objects, namely oscillator functions. They become more complicated once they touch the boundary. In any case, the machinery of solving differential equations can be used to obtain their form and also the eigenvalues ε_k . In particular, an asymptotic analysis is possible and gives the low-lying ones for the case of a large subsystem. This leads to exactly the same density of states as found in the Fisher-Hartwig approach [14, 20]. If either momenta or positions become discrete, the situation is still similar. Working with the other, continuous quantity, one has a commuting differential operator and can discuss its eigenfunctions. One should mention that a lot of this material also appears in random matrix theory, because in the Gaussian unitary ensemble the same integral kernel enters and the eigenvalues ε_k determine the functions of interest, see [21]. The connection to this field was pointed out by Keating and Mezzadri [22, 23] and also used in [15], but again with the focus on the entropy.

The purpose of this paper is to draw attention to the results described above, because they complement the usual approaches and put the entanglement problem into a broader context. Our own contribution is mainly the collection and the presentation, including a number of figures. In section 2 we give a brief general outline of the determination of φ_k via correlation and overlap matrices. In section 3 we discuss the case of an infinite continuum system, where the simple sine kernel and the usual spheroidal functions appear, of which we show some examples. Section 4 treats the case of a finite continuum system, where the correlations still lead to an integral equation. Section 5 deals with an infinite lattice where the same equation appears in momentum space. In this case we also discuss the matrix which commutes with the correlation matrix, as well

as the dispersion relation of the ε_k . Finally, section 6 contains remarks on semi-infinite systems and higher dimensions and a brief conclusion is given in Section 7.

II. CORRELATION MATRICES AND OVERLAP MATRICES

The structure of the problem is best seen from the formulae for a general lattice system with a discrete set of orthonormal single-particle functions $\Phi_q(n)$. A many-particle state $|F\rangle$ in which a set F of these is occupied (the Fermi sea) then is

$$|F\rangle = \prod_{q \in F} c_q^\dagger |0\rangle \quad (2)$$

where c_q^\dagger are creation operators and $|0\rangle$ is the vacuum. With

$$c_n = \sum_q \Phi_q(n) c_q \quad (3)$$

the correlation matrix in state $|F\rangle$ becomes

$$C_{mn} = \langle F | c_m^\dagger c_n | F \rangle = \sum_{q \in F} \Phi_q^*(m) \Phi_q(n) \quad (4)$$

and the RDM in a subsystem S is determined by the eigenvalue problem

$$\sum_{j \in S} C_{ij} \varphi_k(j) = \zeta_k \varphi_k(i), \quad i \in S \quad (5)$$

If S consists of L sites, (5) gives L single-particle eigenfunctions φ_k . The eigenvalues ζ_k with $0 \leq \zeta_k \leq 1$ are their non-integer occupation numbers and related to the ε_k via

$$\varepsilon_k = \ln \frac{1 - \zeta_k}{\zeta_k} \quad \text{or} \quad \zeta_k = \frac{1}{e^{\varepsilon_k} + 1} \quad (6)$$

These quantities can also be obtained by constructing the Schmidt decomposition of $|F\rangle$ directly [7]. In this case, one forms new orthonormal functions Ψ_k from the occupied Φ_q which are orthogonal also in the subsystem (and in the remainder R). This is done by calculating the overlap matrix

$$A_{qq'} = \sum_{j \in S} \Phi_q^*(j) \Phi_{q'}(j) \quad (7)$$

and solving the eigenvalue problem

$$\sum_{q' \in F} A_{qq'} \varphi_k(q') = \zeta_k \varphi_k(q), \quad q \in F \quad (8)$$

Then

$$\Psi_k(i) = \sum_{q \in F} \varphi_k(q) \Phi_q(i) \quad (9)$$

satisfies (5) when restricted to S . Similarly, its restriction to R satisfies the analogue of (5) with eigenvalue $(1 - \zeta_k)$. Moreover, it has norm ζ_k in S and norm $1 - \zeta_k$ in R . Therefore, if φ_k is normalized in S , one has

$$\varphi_k(i) = \frac{1}{\sqrt{\zeta_k}} \Psi_k(i), \quad i \in S \quad (10)$$

which gives the pair of relations

$$\varphi_k(i) = \frac{1}{\sqrt{\zeta_k}} \sum_{q \in F} \varphi_k(q) \Phi_q(i) \quad , \quad \varphi_k(q) = \frac{1}{\sqrt{\zeta_k}} \sum_{i \in S} \varphi_k(i) \Phi_q^*(i) \quad (11)$$

The normalization properties allow to obtain the eigenvalues ζ_k solely from the Ψ_k if these can be found by some other means (as will be the case below). If one arranges the ζ_k in decreasing order, the corresponding Ψ_k are less and less concentrated in S . For L sites in the subsystem, (8) can have only L non-trivial solutions. If the particle number, i.e. the number of states in F , exceeds L , the remaining Ψ_k have no components in the subsystem and $\zeta_k = 0$.

In the following we apply these formulae to the case of plane waves, $\Phi_q(n) \sim e^{iqn}$ or $\Phi_q(x) \sim e^{iqx}$. The two eigenvalue problems (5) and (8) then correspond to working in real space and in momentum space, respectively. Moreover, the state $|F\rangle$ will be a normal Fermi sea ($|q| \leq q_F$) and the subsystem S a single segment. The two functions $\varphi_k(i)$ and $\varphi_k(q)$ are then related by a Fourier transform limited to a window in q space and in real space.

III. INFINITE CONTINUOUS SYSTEM

We now consider free fermions on an infinite line with all momentum states $|q| \leq q_F$ filled. The system then has average density $\bar{n} = q_F/\pi$ and the correlation matrix is

$$C(x - x') = \int_{-q_F}^{q_F} \frac{dq}{2\pi} e^{-iq(x-x')} = \frac{\sin q_F(x - x')}{\pi(x - x')} \quad (12)$$

Choosing the subsystem S as the segment $-\ell/2 \leq x \leq \ell/2$, the eigenvalue problem (5) becomes

$$\int_{-\ell/2}^{\ell/2} dx' C(x - x') \varphi_k(x') = \zeta_k \varphi_k(x) \quad (13)$$

or in reduced variables $y = 2x/\ell$ with $\varphi_k(\ell y/2) = \psi_k(y)$

$$\int_{-1}^1 dy' K(y - y') \psi_k(y') = \zeta_k \psi_k(y) \quad (14)$$

with the *sine kernel*

$$K(y - y') = \frac{\sin c(y - y')}{\pi(y - y')}, \quad c = q_F \ell / 2 \quad (15)$$

Similarly, the overlap matrix is

$$A(q - q') = \int_{-\ell/2}^{\ell/2} \frac{dx}{2\pi} e^{-i(q-q')x} = \frac{\sin(q - q')\ell/2}{\pi(q - q')} \quad (16)$$

and with $p = q/q_F$ the eigenvalue problem (8) becomes

$$\int_{-1}^1 dp' K(p - p') \psi_k(p') = \zeta_k \psi_k(p) \quad (17)$$

Thus the equations in real space and in momentum space are identical. In the following, we will work in real space.

The sine kernel is the “square” of another, even simpler symmetric kernel $\tilde{K}(y, y')$

$$K(y - y') = \int_{-1}^1 dz \tilde{K}(y, z) \tilde{K}^*(z, y'), \quad \tilde{K}(y, z) = \sqrt{\frac{c}{2\pi}} e^{icyz} \quad (18)$$

Therefore, the eigenvalues ζ_k of the sine kernel follow from the eigenvalues μ_k of \tilde{K} via $\zeta_k = |\mu_k|^2$. Moreover, \tilde{K} commutes with the second-order *differential operator* [24]

$$D = -\frac{d}{dy}(1 - y^2)\frac{d}{dy} + c^2 y^2 \quad (19)$$

provided the functions one operates on are regular at $y = \pm 1$. Therefore the (real) eigenfunctions of \tilde{K} and K can be obtained from

$$D\psi = \theta\psi \quad (20)$$

This equation has continuous and bounded solutions for all y only for a discrete set of values $\theta = \theta_k$. The corresponding ψ_k are the prolate spheroidal wave functions of the first kind and order $m = 0$. In the notation of [25] these are called angular functions S_{0k} for $y^2 < 1$ and radial functions R_{0k} for $y^2 > 1$ (which fits with our notations of subsystem and remainder). Both are normalized separately and connected by joining formulae. Their properties have been investigated in great detail, see e.g. [26–28]. Studying the solution of (20) for *all* y gives the quantity Ψ_k of (10). Of particular interest is the case where the subsystem contains many particles. Since the average number is

$$\bar{N} = \ell \bar{n} = \frac{2}{\pi} c \quad (21)$$

this corresponds to large c .

A qualitative picture of the spheroidal functions can be obtained by observing that for small y the operator D reduces to

$$D = -\frac{d^2}{dy^2} + c^2 y^2 \quad (22)$$

and thus to the Hamiltonian of the harmonic oscillator with frequency $\omega = c$. The oscillator functions

$$u_k(y) = A_k e^{-\frac{1}{2}cy^2} H_k(\sqrt{c}y) \quad (23)$$

with the Hermite polynomials H_k have a spatial extension $y_k \simeq \sqrt{(2k+1)/c}$ (using the classical turning point) and therefore "fit" into the subsystem as long as $2k+1 < c$. Under this condition the exact spheroidal functions resemble them closely, in particular those concentrated fully in the interior. A picture gallery is shown in Fig. 1, where we plotted the first 15 spheroidal and oscillator functions for $c = 5\pi$ ($\bar{N} = 10$). Both are normalized to $2/(2k+1)$ in $(-1, 1)$. The function S_{0k} has exactly k zeros there and is alternatingly even and odd. One sees that up to $k \sim 7$ the differences are rather small. As k increases further, the oscillator functions deviate more and have zeros outside the subsystem, while the oscillation of S_{0k} becomes faster near the boundaries. For large c , it is logarithmic up to a distance $1/\sqrt{c}$ from ± 1 , i.e. besides y the variable $\ln[(1+y)/(1-y)]$ enters, as also found in a continuum approximation for a half-filled lattice system [9]. The nature of the eigenfunctions is reflected directly in the occupation numbers ζ_k which are close to 1 for small k and close to zero for large k . As discussed below, the transition takes place at $k \sim \bar{N}$.

If one continues ψ_k to $y^2 > 1$, one finds the eigenfunctions in the remainder R corresponding to the eigenvalue $1 - \zeta_k$. These are a kind of mirror image of those in S . For small k , they are oscillating rapidly near the boundary but have very small amplitudes (the phenomenon has been termed superoscillation [29]), while for large k the behaviour is smooth there and only later an oscillation sets in. This is illustrated in Fig. 2 where the R_{0k} are shown for a number of k values up to $k = 40$. Note that due to the normalization conventions the functions S_{0k} and R_{0k} do not match at $y = 1$. The form for $|y| \gg 1$ can be obtained from D by writing $\psi(y) = \chi(y)/y$ which leads to the operator

$$\hat{D} = y \left(\frac{d^2}{dy^2} + c^2 \right) \quad (24)$$

and gives approximately wave-like solutions $\chi(y) \sim \cos(cy + \alpha) = \cos(q_F x + \alpha)$. This can be seen clearly in the figure.

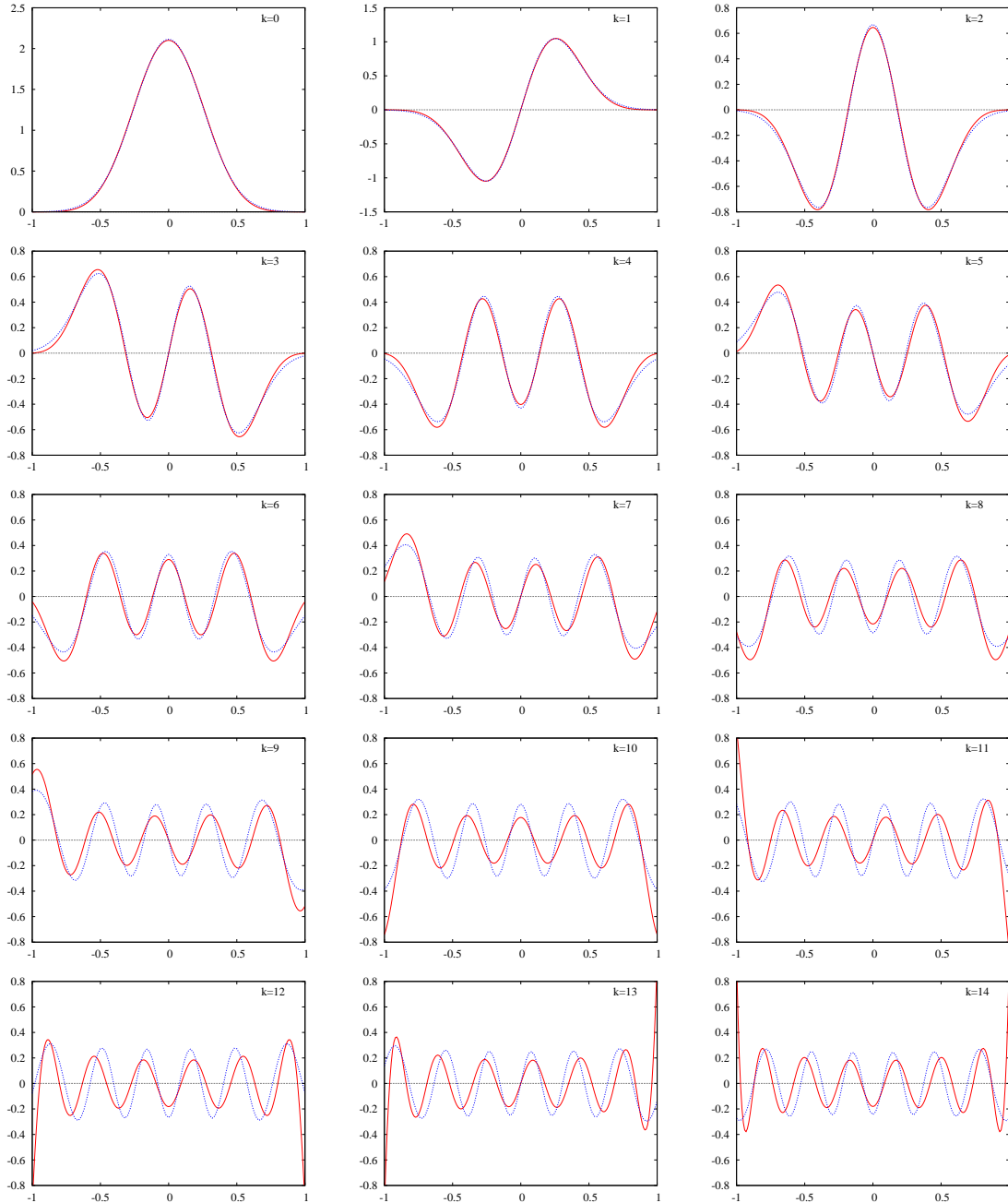


FIG. 1: The first 15 spheroidal functions $S_{0k}(c, y)$ for $c = 5\pi$ (full lines, red) and, for comparison, the oscillator functions $u_k(y)$ (dotted lines, blue).

Turning to the eigenvalues ζ_k (usually called λ_k in the literature), they can be obtained from the relation [27]

$$\int_{-1}^1 dy e^{icyz} S_{0k}(c, y) = 2i^n R_{0k}(c, 1) S_{0k}(c, z) \quad (25)$$

which is, up to a factor, the eigenvalue equation of the integral operator \tilde{K} . This gives the general

formula

$$\zeta_k = |\mu_k|^2 = \frac{2c}{\pi} [R_{0k}(c, 1)]^2 \quad (26)$$

which can be evaluated numerically. To obtain analytical expressions for large c , Slepian considered the solutions of (20) in the various regions of y and connected them in the domains of overlap [17]. While he considered small and large k separately, des Cloizeaux and Mehta using WKB formulae could later obtain a single expression [30] and Landau and Widom gave a mathematical proof [31]. The procedure is rather tedious, but in the end a relatively simple result for ε_k emerges if $k \simeq \bar{N}$, c.f. (1.37), (1.38) in [17]. Namely, it is given by the root of smallest absolute value of the equation

$$c + \frac{\varepsilon_k}{\pi} \ln(2\sqrt{c}) - \varphi\left(\frac{\varepsilon_k}{2\pi}\right) = \frac{\pi}{2}\left(k - \frac{1}{2}\right) \quad (27)$$

where $\varphi(z) = \arg\Gamma(1/2 + iz)$ and $\Gamma(z)$ is the gamma function. This has solutions $|\varepsilon_k| \ll 1$ which are obtained by expanding $\varphi(z)$

$$\frac{\varepsilon_k}{2\pi} (\ln(4c) - \varphi'(0)) = \frac{\pi}{2}(k - 1/2 - \bar{N}) \quad (28)$$

or, with c inserted,

$$\varepsilon_k = \frac{\pi^2(k - 1/2 - \bar{N})}{\ln(2\pi\bar{N}) - \psi(1/2)} \quad (29)$$

where $\psi(1/2) = -\gamma - 2\ln 2 = -1.963\dots$, γ is Euler's constant and $\psi(z)$ denotes the digamma function. Thus ε_k goes through zero (ζ_k through $1/2$) for $k \simeq \bar{N} \gg 1$ and the slope vanishes logarithmically with c or \bar{N} . A similar formula was found in [9] for a half-filled lattice system. For larger ε_k one really has to solve (27). It is simpler, however, to view it as a relation $k = k(\varepsilon)$ which leads to a density of states $n(\varepsilon) = dk/d\varepsilon$ given by

$$n(\varepsilon) = \frac{1}{\pi^2} \left[\ln(4c) - \varphi'\left(\frac{\varepsilon}{2\pi}\right) \right] \quad (30)$$

where explicitly

$$\varphi'(z) = \frac{1}{2} \left[\psi\left(\frac{1}{2} + iz\right) + \psi\left(\frac{1}{2} - iz\right) \right] \quad (31)$$

This is the result found and plotted in [20] and implicit already in [14]. Inserting it into the expression for the entanglement entropy, one finds the leading logarithmic term and the first correction. We will come back to it in Section 5.

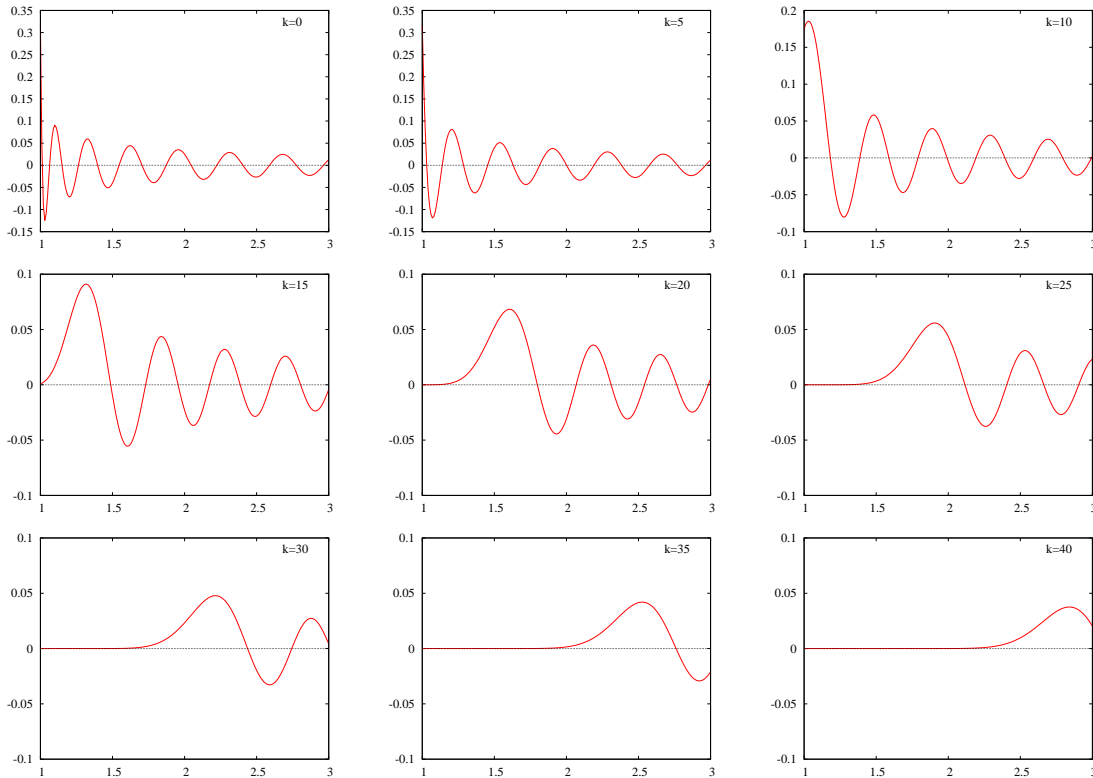


FIG. 2: Spheroidal functions $R_{0k}(c, y)$ for $c = 5\pi$, $1 \leq y \leq 3$ and various k .

IV. FINITE CONTINUOUS SYSTEM

Consider now a finite system in the form of a ring with circumference L . The momenta are quantized according to $q = 2\pi n/L$ with integer n and the Fermi momentum is written as $q_F = 2\pi m/L$. This gives a total particle number $N = 2m + 1$ and a correlation matrix

$$C(x - x') = \frac{1}{L} \sum_{n=-m}^m e^{-i2\pi(x-x')n/L} = \frac{1}{L} \frac{\sin(N\pi/L)(x-x')}{\sin(\pi/L)(x-x')} \quad (32)$$

With the same subsystem as before, $-\ell/2 \leq x \leq \ell/2$, the eigenvalue equation (13) retains its form. However, here it is preferable to define the reduced variable as $z = x/L$ such that $|z| \leq 1/2$. Then the equation becomes

$$\int_{-W}^W dz' K'(z - z') \psi_k(z') = \zeta_k \psi_k(z) \quad (33)$$

with $W = \ell/2L < 1/2$ and the *modified sine kernel*

$$K'(z - z') = \frac{\sin \pi N(z - z')}{\sin \pi(z - z')} \quad (34)$$

The overlap matrix is

$$A(q - q') = \int_{-\ell/2}^{\ell/2} \frac{dx}{L} e^{-i(q-q')x} = \frac{\sin(q - q')\ell/2}{(q - q')L/2} \quad (35)$$

but since the momenta are discrete, one can write it as

$$A_{nn'} = \frac{\sin(\pi\ell/L)(n - n')}{\pi(n - n')} \quad (36)$$

and the eigenvalue equation is a genuine matrix equation with a Toeplitz matrix.

The problem is now in exactly the form as studied by Slepian in 1978 [18]. In particular, (33) is his equation (10) and the ψ_k are his functions U_k . There are only N of them with non-zero eigenvalue (corresponding to the N eigenvalues of the overlap matrix) and he calls them *discrete prolate spheroidal wave functions*. The treatment of the infinite case can be repeated, because there is again a commuting differential operator, namely

$$D' = -\frac{1}{4\pi^2} \frac{d}{dz} (\cos 2\pi z - \cos 2\pi W) \frac{d}{dz} - \frac{1}{4} (N^2 - 1) \cos 2\pi z \quad (37)$$

One sees that, in comparison with (19), the powers have been replaced by cosine functions, which reflect the ring geometry. The first term is a kinetic energy with different sign in S and R , as in the infinite case. The second term is a potential with a minimum at the origin. In the limit of small z and W one can expand the cosine functions and recovers the operator D of the infinite case. The finite size is then no longer visible. The same holds for the integral operator K' which reduces to K . The N lowest eigenfunctions of the differential operator give the solution both in the subsystem and in the remainder, and determining the respective norms allows to calculate the eigenvalues ζ_k . Pictures of the functions for $N = 4, 5$ and $W = 0.2, 0.4$ are shown in [18] and one sees the similarity to the oscillator functions in particular for the lowest state $k = 0$.

The analysis of the eigenfunctions of D' for large N leads to formulae for ε_k which are very similar to those of the infinite system, see equs. (53), (60) and (61) in [18]. Instead of (27) one finds the equation

$$\pi N W + \frac{\varepsilon_k}{2\pi} \ln(2N \sin 2\pi W) - \varphi\left(\frac{\varepsilon_k}{2\pi}\right) = \frac{\pi}{2} \left(k - \frac{1}{2}\right) \quad (38)$$

and in the linear region this gives after inserting W

$$\varepsilon_k = \frac{\pi^2(k - 1/2 - \bar{N})}{\ln(2N \sin(\pi\ell/L)) - \psi(1/2)} \quad (39)$$

For $L \rightarrow \infty$, keeping $N/L = \bar{n}$ constant, this reduces to (29).

The existence of the commuting operator D' also has consequences for the other eigenvalue problem. This will be discussed in the following section.

V. INFINITE LATTICE SYSTEM

In the entanglement investigations, this is the most studied case. Let the system be the limit of a ring with a total of M sites. The correlation matrix is

$$C_{nn'} = \int_{-q_F}^{q_F} \frac{dq}{2\pi} e^{-iq(n-n')} = \frac{\sin q_F(n-n')}{\pi(n-n')} \quad (40)$$

which corresponds to (12) but with discrete sites. We will choose the subsystem here as the L sites $n = 1, 2, \dots, L$. Then the eigenvalue equation is

$$\sum_{n'=1}^L C_{nn'} \varphi_k(n') = \zeta_k \varphi_k(n) \quad (41)$$

and for the overlap matrix one finds

$$\begin{aligned} A(q-q') &= \frac{1}{M} \sum_{n=1}^L e^{-i(q-q')n} \\ &= e^{-iq(L+1)/2} \left(\frac{1}{M} \frac{\sin(q-q')L/2}{\sin(q-q')/2} \right) e^{iq'(L+1)/2} \end{aligned} \quad (42)$$

The exponential factors reflect the location of the subsystem, but do not affect the spectrum. The eigenvalue equation can be written

$$\int_{-q_F}^{q_F} \frac{dq'}{2\pi} \frac{\sin(q-q')L/2}{\sin(q-q')/2} \tilde{\varphi}_k(q') = \zeta_k \tilde{\varphi}_k(q), \quad \tilde{\varphi}_k(q) = e^{iq(L+1)/2} \varphi_k(q) \quad (43)$$

With $p = q/2\pi$, $W = q_F/2\pi = \bar{n}/2$ and $\tilde{\varphi}_k(2\pi p) = \psi(p)$ this leads to

$$\int_{-W}^W dp' K'(p-p') \psi_k(p') = \zeta_k \psi_k(p) \quad (44)$$

which is (33) with the substitution $N \rightarrow L$ in the kernel K' .

Therefore, as noted in previous work [10, 11], the infinite lattice and the finite continuum problem are actually the same with the role of positions and momenta, i.e. of correlation and overlap matrices, interchanged. Thus the discrete spheroidal functions appear here in momentum space, and the same holds for the commuting differential operator. As mentioned above, this operator has a consequence for the other eigenvalue problem (41). From (11)

$$\tilde{\varphi}_k(q) = \frac{1}{\sqrt{\zeta_k}} e^{iq(L+1)/2} \frac{1}{\sqrt{M}} \sum_{n=1}^L \varphi_k(n) e^{-iqn} \quad (45)$$

and inserting this into the eigenvalue equation $D'\tilde{\varphi} = \theta'\tilde{\varphi}$ one finds a three-term recursion relation for the $\varphi_k(n)$ which involves only the sites $n-1, n$ and $n+1$. In other words, the $\varphi_k(n)$ are also

the eigenfunctions of a tridiagonal matrix T which therefore commutes with C (in the subsystem). Thus the relation $[K', D'] = 0$ has an equivalent $[C, T] = 0$ in real space.

Writing T in the form

$$T = \begin{pmatrix} d_1 & t_1 & & & \\ t_1 & d_2 & t_2 & & \\ & t_2 & d_3 & t_3 & \\ & & & \ddots & \ddots \\ & & & & t_{L-1} & d_L \end{pmatrix} \quad (46)$$

the matrix elements are

$$t_n = \frac{1}{2}n(L-n), \quad d_n = \left(\frac{L+1}{2} - n\right)^2 \cos q_F \quad (47)$$

Both coefficients vary parabolically around the center of the system. Viewed as a hopping Hamiltonian, T describes an inhomogeneous system where the hopping is largest in the middle. The potential energy is also largest there if $q_F > \pi/2$, but smallest if $q_F < \pi/2$. For a half-filled system, $q_F = \pi/2$, it vanishes.

This matrix was later rediscovered in [9] on the basis that the Hamiltonian in (1) when calculated numerically shows a very similar structure. Note that T is only determined up to a multiplicative factor and an additive constant. The matrix elements given in [9] differ from (47) by the factor $2/L^2$ and a constant in d_n . Using T , one can obtain the eigenfunctions φ_k numerically for much larger systems than via the correlation matrix. They resemble the spheroidal functions of the continuum and were termed *discrete prolate spheroidal sequences* by Slepian. In Fig. 3 we show some of them for a system of $L = 50$ sites and $q_F = \pi/2$. For $q_F = 0, \pi$ they are given by Hahn polynomials and the eigenvalues of T are very simple [32]. In the limit $q_F \rightarrow 0$ and $L \rightarrow \infty$ keeping q_FL constant, the problem becomes continuous in $y = n/L$ and one comes back to the usual spheroidal functions. Expanding the quantities in $T\varphi = \theta'\varphi$, one can also derive the differential operator D directly.

The eigenvalues ε_k follow directly from the formulae in section 4 with $N \rightarrow L$ and $2\pi W = q_F$. Then (39) becomes

$$\varepsilon_k = \frac{\pi^2(k - 1/2 - \bar{N})}{\ln(2L \sin q_F) - \psi(1/2)} \quad (48)$$

For a half-filled system ($q_F = \pi/2$) this gives the asymptotic result found in [9], whereas for $q_F \rightarrow 0$ and $L \rightarrow \infty$ it reduces to (29). The density of states $n(\varepsilon)$ which decreases with ε is clearly seen in numerical calculations of the ε_k [2]. This is illustrated in Fig. 4, where the eigenvalues obtained

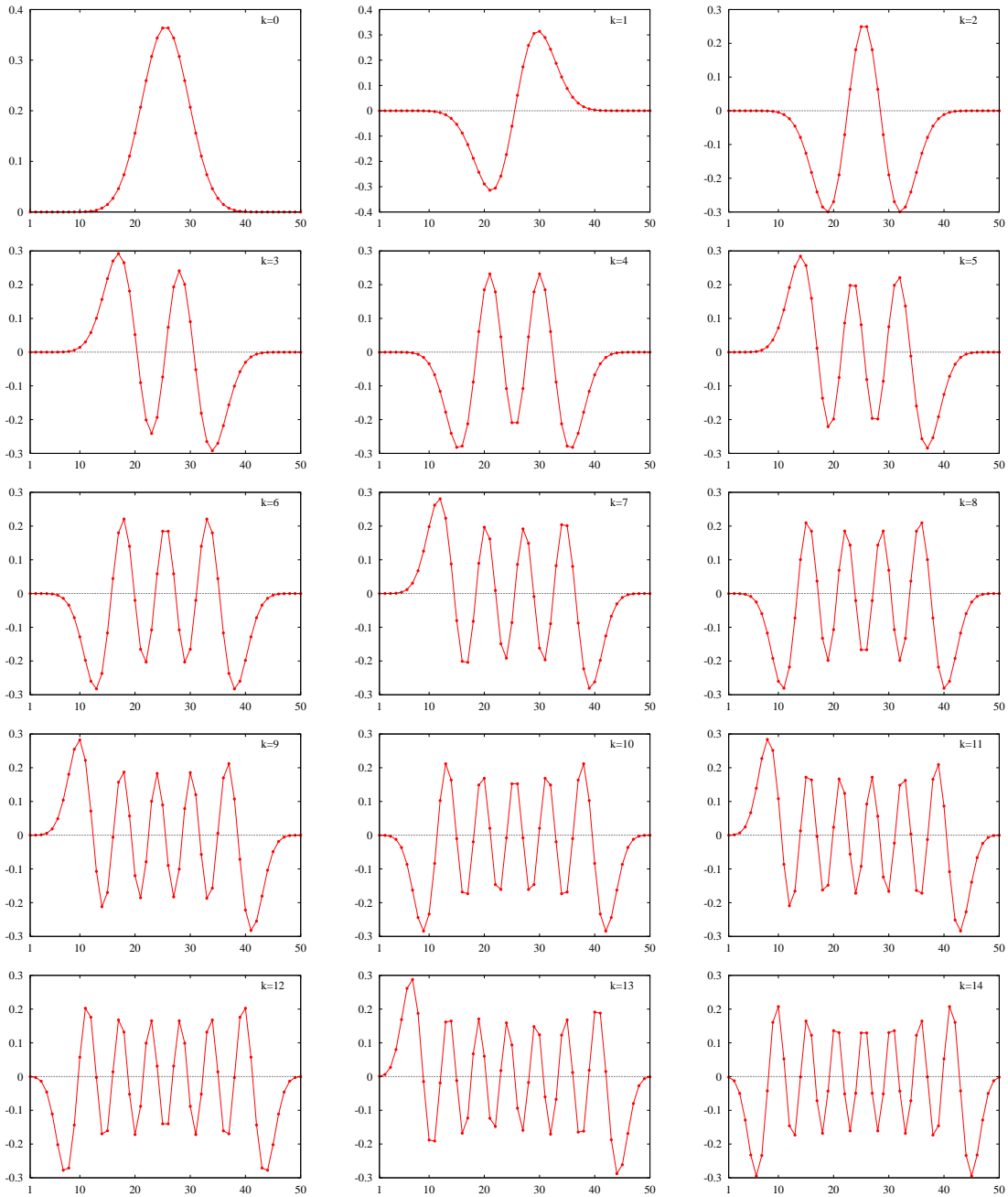


FIG. 3: The first 15 eigenfunctions φ_k for a subsystem of $L = 50$ sites in a half-filled infinite chain.

directly from (41) are shown together with the theoretical formula for $k = k(\varepsilon)$, viewing k as a continuous variable. The curves are not exactly linear, but show an upward (downward) bend on the positive (negative) side. One sees that for $L = 20$ there are small differences between both results, but for the larger L there is an excellent agreement. One also sees that even there the linear region is still quite small.

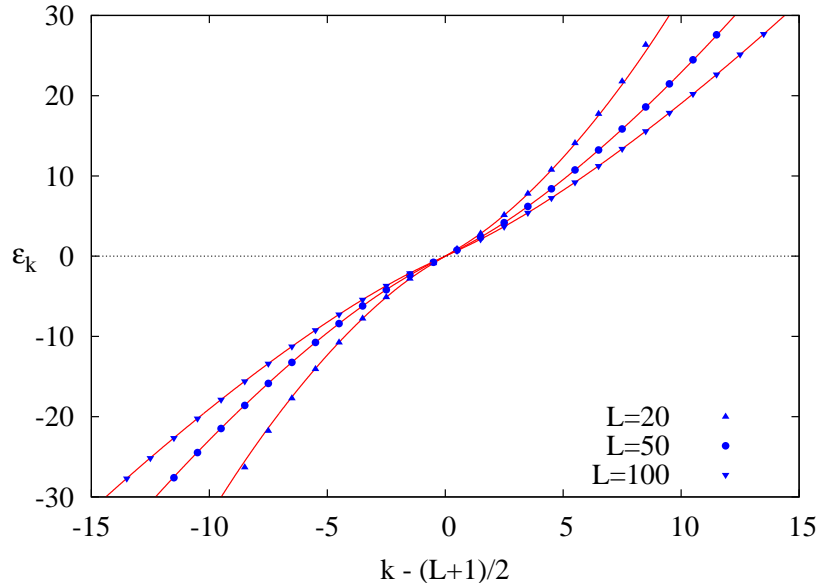


FIG. 4: Dispersion relation of the ε_k for a half-filled infinite lattice and three different sizes of the subsystem. Symbols: numerical data, lines: analytical result for $k(\varepsilon)$.

VI. FURTHER ASPECTS

So far, we have considered only systems without boundaries. However, the results cover also the case of a semi-infinite geometry when the subsystem is located next to the boundary. The Φ_q are then sine functions and, in the continuum case, lead to the correlation matrix

$$C_s(x, x') = C(x - x') - C(x + x'), \quad x, x' \geq 0 \quad (49)$$

where $C(x - x')$ is the result (12). But if the subsystem is the interval $0 \leq x \leq \ell/2$, the eigenvalue problem

$$\int_0^{\ell/2} dx' C_s(x - x') \varphi_k(x') = \zeta_k \varphi_k(x) \quad (50)$$

is solved by the *odd* eigenfunctions of (13). Thus one can take over the previous results, confining oneself to the odd k -values. This means in particular that the spacing of the low-lying ε_k doubles and the density of states halves. As a result, the entanglement entropy is also halved.

The argument also holds for the lattice case, where C_s has the form (49) with $x, x' \rightarrow n, n'$ and $n, n' \geq 1$. However, the solutions of the analogue of (50) then vanish at the point $n = 0$. Therefore, one has to compare with an infinite lattice problem, where this point is the center of the subsystem. This means, that it has to consist of $2L + 1$ sites (an odd number), if in the semi-infinite case the subsystem has L sites. The connection between infinite and semi-infinite system is also

seen at the level of the commuting matrices. There exists a tridiagonal matrix T_s with the property $[C_s, T_s] = 0$ and it is just the right half of the matrix T [9].

Returning to closed systems, one should mention that a finite ring of M lattice sites filled with $N = 2m + 1$ particles leads to the correlation matrix (32) with $x \rightarrow n$ and $L \rightarrow M$. For a segment of L sites, one can then also find a commuting tridiagonal matrix [33] which is a generalization of T and leads to another discrete version of the spheroidal functions. The parabolic form of the t_n and d_n is then replaced by trigonometric expressions. For example $t_n \sim \sin(\pi n/M) \sin(\pi(L - n)/M)$, and for $M \rightarrow \infty$ one reobtains (47).

Another generalization concerns higher dimensions. The case of an infinite continuum with spherical Fermi surface and a spherical subsystem has also been studied in detail [34]. Due to the rotational symmetry, the eigenfunctions are products of an angular and a radial factor. For the latter, one finds an integral equation with a Bessel function as kernel. Again a commuting differential operator exists and is closely related to D . For $d = 2$ and with $y \rightarrow r$

$$D_r = D + \frac{m^2 - 1/4}{r^2}, \quad r > 0 \quad (51)$$

where $m = 0, \pm 1, \pm 2, \dots$ is the azimuthal quantum number. Physically, the additional term can be viewed as a centrifugal potential. As a result, the eigenfunctions have to vanish at the origin. They were called *generalized spheroidal functions* and some are shown in [34]. For the eigenvalues ε_{km} for fixed m one finds very similar results as in one dimension.

VII. CONCLUSION

We have considered the ground state of free fermions and discussed an approach which determines the reduced density matrix directly via its single-particle eigenfunctions. It circumvents the original matrices or integral kernels and works instead with differential operators. In the continuum case, this leads to spheroidal functions which are well known in mathematics and appear in various other areas. Physically, they have the character of either bulk or boundary-like states, and it is amusing that, in the first instance, they are close to harmonic oscillator functions. In hindsight, however, one could have guessed that from the appearance of their lattice counterparts. In the lattice case, the asymptotic results for the single-particle eigenvalues bridge a gap between the numerical calculations and the Fisher-Hartwig determinantal formulae which only give a density of states. We have demonstrated in Fig. 4 how well the results match.

On the technical level, the approach is rather tedious and inferior to Fisher-Hartwig calculations.

However, the concept of a commuting operator is interesting and reminiscent of transfer matrix problems in integrable classical lattice models. It is also interesting that this feature carries over to higher dimensions for spherical subsystems. As to the one-dimensional problem, one has now an almost complete overview over the properties of the entanglement Hamiltonian \mathcal{H} , but an explicit form is still lacking.

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