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Many-body density matrices for free fermions

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Building upon an analytical technique introduced by Chung and Peschel [Phys. Rev. B **64**, 064412 (2001)], we calculated the many-body density matrix ρ_B of a finite block of B sites within an infinite system of free spinless fermions in arbitrary dimensions. In terms of the block Green function matrix G (whose elements are $G_{ij} = \langle c_i^\dagger c_j \rangle$, where $c_i^\dagger$ and c_j are fermion creation and annihilation operators acting on sites i and j within the block, respectively), the density matrix can be written as $\rho_B = \det(1 - G) \exp(\sum_{ij} [\ln G(1 - G)^{-1}]_{ij} c_i^\dagger c_j)$. Our results suggest that Hilbert space truncation schemes should retain the states created by a subset of the $c_i^\dagger$'s (in any combination), rather than selecting eigenvectors of ρ_B independently based on the eigenvalue.

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I. INTRODUCTION

Exact solutions are hard to come by in many-body problems, and every so often we have to resort to numerical solutions. The traditional approaches, applied to finite systems, are exact diagonalization and quantum Monte Carlo. For quantum lattice models of fermions, the former is constrained by the size of the Hilbert space, which grows exponentially with the number of sites, while the latter is plagued by the “minus-sign problem.” For quantum lattice models of bosons, the Hilbert space is infinite dimensional even for finite systems. In either case, because of the enormous computational complexity involved, there is no hope of getting to the thermodynamic limit of infinite system size. In view of these difficulties, one then hopes for the next best thing: approximate solutions that capture the essence of the physics.

This is where renormalization group (RG) approaches come in. In such approaches^{1–11} to the approximate solution of otherwise intractable problems, the size of the Hilbert space is kept in check by aggressive truncation, with the hope that the small number of states kept will reproduce the more important features of the physics. Whatever the RG scheme, ultimately its success will lie in how the truncation is done. Since the quantum-mechanical state of a block embedded in a larger system must in general be described by a density matrix, it is therefore natural to use it to guide the truncations.

With the goal of understanding the structure and spectrum of the density matrix, and their implications on RG truncation schemes in mind, Peschel *et al.* calculated exactly the half-chain density matrix for several models.^{12–14} For a chain of coupled harmonic oscillators and spinless Bogoliubov fermions, they found that the half-chain density matrices can be expressed exactly as the exponential of a pseudo-Hamiltonian, whose spectrum is generated by a set of independent bosonic and fermionic operators, respectively. In this paper, we pursue their analysis further for a system of free spinless fermions to obtain a closed-form formula relating the density matrix ρ_B of a subsystem and the subsystem Green function matrix G (to be defined in Sec. II C).

The organization of the paper will be as follows: we will start Sec. II by reviewing the density-matrix formulation of

quantum mechanics, and how the density matrix ρ_B of a subsystem can be obtained from the density matrix ρ_0 of the overall system. Following this, we will describe an alternative approach to calculating the density matrix elements as expectations of referencing operators. We shall show that the real-space structure, and the strong signs that point to a closed-form expression for ρ_B , is most readily discerned within this alternative formulation. Then, in Sec. III, we derive this closed-form expression for ρ_B in terms of the subsystem Green function matrix G by adapting the technique put forward by Chung and Peschel.¹⁴ The existence of such a relation between ρ_B and G tells us that ρ_B is completely determined by its 0- and 1-particle sectors. We discuss the implications of this in Sec. IV, where we illustrate how the eigenvectors and eigenvalues of the ($F > 1$) sectors of ρ_B can be constructed out of the eigenvectors and eigenvalues of the 1-particle sector. We also show how symmetries of the Hamiltonian that are realized in ρ_B affect the pattern of degeneracies in the eigenvalues of these sectors, an understanding of which is important in formulating a consistent truncation scheme.

II. DENSITY MATRIX OF A FINITE BLOCK

In this section, we first review the density-matrix notions that will be used throughout this paper. Following this we develop the first of our two paths to calculate the density matrix ρ_B for a particular block within a large system of noninteracting fermions. By analyzing the index structure of the matrices involved, we arrived at a conjecture for a closed-form expression for the 1-particle sector of the block density matrix ρ_B in terms of the block Green function matrix G .

A. Density-matrix formulation of quantum mechanics

In quantum mechanics one distinguishes between *pure states*, which occur, for example, at $T=0$ when the system is totally decoupled from the rest of the universe, and *mixed states*, which occur, for example, at $T>0$ when the system is in thermodynamic equilibrium with the rest of the universe. A pure state can be described by a wave function $|\Psi\rangle$ in the usual formulation of quantum mechanics, whereas a mixed

state cannot. Both types of states are treated on equal footing in the density-matrix formulation of quantum mechanics, in which the state of a system is described by a density matrix ρ_0 (see, for example, Ref. 15). In this formulation of quantum mechanics, the expectation of an operator A in a state described by ρ_0 is given by

$$\langle A \rangle = \text{Tr}(\rho_0 A). \quad (2.1)$$

If the state so described is pure, i.e., given in the usual formulation by the wave function $|\Psi\rangle$, so that $\langle A \rangle = \langle \Psi | A | \Psi \rangle$, then it is clear that $\rho_0 = |\Psi\rangle\langle\Psi|$.

In this paper, we shall be mainly interested in a finite subsystem of B sites, which we call the *block*, embedded within a larger system of N sites, with periodic boundary conditions in d dimensions. The latter can then be taken to the thermodynamic limit of infinite number of sites, i.e., $N \rightarrow \infty$. The system minus the block is called the *environment* of the block. If the overall system is known to be in a pure state $|\Psi\rangle$, then in general the quantum-mechanical state of the block cannot be described by a pure state wave function. Instead, the mixed state of the block must be described by a block density matrix ρ_B (see arguments in Ref. 16), so defined that

$$\langle A \rangle = \text{Tr}(\rho_B A), \quad (2.2)$$

if the operator A acts entirely within the block.

There are two useful formulas to relate the block density matrix ρ_B to the density matrix ρ_0 of the entire system. The first formula, which we will use in Sec. III, follows from Eqs. (2.1) and (2.2). Using the subscripts B and E , respectively, to make the trace over the degrees of freedom associated with the block and its environment more explicit, we can rewrite Eq. (2.1) as

$$\langle A \rangle = \text{Tr}(\rho_0 A) = \text{Tr}_{B,E}(\rho_0 A). \quad (2.3)$$

Since A does not act on the environment, we can trivially trace over environmental degrees of freedom to get

$$\langle A \rangle = \text{Tr}_B\{\text{Tr}_E(\rho_0) A\}. \quad (2.4)$$

Comparing this with Eq. (2.2), we find a consistent expectation for A whether it is taken over the entire system or just over the block, if the block density matrix is defined as

$$\rho_B = \text{Tr}_E(\rho_0). \quad (2.5)$$

The second formula for ρ_B allows us to write down its matrix elements explicitly when the overall system is in a pure state. To arrive at this formula, let us first note that any pure state of the overall system can be written as $|\Psi\rangle = \sum_b |b\rangle |e_b\rangle$, where $|b\rangle$ is a complete orthonormal (many-body) basis for the block and $|e_b\rangle$ is the (unnormalized) state of the environment associated with the state $|b\rangle$ on the block. Using this form for $|\Psi\rangle$ in Eq. (2.1), we find that

$$\langle A \rangle = \sum_{b,b'} \langle e_b | \langle b | A | b' \rangle | e_{b'} \rangle = \text{Tr}_B(\rho_B A) \quad (2.6)$$

if the block density matrix ρ_B is defined such that

$$(\rho_B)_{b'b} = \langle e_b | e_{b'} \rangle, \quad (2.7)$$

i.e., the matrix element of ρ_B between $|b\rangle$ and $|b'\rangle$ is none other than the overlap between their associated environmental states $|e_b\rangle$ and $|e_{b'}\rangle$.

B. Free spinless fermions

Let us now apply Eq. (2.7) to calculate the block density matrix from the ground state of a ring of $N \rightarrow \infty$ free spinless fermions, the simplest realization of which is described by a translationally invariant Hamiltonian with nearest-neighbor hopping

$$H = -t \sum_{\langle ij \rangle} (c_i^\dagger c_j + c_j^\dagger c_i), \quad (2.8)$$

where c_i and $c_i^\dagger$ are the fermion annihilation and creation operators acting on site i , and $\langle ij \rangle$ runs once over each pair of neighbor sites.

The Hamiltonian given in Eq. (2.8) is diagonal in momentum space, and can be written as

$$H = \sum_k \epsilon_k \tilde{c}_k^\dagger \tilde{c}_k. \quad (2.9)$$

Here

$$\begin{aligned} \tilde{c}_k &\equiv N^{-1/2} \sum_j c_j e^{ik \cdot r_j}, \\ \tilde{c}_k^\dagger &\equiv N^{-1/2} \sum_j c_j^\dagger e^{-ik \cdot r_j} \end{aligned} \quad (2.10)$$

are the momentum space annihilation and creation operators, r_i is the position of site i , and ϵ_k the single-particle energy associated with wave vector k . The ground state of such a system is just a Fermi sea,

$$|\Psi_F\rangle = \prod_{k \text{ filled}} \tilde{c}_k^\dagger |0\rangle, \quad (2.11)$$

where $|0\rangle$ is the vacuum and the product is over the wave vectors inside the Fermi surface.

As noted in Eq. (2.7), when the ground-state wave function is written as $|\Psi_F\rangle = \sum_b |b\rangle |e_b\rangle$, the block density-matrix elements are $(\rho_B)_{b'b} = \langle e_b | e_{b'} \rangle$. When dealing with a finite block and an infinite environment, it makes no sense to evaluate these environmental overlaps by first calculating $|e_b\rangle$ and $|e_{b'}\rangle$. Instead, we find that it is possible to evaluate such environmental overlaps with the help of operator products that are defined entirely within the block. To do so, let us first write the many-body states $|b\rangle$ on the block in the occupation number representation as $|b\rangle = |n_1^b n_2^b \cdots n_B^b\rangle$, where $n_j^b = 0$ or 1 depending on whether the site j on the block is empty or occupied in the state $|b\rangle$. We then define the *referencing operators*

$$K_b = \prod_{j=1}^B [n_j^b c_j + (1 - n_j^b) c_j^\dagger], \quad (2.12)$$

such that the effect of K_b acting on a state $|b'\rangle$ is $K_b|b'\rangle = \delta_{bb'}|0\rangle_B$, where $|0\rangle_B$ is the *reference state* for which all sites on the block are empty. Letting K_b act on $|\Psi_F\rangle$ gives $K_b|\Psi_F\rangle = \sum_{b''} K_b|b''\rangle|e_{b''}\rangle = |0\rangle_B|e_b\rangle$. Hence, in terms of the operators K_b and their conjugates $K_b^\dagger$, the density-matrix elements are found to be

$$(\rho_B)_{b'b} = \langle e_b|e_{b'}\rangle = \langle \Psi_F|K_b^\dagger K_{b'}|\Psi_F\rangle = \langle K_b^\dagger K_{b'}\rangle. \quad (2.13)$$

From the way the operators K_b are defined, we know that ρ_B is real and symmetric. Furthermore, $(\rho_B)_{b'b}$ vanishes if the states $|b\rangle$ and $|b'\rangle$ do not contain the same number of fermions F . Consequently, the nonzero matrix elements of ρ_B are found in a total of $(B+1)$ submatrices along the diagonal, corresponding to the various F -particle sectors, for $F=0,1,\dots,B$. We shall call such submatrices $\rho_{B,F,l}$, and their eigenvalues the *density-matrix weights* $w_{B,F,l}$, where $l=1,\dots,\text{rank}(\rho_{B,F})$.

C. Conjecture based on index structure

In general, for a block of B sites, there are a total of $2^B K_b$ operators we need to write down explicitly to calculate the $\sim 2^B$ density-matrix elements. For large blocks, this is extremely tedious and has to be automated (see Appendix A), but for small blocks, it is not difficult to work out exact expressions for $(\rho_B)_{b'b}$ in terms of the $2n$ -point functions:

$$G_{\bar{i}j} \equiv \langle c_i^\dagger c_j \rangle, \quad (2.14a)$$

$$G_{\bar{i}jkl} \equiv \langle c_i^\dagger c_j^\dagger c_k c_l \rangle = (-1)^{2(2-1)/2} \begin{vmatrix} G_{\bar{i}k} & G_{\bar{i}l} \\ G_{\bar{j}k} & G_{\bar{j}l} \end{vmatrix}, \quad (2.14b)$$

$$G_{\bar{i}jklmn} \equiv \langle c_i^\dagger c_j^\dagger c_k^\dagger c_l c_m c_n \rangle = (-1)^{3(3-1)/2} \begin{vmatrix} G_{\bar{i}l} & G_{\bar{i}m} & G_{\bar{i}n} \\ G_{\bar{j}l} & G_{\bar{j}m} & G_{\bar{j}n} \\ G_{\bar{k}l} & G_{\bar{k}m} & G_{\bar{k}n} \end{vmatrix}, \quad (2.14c)$$

and so forth, where $i,j,k,l,\dots=1,\dots,B$ are sites on the block. As shown explicitly above, the $2n$ -point functions $G_{\bar{i}_1\dots\bar{i}_n j_1\dots j_n}$ Wick factorize into sums of products of 2-point functions $G_{\bar{i}j}$ for our noninteracting system, with an overall fermion factor of $(-1)^{n(n-1)/2}$.

At this point let us note that since the 2-point functions $G_{\bar{i}j}$ are labeled by two indices, it is convenient to organize them into a *system Green function matrix* $\mathcal{G}$ given by

$$\mathcal{G} = \begin{bmatrix} G_{\bar{1}1} & \cdots & G_{\bar{1}B} & G_{\bar{1}B+1} & \cdots & G_{\bar{1}N} \\ G_{\bar{2}1} & \cdots & G_{\bar{2}B} & G_{\bar{2}B+1} & \cdots & G_{\bar{2}N} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ G_{\bar{B}1} & \cdots & G_{\bar{B}B} & G_{\bar{B}B+1} & \cdots & G_{\bar{B}N} \\ G_{\bar{B+1}1} & \cdots & G_{\bar{B+1}B} & G_{\bar{B+1}B+1} & \cdots & G_{\bar{B+1}N} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ G_{\bar{N}1} & \cdots & G_{\bar{N}B} & G_{\bar{N}B+1} & \cdots & G_{\bar{N}N} \end{bmatrix}, \quad (2.15)$$

of which

$$G = \begin{bmatrix} G_{\bar{1}1} & G_{\bar{1}2} & \cdots & G_{\bar{1}B} \\ G_{\bar{2}1} & G_{\bar{2}2} & \cdots & G_{\bar{2}B} \\ \vdots & \vdots & \ddots & \vdots \\ G_{\bar{B}1} & G_{\bar{B}2} & \cdots & G_{\bar{B}B} \end{bmatrix} \quad (2.16)$$

is its *restriction to the block*. We call G the *block Green function matrix*. As a result of the translational invariance of H , $\mathcal{G}$ is also translationally invariant. In real space, this means that its matrix elements $\mathcal{G}_{ij} = G_{\bar{i}j} = \langle c_i^\dagger c_j \rangle$ are functions only of $r_i - r_j$. When $\mathcal{G}$ is restricted to the block to give G , however, this translational invariance is lost due to the fact that the presence of a block in the system allows an unambiguous definition of the origin.

Anyway, from Eqs. (2.12) and (2.13), we see on the one hand that $(\rho_B)_{bb'}$ can be written as sums of $2n$ -point functions—which themselves factor into sums of products of 2-point functions—and so we find that $(\rho_B)_{bb'}$ are all functions of $G_{\bar{k}l}$. On the other hand, the 1-particle sector of ρ_B contains matrix elements $(\rho_B)_{bb'}$, connecting the states $|b\rangle$ and $|b'\rangle$, which contain one particle each at sites, say i and j , respectively. Therefore, the matrix elements within $\rho_{B,1}$ may be indexed using i and j instead of b and b' . Diligently writing down the polynomial expressions

$$(\rho_{B,1})_{ij} = \sum_{k_1,l_1}^B \alpha_{ij;k_1,l_1}^{(1)} G_{\bar{k}_1 l_1} + \sum_{\substack{k_1,k_2, \\ l_1,l_2}}^B \alpha_{ij;k_1,k_2,l_1,l_2}^{(2)} G_{\bar{k}_1 l_1} G_{\bar{k}_2 l_2} \\ + \cdots + \sum_{\substack{k_1,\dots,k_B, \\ l_1,\dots,l_B}}^B \alpha_{ij;k_1,\dots,k_B,l_1,\dots,l_B}^{(B)} G_{\bar{k}_1 l_1} \times \cdots \\ \times G_{\bar{k}_B l_B}, \quad (2.17)$$

we find that (a) the coefficients $\alpha_{ij;k_1,\dots,k_n,l_1,\dots,l_n}^{(n)}$ are independent of i and j ; and (b) indices other than i and j always appear in pairs, as if they are summed over.

Exhaustively comparing the matrix elements of $\rho_{B,1}$ and powers of G for $2 \leq B \leq 5$, we find that

$$\rho_{B,1} = G + G^2 - G \text{Tr}(G) + G^3 - G^2 \text{Tr}(G) - \frac{1}{2} \{ \text{Tr}(G^2) \\ - [\text{Tr}(G)]^2 \} G + G^4 - G^3 \text{Tr}(G) - \frac{1}{2} \{ \text{Tr}(G^2) \\ - [\text{Tr}(G)]^2 \} G^2 - \left\{ \frac{1}{3} \text{Tr}(G^3) - \frac{1}{2} \text{Tr}(G) \text{Tr}(G^2) \right. \\ \left. + \frac{1}{6} [\text{Tr}(G)^3] \right\} G + \cdots. \quad (2.18)$$

What is most fascinating about this series is that for $B=2$, Eqs. (2.12) and (2.13) tell us that $\rho_{B,1}$ can be at most $O(G^2)$, since its matrix elements never contain terms with more than two creation and annihilation operators each. Yet Eq. (2.18) is perfectly valid for $B=2$ because terms higher order in G vanish. For $B=3$ and $B=4$, we find similarly that terms higher order than $O(G^3)$ and $O(G^4)$ vanish, respectively. If

we conjecture that Eq. (2.18) gives the leading terms to an infinite series that holds true for all $B > 5$, then we can factorize it into

$$\rho_{B,1} = (G + G^2 + G^3 + \dots) \times \exp \left[-\text{Tr} \left(G + \frac{1}{2}G^2 + \frac{1}{3}G^3 + \dots \right) \right]. \quad (2.19)$$

Noting that the series inside the trace is just $-\ln(1-G)$, Eq. (2.19) can be compactly written as

$$\rho_{B,1} = G(1-G)^{-1} \det(1-G). \quad (2.20)$$

III. DERIVATION AND PROPERTIES OF ρ_B

In passing from Eq. (2.18) to Eq. (2.20), a leap of faith was required, and it would appear forbiddingly difficult to actually prove Eq. (2.20) for arbitrary block sizes B , by the algebraic manipulations used in Sec. II C. Fortunately, an alternate technique introduced by Chung and Peschel¹⁴ can be adapted and extended for calculating the density matrix of a finite block, although it comes with its own set of technical difficulties. It turns out that if the whole system were in the Fermi sea ground state, the derivation would require the inversion of singular matrices. In the end, the singularities do cancel and give a well-defined answer, but a regularization is needed to avoid divergences in the intermediate steps. The most natural way to do so would be to generalize our problem to nonzero temperature, in which case the limit $T \rightarrow 0$ then provides the needed regularization.¹⁹

In essence, the calculations are just that of evaluating a Gaussian integral with the usual shift in integration variables. However, because we are dealing with fermions, whose creation and annihilation operators anticommute rather than commute, additional machinery is needed to accomplish the feat of Gaussian integration. After casting the system density matrix ρ_0 as a Gaussian of the fermion operators, we introduce fermionic coherent states with the aid of anticommuting Grassmann variables. The matrix elements of ρ_0 between such coherent states, obtained via a translation machinery, are similarly of Gaussian form, but are now easier to handle. A Gaussian integration over the environmental degrees of freedom then yields elements of the block density matrix ρ_B , following which reverse translation gives ρ_B proper.

A. Exponential form for ρ_0

To get the calculations underway, we consider the grand-canonical $T > 0$ density matrix ρ_0 of the overall system that the block is embedded in. As always, this is given by

$$\rho_0 = \mathcal{Q}^{-1} \exp[-\beta(H - \mu F)], \quad (3.1)$$

where $\beta \equiv 1/k_B T$, μ is the chemical potential, and $F \equiv \sum_k \tilde{c}_k^\dagger \tilde{c}_k = \sum_i c_i^\dagger c_i$ is the fermion number operator. The prefactor $\mathcal{Q}^{-1}$ in Eq. (3.1) is just the reciprocal of the grand partition function to ensure that $\text{Tr}(\rho_0) = 1$.

The notations can be made more compact if we introduce the matrices Γ and its Fourier transform $\tilde{\Gamma}$, such that

$$\rho_0 = \mathcal{Q}^{-1} \exp \left(\sum_{i,j} \Gamma_{ij} c_i^\dagger c_j \right) = \mathcal{Q}^{-1} \exp \left(\sum_k \tilde{\Gamma}_{kk} \tilde{c}_k^\dagger \tilde{c}_k \right), \quad (3.2)$$

where we have made use of the fact that $H - \mu F$, and hence $\tilde{\Gamma}$ is diagonal in momentum space. The matrix elements of Γ can be read off from Eq. (2.8) as

$$\Gamma_{ij} = \begin{cases} \beta\mu & \text{if } i=j \\ \beta t & \text{if } i \text{ and } j \text{ are nearest neighbors} \\ 0 & \text{otherwise,} \end{cases} \quad (3.3)$$

while those of $\tilde{\Gamma}$ can be read off from Eq. (2.9) as

$$\tilde{\Gamma}_{kk} = -\beta E_k, \quad (3.4)$$

where $E_k \equiv \epsilon_k - \mu$ is the single-particle energy measured relative to μ .

In order to prove our conjecture (2.20), it is clear that we need to somehow relate Γ to $\mathcal{G}$. To do this, let us note that since $\mathcal{G}$ is translationally invariant, its Fourier transform $\tilde{\mathcal{G}}$ is diagonal in momentum space, with matrix elements given in the grand-canonical ensemble as

$$\tilde{\mathcal{G}}_{kk} = \langle \tilde{c}_k^\dagger \tilde{c}_k \rangle = \frac{1}{\exp \beta E_k + 1}, \quad (3.5)$$

observing which we find that

$$\tilde{\mathcal{G}}_{kk} = \exp(\tilde{\Gamma}_{kk}) [\exp(\tilde{\Gamma}_{kk}) + 1]^{-1}. \quad (3.6)$$

But since both $\tilde{\mathcal{G}}$ and $\tilde{\Gamma}$ are diagonal matrices, we have the relation

$$e^{\tilde{\Gamma}} = \tilde{\mathcal{G}}(1 - \tilde{\mathcal{G}})^{-1}, \quad (3.7)$$

where $e^{\tilde{\Gamma}}$ is the matrix exponential of $\tilde{\Gamma}$.

Of course, $\mathcal{G}$ and $\tilde{\mathcal{G}}$ correspond merely to the matrix of the same Hilbert space operator evaluated in two different bases, and the same is true of Γ and $\tilde{\Gamma}$. As such, the matrix relation (3.7) between $e^{\tilde{\Gamma}}$ and $\tilde{\mathcal{G}}$ holds true for e^Γ and $\mathcal{G}$ as well, i.e., we have

$$e^\Gamma = \mathcal{G}(1 - \mathcal{G})^{-1}. \quad (3.8)$$

B. Key formulas involving Grassmann variables

In the next stage of our derivations, we need to make use of Grassmann variables. These are anticommuting c numbers familiar in the context of field theory (see, for example, Ref. 17). If ξ_i and ξ_j are Grassmann variables, where $i \neq j$, then we have $\xi_i \xi_j = -\xi_j \xi_i$ and $\xi_i^2 = 0 = \xi_j^2$. The purpose of introducing these is to define the fermionic coherent states

$$|\xi\rangle = |\xi_1 \xi_2 \dots \xi_N\rangle = \exp \left(- \sum_{i=1}^N \xi_i c_i^\dagger \right) |0\rangle, \quad (3.9)$$

which are eigenstates of the fermion annihilation operators, i.e., $c_i |\xi\rangle = -\xi_i |\xi\rangle$. The value of coherent states in general is

that one can replace the manipulation of noncommuting operators by the manipulation of c -number matrix elements. In the present case of fermions, anticommuting operators may be made to commute by the insertion of Grassmann coefficients.

There are three key formulas involving Grassmann algebra that we need for the derivations in this section. The first involves the matrix element of an exponentiated bilinear operator $\exp(\sum_{i,j} \Gamma_{ij} c_i^\dagger c_j)$ between fermionic coherent states $|\xi\rangle$ and $|\xi'\rangle$, given by

$$\left\langle \xi \left| \exp \left(\sum_{i,j} \Gamma_{ij} c_i^\dagger c_j \right) \right| \xi' \right\rangle = \exp \left[\sum_{i,j} (e^\Gamma)_{ij} \xi_i^* \xi_j' \right], \quad (3.10)$$

where e^Γ is the exponential of the matrix Γ . The second formula expresses the trace of an operator A as a Grassmann integral over its coherent-state matrix elements as

$$\text{Tr}(A) = \int \prod_i d\xi_i^* d\xi_i e^{-\sum_i \xi_i^* \xi_i} \langle -\xi | A | \xi \rangle. \quad (3.11)$$

The third formula that we would need is the Gaussian integral over Grassmann variables,

$$\int \prod_i d\xi_i^* d\xi_i e^{\sum_{j,k} \xi_j^* A_{jk} \xi_k} = \det A. \quad (3.12)$$

The strategy then would be to evaluate the matrix elements of ρ_0 in Eq. (3.2) using Eq. (3.10), follow the prescription in Eq. (2.5) where we trace over the environmental degrees of freedom using Eq. (3.11), and then use Eq. (3.10) in reverse to recover ρ_B from its coherent-state matrix elements. Before we do so, let us first tidy up the notations by relabeling the coherent states as

$$\begin{aligned} |\xi \eta\rangle &= |\xi_1 \cdots \xi_B; \eta_1 \cdots \eta_{N-B}\rangle \\ &= \exp \left(-\sum_{i=1}^B \xi_i c_i^\dagger - \sum_{j=1}^{N-B} \eta_j c_j^\dagger \right) |0\rangle, \end{aligned} \quad (3.13)$$

where $\xi = \{\xi_1, \dots, \xi_B\}$ are Grassmann coordinates associated with sites on the block, and $\eta = \{\eta_1, \dots, \eta_{N-B}\}$ are Grassmann coordinates associated with sites in the environment.

C. Matrix block form

Seeing that ρ_0 is written in Eq. (3.2) as the exponential of a quadratic form with coefficient matrix Γ , we make use of Eq. (3.10) to write down its matrix element between the fermionic coherent states $|\xi \eta\rangle$ and $|\xi' \eta'\rangle$ as a Gaussian in Grassmann variables:

$$\langle \xi \eta | \rho_0 | \xi' \eta' \rangle = \mathcal{Q}^{-1} \exp \left[(\xi^* \eta^*) e^\Gamma \begin{pmatrix} \xi' \\ \eta' \end{pmatrix} \right]. \quad (3.14)$$

Our task now is to derive the matrix elements of ρ_B in the same Gaussian form, after tracing out the environment.

To find the matrix elements $\langle \xi | \rho_B | \xi' \rangle$ of the density matrix ρ_B on the block of B sites, we use Eq. (3.11) and perform a partial trace over the environment to give

$$\begin{aligned} \langle \xi | \rho_B | \xi' \rangle &= \int d\eta^* d\eta e^{-\eta^* 1 \eta} \langle \xi - \eta | \rho_0 | \xi' \eta \rangle \\ &= \mathcal{Q}^{-1} \int d\eta^* d\eta \exp \left[(\xi^* - \eta^*) \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \xi' \\ \eta \end{pmatrix} \right] \\ &\quad \times \exp \left[(\xi^* - \eta^*) e^\Gamma \begin{pmatrix} \xi' \\ \eta \end{pmatrix} \right] \\ &= \mathcal{Q}^{-1} e^{-\xi^* 1 \xi'} \int d\eta^* d\eta \\ &\quad \times \exp \left[(\xi^* - \eta^*) (1 + e^\Gamma) \begin{pmatrix} \xi' \\ \eta \end{pmatrix} \right]. \end{aligned} \quad (3.15)$$

Following this we must express these matrix elements in a form that would allow us to trace over the environment. To do so, let us first write $(1 + e^\Gamma)$ in matrix block form as

$$1 + e^\Gamma = \begin{bmatrix} A & B \\ B^T & C \end{bmatrix}, \quad (3.16)$$

where A is the $B \times B$ *block submatrix*, obtained by restricting the indices i and j of $(1 + e^\Gamma)$ in coordinate space to range only over sites on the block, C is the $(N-B) \times (N-B)$ *environment submatrix*, obtained by restricting the indices i and j of $(1 + e^\Gamma)$ to range only over sites in the environment, and B is the $B \times (N-B)$ *decoherence submatrix* of $(1 + e^\Gamma)$, obtained by restricting the row index to range only over sites on the block and the column index to range only over sites in the environment.

D. Tracing down ρ_0

With Eqs. (3.15) and (3.16), the block density-matrix elements can then be written as

$$\langle \xi | \rho_B | \xi' \rangle = \mathcal{Q}^{-1} e^{\xi^* (A-1) \xi'} \int d\eta^* d\eta e^{\xi^* B \eta - \eta^* B^T \xi' - \eta^* C \eta}. \quad (3.17)$$

Here we have made use of the fact that since the Grassmann variables occur quadratically in each term in the exponential, they commute with one another and we may thus factor the exponential as if it is an exponential of c numbers.

By performing a shift of the integration variables η and η^* , and then evaluating the Grassmann Gaussian integral using Eq. (3.12), we find that

$$\langle \xi | \rho_B | \xi' \rangle = \mathcal{Q}^{-1} \det C e^{\xi^* [A - 1 - B C^{-1} B^T] \xi'}, \quad (3.18)$$

which parallels Eq. (14) in Ref. 14. From Eq. (3.18), we see that the expression for $\langle \xi | \rho_B | \xi' \rangle$ involves only the Grassmann coordinates ξ_i and ξ_i' associated with sites on the block. This is good. But it also involves the decoherence submatrix B as well as the environment submatrix C , with the latter appearing both in the exponential and in the normalization constant.

These matrices have indices that range over sites outside the block, which we are supposed to have traced out and gotten over with.

Indeed, this must have been successfully done, since $A - \mathbb{1} - BC^{-1}B^T$ is a $B \times B$ matrix whose indices range only over sites on the block. In fact, using Eq. (B5) in Appendix B, we can express this matrix entirely in terms of submatrices on the block, and write Eq. (3.18) as

$$\langle \xi | \rho_B | \xi' \rangle = \mathcal{Q}^{-1} \det C e^{\xi^* [D^{-1} - \mathbb{1}] \xi'}, \quad (3.19)$$

where D is the block submatrix of $(\mathbb{1} + e^\Gamma)^{-1}$, obtained by restricting its indices to range only over sites on the block. This leaves only the $\det C$ in the normalization that we have to deal with.

To express $\mathcal{Q}^{-1} \det C$ in terms of submatrices whose indices range only over sites on the block, we make use of the fact that

$$\begin{aligned} \text{Tr}(\rho_B) &= 1 = \int d\xi^* d\xi e^{-\xi^* \mathbb{1} \xi} \langle -\xi | \rho_B | \xi \rangle \\ &= \mathcal{Q}^{-1} \det C \int d\xi^* d\xi e^{-\xi^* D^{-1} \xi} \\ &= \mathcal{Q}^{-1} \det C \det D^{-1}, \end{aligned} \quad (3.20)$$

which means that

$$\mathcal{Q}^{-1} \det C = \det D. \quad (3.21)$$

With this we have succeeded in writing down a Gaussian form for the coherent-state matrix elements of ρ_B involving only degrees of freedom on the block. Using the translation machinery provided by Eq. (3.10), we then establish the exponentiated form

$$\rho_B = \det D \exp \left\{ \sum_{i,j} [\ln(D^{-1} - \mathbb{1})]_{ij} c_i^\dagger c_j \right\} \quad (3.22)$$

of Chung and Peschel.

At this point, let us remark that the above formula for ρ_B is of no practical use, if to find the matrix D , we actually have to evaluate the matrix $(\mathbb{1} + e^\Gamma)$, whose indices run over the entire system, take its inverse $(\mathbb{1} + e^\Gamma)^{-1}$, and then from this identify the block submatrix D . This is essentially what was done in Ref. 14, where the matrix parallel to $D^{-1} - \mathbb{1}$ was computed numerically, for the case of an environment equal in size to the block. For our problem, identifying $A - BC^{-1}B^T$ as D^{-1} with the aid of our analytic relation (B5) allows us to work with arbitrary, even infinite, environment sizes.

Furthermore, armed with the relationship (3.8) obtained in Sec. III A, we can find the normalization and matrix of coefficients appearing in Eq. (3.19) in terms of the block Green function matrix G . From

$$\mathbb{1} + e^\Gamma = \mathbb{1} + \mathcal{G}(\mathbb{1} - \mathcal{G})^{-1} = (\mathbb{1} - \mathcal{G})^{-1} \quad (3.23)$$

we see that D is just $(\mathbb{1} - \mathcal{G})$ restricted to the block, i.e., $D = \mathbb{1} - G$, and consequently, $D^{-1} = (\mathbb{1} - G)^{-1}$. With this, the

normalization constant for ρ_B can be written as $\det D = \det(\mathbb{1} - G)$. For the matrix of coefficients $(D^{-1} - \mathbb{1})$ in the exponential, we see that

$$D^{-1} - \mathbb{1} = (\mathbb{1} - G)^{-1} - \mathbb{1} = G(\mathbb{1} - G)^{-1}. \quad (3.24)$$

With this substitution, the matrix elements of ρ_B now read as

$$\langle \xi | \rho_B | \xi' \rangle = \det(\mathbb{1} - G) \exp[\xi^* G(\mathbb{1} - G)^{-1} \xi'] \quad (3.25)$$

so that, after using Eq. (3.10) in reverse translation, we can read off the operator form of ρ_B as

$$\rho_B = \det(\mathbb{1} - G) \exp \left\{ \sum_{ij} [\ln G(\mathbb{1} - G)^{-1}]_{ij} c_i^\dagger c_j \right\}. \quad (3.26)$$

In a suitable basis diagonalizing $\ln G(\mathbb{1} - G)^{-1}$, this becomes

$$\rho_B = \det(\mathbb{1} - G) \exp \left[- \sum_l \varphi_l f_l^\dagger f_l \right], \quad (3.27)$$

where the f_l 's are linear combinations of c_j 's, and φ_l is the associated pseudoenergy [see Eq. (3.33) for definition]. With Eq. (3.27), we see that to find ρ_B , we need only calculate the $B \times B$ block Green function matrix G from the ground-state wave function with the aid of operators local to the block, and diagonalize it to determine f_l and subsequently φ_l .

To connect this with the results that we obtained in Sec. II C, let us evaluate the matrix elements for the 0- and 1-particle sectors of ρ_B . Taylor expanding the exponential in Eq. (3.27) gives us

$$\rho_B = \det(\mathbb{1} - G) \prod_l [1 + (e^{-\varphi_l} - 1) f_l^\dagger f_l], \quad (3.28)$$

and so we see that the 0-particle sector is given by

$$\rho_{B,0} = {}_B \langle 0 | \rho_B | 0 \rangle_B = \det(\mathbb{1} - G), \quad (3.29)$$

while in the basis diagonalizing ρ_B , the matrix elements in the 1-particle sector are given by

$$\begin{aligned} {}_B \langle 0 | f_l \rho_{B,1} f_l^\dagger | 0 \rangle_B &= \det(\mathbb{1} - G) \left[{}_B \langle 0 | f_l \mathbb{1} f_l^\dagger | 0 \rangle_B \right. \\ &\quad \left. + \sum_{l'} (e^{-\varphi_{l'}} - 1) {}_B \langle 0 | f_l f_{l'}^\dagger f_{l'} f_l^\dagger | 0 \rangle_B \right] \\ &= \det(\mathbb{1} - G) e^{-\varphi_l} \\ &= \det(\mathbb{1} - G) [G(\mathbb{1} - G)^{-1}]_{ll}. \end{aligned} \quad (3.30)$$

This completes the proof of our conjecture at the end of Sec. II that as a matrix, $\rho_{B,1}$ is related to G by Eq. (2.20).

E. The pseudoenergies φ_l

With the closed-form formula (3.27) for ρ_B at hand, we are now ready to understand its structure and spectra. To begin with, we find that the exponential form

$$\begin{aligned}\rho_B &= \det(1-G) \exp \left[\sum_{ij} [\ln G(1-G)^{-1}]_{ij} c_i^\dagger c_j \right] \\ &= \det(1-G) \exp \left[- \sum_{ij} \Phi_{ij} c_i^\dagger c_j \right],\end{aligned}\quad (3.31)$$

where we define the matrix Φ to be

$$\Phi = -\ln G(1-G)^{-1} = -\ln G + \ln(1-G), \quad (3.32)$$

implies that the weights and eigenvectors of the $(F>1)$ -particle sectors of ρ_B are determined completely by those in the 0- and 1-particle sectors. Defining the set of *pseudoenergies*

$$\varphi_l = -[\ln G(1-G)^{-1}]_{ll}, \quad (3.33)$$

for $l=1, \dots, B$, which are the eigenvalues of Φ , and $\varphi_0 = -\ln \det(1-G)$, we find that the weights of the 1-particle block can be written as

$$w_l = \exp[-(\varphi_0 + \varphi_l)], \quad (3.34)$$

and ρ_B can be written in the form

$$\rho_B = e^{-\varphi_0} \exp \left[- \sum_l \varphi_l f_l^\dagger f_l \right] = e^{-\varphi_0} \exp[-\tilde{H}]. \quad (3.35)$$

Inspired by the resemblance of the form of ρ_B to the density matrix of a quantum canonical ensemble, we call $\tilde{H}$ the *pseudo-Hamiltonian*.

F. Particle-hole symmetry at half-filling

To complete our understanding of the structure and spectrum of ρ_B , we want to know how symmetries of the original problem are built into ρ_B . In particular, we will consider particle-hole symmetry on a bipartite lattice, on which we define a “charge-conjugation” operator $\mathcal{C}$, with $\mathcal{C}^2 = 1$.²⁰ The action of $\mathcal{C}$ on the coordinate space fermion operators can be defined to be

$$\mathcal{C} c_i \mathcal{C} = -(-1)^i c_i^\dagger, \quad \mathcal{C} c_i^\dagger \mathcal{C} = -(-1)^i c_i, \quad (3.36)$$

where $(-1)^i$ is defined to be $+1$ (-1) whenever the site i belongs to the even (odd) sublattice. In a d -dimensional hypercubic lattice, where the site index is $i = \{i_1, i_2, \dots, i_d\}$, the factor $(-1)^i$ is rightfully given by $(-1)^{i_1 + i_2 + \dots + i_d}$.

There are two conditions, one on the dispersion relation ϵ_k and the other on the chemical potential μ , implied by particle-hole symmetry. To derive the first condition on the dispersion relation, we note from Eq. (3.36) that in momentum space, when the lattice is a Bravais lattice

$$\mathcal{C} \tilde{c}_k \mathcal{C} = -\tilde{c}_{-k-Q}^\dagger, \quad \mathcal{C} \tilde{c}_k^\dagger \mathcal{C} = -\tilde{c}_{-k+Q}, \quad (3.37)$$

where the wave vector Q is defined by $e^{iQ \cdot r_i} = (-1)^{i_1}$.²¹ We can then check, with Eqs. (2.9) and (3.37), that

$$\begin{aligned}CHC &= \sum_k \epsilon_k \tilde{c}_{-k+Q} \tilde{c}_{-k-Q}^\dagger \\ &= \sum_{k'} \epsilon_{-k'-Q} \tilde{c}_{k'+2Q} \tilde{c}_{k'}^\dagger.\end{aligned}\quad (3.38)$$

Now, from the definition of Q , it is clear that

$$\begin{aligned}\tilde{c}_{k'+2Q} &= N^{-1/2} \sum_j e^{i(k'+2Q) \cdot r_j} c_j \\ &= N^{-1/2} \sum_j e^{ik' \cdot r_j} [(-1)^j]^2 c_j = \tilde{c}_{k'},\end{aligned}\quad (3.39)$$

and thus (dropping the prime on the dummy wave vector k' that is summed over)

$$CHC = \sum_k \epsilon_{-k-Q} \tilde{c}_k \tilde{c}_k^\dagger = \sum_k \epsilon_{-k-Q} + \sum_k -\epsilon_{-k-Q} \tilde{c}_k^\dagger \tilde{c}_k. \quad (3.40)$$

For time-reversal invariant systems, $\epsilon_{-k} = \epsilon_k$. Also, for our choice of Hamiltonian, $\sum_k \epsilon_{-k-Q} = \sum_{k'} \epsilon_{k'} = \text{Tr } H = 0$. Thus Eq. (3.40) simplifies to

$$CHC = \sum_k -\epsilon_{k+Q} \tilde{c}_k^\dagger \tilde{c}_k. \quad (3.41)$$

Since it is clear from Eqs. (2.8) and (3.36) that $CHC = H$, Eq. (3.41) tells us that the dispersion relation associated with the particle-hole symmetric Hamiltonian H must satisfy the condition

$$\epsilon_{k+Q} = -\epsilon_k. \quad (3.42)$$

Next, to understand how the second condition on the chemical potential comes about, let us note the trivial fact that since ρ_B is a reduced density matrix of ρ_0 , for there to be any sense in talking about the manifestation of particle-hole symmetry in ρ_B , ρ_0 must first be particle-hole symmetric, i.e., $\mathcal{C} \rho_0 \mathcal{C} = \rho_0$. When ρ_0 is the density matrix of the ground state at $T=0$, then it is particle-hole symmetric whenever the ground state $|\Psi_F\rangle$ is. For $|\Psi_F\rangle$ to be particle-hole symmetric, it must have the transformation property

$$\mathcal{C} |\Psi_F\rangle = \eta_{\mathcal{C}} |\Psi_F\rangle, \quad (3.43)$$

where $\eta_{\mathcal{C}} = \pm 1$ is a phase factor associated with $\mathcal{C}$. We know that this is satisfied only by the half-filled ground-state. At finite temperature, when ρ_0 is taken from the grand-canonical ensemble and has the form given in Eq. (3.1), what, if any, extra conditions must be satisfied in order for ρ_0 to be particle-hole symmetric?

Indeed, there appears to be cause for concern: unlike H , which is invariant under “charge-conjugation,” the fermion number operator F transforms under $\mathcal{C}$ as

$$\mathcal{C} F \mathcal{C} = \sum_i \mathcal{C} c_i^\dagger c_i \mathcal{C} = \sum_i c_i c_i^\dagger = N - F, \quad (3.44)$$

and so for ρ_0 to be particle-hole symmetric, i.e.,

$$C\rho_0 C = Q^{-1} \exp \beta[H - \mu(N - F)] = \rho_0, \quad (3.45)$$

we must have $\mu = 0$. For a dispersion relation satisfying Eq. (3.42), $\mu = 0$ corresponds to precisely the situation of half filling. At least for the grand-canonical ensemble, there appears to be no other conditions necessary for ρ_0 to be particle-hole symmetric.

With these conditions in mind, we may now proceed to investigate how particle-hole symmetry shows up in the pseudoenergy spectrum (and hence the spectrum of the block density matrix ρ_B). But first, we must understand how the symmetry is manifested in the Green function matrix $\mathcal{G}$, and its restriction to the block, G . Knowing from our arguments above that $\mu = 0$, we see that the matrix elements of $\tilde{\mathcal{G}}$ in momentum space simplifies to

$$\tilde{\mathcal{G}}_{kk} = \frac{1}{\exp \beta \epsilon_k + 1}. \quad (3.46)$$

Furthermore, using Eq. (3.42), we can relate $\tilde{\mathcal{G}}_{k+Q, k+Q}$ to $\tilde{\mathcal{G}}_{kk}$ by

$$\tilde{\mathcal{G}}_{k+Q, k+Q} = \frac{1}{\exp \beta \epsilon_{k+Q} + 1} = \frac{1}{\exp(-\beta \epsilon_k) + 1} = 1 - \tilde{\mathcal{G}}_{kk}. \quad (3.47)$$

This gives rise to the condition

$$\mathcal{G}_{ij} = \delta_{ij} - (-1)^{(i-j)} \mathcal{G}_{ij} \quad (3.48)$$

that must be satisfied by the matrix elements of $\mathcal{G}$ in coordinate space.

This same result can be derived more transparently for the special case of $T=0$: using the fact that $C^2=1$, $\eta_C^2=1$, as well as Eqs. (3.36) and (3.43), we find that

$$\begin{aligned} \mathcal{G}_{ij} &= \langle \Psi_F | c_i^\dagger c_j | \Psi_F \rangle = \langle \Psi_F | C(C c_i^\dagger C)(C c_j C) C | \Psi_F \rangle \\ &= (-1)^{i+j} \langle \Psi_F | c_i c_j^\dagger | \Psi_F \rangle \\ &= (-1)^{i+j} \delta_{ij} - (-1)^{i+j} \langle \Psi_F | c_j^\dagger c_i | \Psi_F \rangle \\ &= \delta_{ij} - (-1)^{i+j} \mathcal{G}_{ij}, \end{aligned} \quad (3.49)$$

where we have made use of the fact that $\mathcal{G}$ is symmetric, i.e., $\mathcal{G}_{ji} = \mathcal{G}_{ij}$.

Since Eq. (3.49) is a condition satisfied by the matrix elements of $\mathcal{G}$ individually, it holds just as well to those restricted to the block, i.e., G_{ij} . In particular, we note that Eq. (3.49) can actually be written as a matrix equation, which when restricted to the block reads as

$$G = 1 - J G J, \quad (3.50)$$

where $J = \text{diag}(e^{iQ \cdot r_i}) = \text{diag}(1, -1, 1, -1, \dots)$ in coordinate space, and $J^2 = 1$.

To appreciate the implications of Eq. (3.50), let us consider an eigenvector $|\lambda_l\rangle$ of G correspond to the eigenvalue λ_l , such that

$$G|\lambda_l\rangle = \lambda_l |\lambda_l\rangle. \quad (3.51)$$

By Eq. (3.32), this is also the eigenvector of ρ_B , with corresponding pseudoenergy

$$\varphi_l = -\ln \lambda_l + \ln(1 - \lambda_l). \quad (3.52)$$

Using Eq. (3.50), we find that

$$\begin{aligned} GJ|\lambda_l\rangle &= (1 - JGJ)J|\lambda_l\rangle = J|\lambda_l\rangle - JGJ^2|\lambda_l\rangle \\ &= J|\lambda_l\rangle - JG|\lambda_l\rangle \\ &= J|\lambda_l\rangle - \lambda_l J|\lambda_l\rangle \\ &= (1 - \lambda_l)J|\lambda_l\rangle, \end{aligned} \quad (3.53)$$

i.e., the state $|\lambda_{l'}\rangle \equiv J|\lambda_l\rangle$ generated by particle-hole symmetry from $|\lambda_l\rangle$ is also an eigenvector of G , with eigenvalue $\lambda_{l'} = (1 - \lambda_l)$. The pseudoenergy $\varphi_{l'}$ associated with $|\lambda_{l'}\rangle$ is then

$$\varphi_{l'} = -\ln \lambda_{l'} + \ln(1 - \lambda_{l'}) = -\varphi_l. \quad (3.54)$$

It is interesting to note how the weights $w_{B,1,l}$, being exponentials of the pseudoenergies φ_l , hide this particular aspect of particle-hole symmetry.

IV. THE ($F > 1$)-PARTICLE SECTORS

Up to this point, our discussions have been for arbitrary dimensions. To demonstrate how the ($F > 1$)-particle sectors can be constructed from the 0- and 1-particle sectors, we specialize to the one-dimensional case, wherein the Fermi sea is

$$|\Psi_F\rangle = \prod_{|k|=\bar{n}}^{\bar{n}(\pi/a)} \tilde{c}_k^\dagger |0\rangle, \quad (4.1)$$

where a is the lattice constant and $\bar{n}$ is the filling fraction. The 2-point functions can be computed explicitly as

$$G_{ij} = \frac{\sin \pi \bar{n} |i-j|}{\pi |i-j|}. \quad (4.2)$$

We now illustrate how to construct the weights and eigenvectors of the ($F > 1$)-particle sectors of ρ_B starting from φ_0 , φ_l , and f_l , using the example of $B=3$ at half filling.

At half filling, $\bar{n} = \frac{1}{2}$, the 2-point functions G_{ij} take on particularly simple values

$$G_{11} = G_{22} = G_{33} = \frac{1}{2}, \quad G_{12} = G_{23} = \frac{1}{\pi}, \quad G_{13} = 0, \quad (4.3)$$

with which we find, using the machinery developed in Sec. II B, the 0-particle and 1-particle sectors of ρ_3 to be

$$\rho_{3,0} = \langle 000 | \rho_3 | 000 \rangle = \frac{1}{8} - \frac{1}{\pi^2},$$

$$\rho_{3,1} = \begin{bmatrix} \langle 100 | \rho_3 | 100 \rangle & \langle 100 | \rho_3 | 010 \rangle & \langle 100 | \rho_3 | 001 \rangle \\ \langle 010 | \rho_3 | 100 \rangle & \langle 010 | \rho_3 | 010 \rangle & \langle 010 | \rho_3 | 001 \rangle \\ \langle 001 | \rho_3 | 100 \rangle & \langle 001 | \rho_3 | 010 \rangle & \langle 001 | \rho_3 | 001 \rangle \end{bmatrix}$$

$$= \begin{bmatrix} \frac{1}{8} & \frac{1}{2\pi} & \frac{1}{\pi^2} \\ \frac{1}{2\pi} & \frac{1}{8} + \frac{1}{\pi^2} & \frac{1}{2\pi} \\ \frac{1}{\pi^2} & \frac{1}{2\pi} & \frac{1}{8} \end{bmatrix}. \quad (4.4)$$

Diagonalizing these, we find

$$w_{3,0,1} = \left(\frac{1}{\sqrt{8}} - \frac{1}{\pi} \right) \left(\frac{1}{\sqrt{8}} + \frac{1}{\pi} \right), \quad (4.5a)$$

$$w_{3,1,1} = \left(\frac{1}{\sqrt{8}} + \frac{1}{\pi} \right)^2,$$

$$w_{3,1,2} = \left(\frac{1}{\sqrt{8}} - \frac{1}{\pi} \right) \left(\frac{1}{\sqrt{8}} + \frac{1}{\pi} \right), \quad (4.5b)$$

$$w_{3,1,3} = \left(\frac{1}{\sqrt{8}} - \frac{1}{\pi} \right)^2,$$

and thus

$$\varphi_0 = -\ln \left(\frac{1}{\sqrt{8}} - \frac{1}{\pi} \right) \left(\frac{1}{\sqrt{8}} + \frac{1}{\pi} \right) = +3.743\,17\dots, \quad (4.6a)$$

$$\varphi_1 = -\ln \frac{\frac{1}{\sqrt{8}} + \frac{1}{\pi}}{\frac{1}{\sqrt{8}} - \frac{1}{\pi}} = -2.947\,77\dots,$$

$$\varphi_2 = -\ln 1 = 0, \quad (4.6b)$$

$$\varphi_3 = -\ln \frac{\frac{1}{\sqrt{8}} - \frac{1}{\pi}}{\frac{1}{\sqrt{8}} + \frac{1}{\pi}} = +2.947\,77\dots$$

Since $\varphi_1 = -\varphi_3$, we call these a *particle-hole conjugate pair* of pseudo-energies, and say that φ_3 is the particle-hole conjugate of φ_1 . The eigenvectors of the 1-particle sector are

$$f_1^\dagger = \frac{1}{2} c_1^\dagger + \frac{1}{\sqrt{2}} c_2^\dagger + \frac{1}{2} c_3^\dagger, \quad (4.7a)$$

$$f_2^\dagger = \frac{1}{\sqrt{2}} c_1^\dagger - \frac{1}{\sqrt{2}} c_3^\dagger, \quad (4.7b)$$

$$f_3^\dagger = \frac{1}{2} c_1^\dagger - \frac{1}{\sqrt{2}} c_2^\dagger + \frac{1}{2} c_3^\dagger, \quad (4.7c)$$

corresponding to φ_1 , φ_2 , and φ_3 , respectively.

We can easily check that the $f_i^\dagger$'s obey the same anticommutator relation as the $c_i^\dagger$'s, i.e., they obey Pauli's exclusion principle, and so the eigenvectors of the 2-particle sector of ρ_3 are created by

$$f_1^\dagger f_2^\dagger = -\frac{1}{2} c_2^\dagger c_3^\dagger - \frac{1}{\sqrt{2}} c_1^\dagger c_3^\dagger - \frac{1}{2} c_1^\dagger c_2^\dagger, \quad (4.8a)$$

$$f_1^\dagger f_3^\dagger = \frac{1}{\sqrt{2}} c_2^\dagger c_3^\dagger - \frac{1}{\sqrt{2}} c_1^\dagger c_2^\dagger, \quad (4.8b)$$

$$f_2^\dagger f_3^\dagger = -\frac{1}{2} c_2^\dagger c_3^\dagger + \frac{1}{\sqrt{2}} c_1^\dagger c_3^\dagger - \frac{1}{2} c_1^\dagger c_2^\dagger, \quad (4.8c)$$

with associated pseudoenergies $\varphi_1 + \varphi_2 = \varphi_1$, $\varphi_1 + \varphi_3 = 0 = \varphi_2$, and $\varphi_2 + \varphi_3 = \varphi_3$, respectively. Here we see that because of the particle-hole symmetry in the ground-state wave function, the pseudoenergies of the 2-particle sector are identical to those in the 1-particle sector, which implies that the density-matrix weights of the 2-particle sector are identical to those in the 1-particle sector.

For the 3-particle sector, we find that the eigenvector is created by the operator $f_1^\dagger f_2^\dagger f_3^\dagger = c_1^\dagger c_2^\dagger c_3^\dagger$, associated with pseudoenergy $\varphi_1 + \varphi_2 + \varphi_3 = 0$, and hence $w_{3,3,1} = e^{-\varphi_0} = w_{3,0,1}$. This method of generating all ($F > 1$)-particle sectors, starting from the 0- and 1-particle sectors, for larger block sizes at various filling fractions $\bar{n}$ was verified numerically.

Another manifestation of particle-hole symmetry is a queer degeneracy between weights in the F - and $(F+2)$ -particle sectors. This we understand as follows: if $\varphi_{l_1} + \dots + \varphi_{l_F}$ is a weight in the F -particle sector, then in general we can find weights $(\varphi_{l_1} + \dots + \varphi_{l_F}) + \varphi_{l_{F+1}} + \varphi_{l_{F+2}} = (\varphi_{l_1} + \dots + \varphi_{l_F})$ in the $(F+2)$ -particle sector, where $\varphi_{l_{F+1}}$ and $\varphi_{l_{F+2}}$ are particle-hole conjugates of each other.

In fact, from the construction outlined above, we also know the pattern of degeneracy. For example, for $B=6$ at half filling, the pseudoenergies are of the form $-\varphi_a$, $-\varphi_b$, $-\varphi_c$, φ_c , φ_b , and φ_a , corresponding to the eigenstates created by $f_{-a}^\dagger$, $f_{-b}^\dagger$, $f_{-c}^\dagger$, $f_c^\dagger$, $f_b^\dagger$, and $f_a^\dagger$ respectively, where $\varphi_a > \varphi_b > \varphi_c$. We then see in the 3-particle sector that $f_b^\dagger f_{-b}^\dagger f_{-a}^\dagger |0\rangle$ and $f_c^\dagger f_{-c}^\dagger f_{-a}^\dagger |0\rangle$ have the same

pseudoenergy of $\varphi_b - \varphi_b - \varphi_a = \varphi_a = \varphi_c - \varphi_c + \varphi_a$, and are thus degenerate, whereas $f_c^\dagger f_b^\dagger f_a^\dagger |0\rangle$ is nondegenerate with pseudoenergy $\varphi_c - \varphi_b - \varphi_a$.

V. CONCLUSIONS

To summarize, in this paper we showed that elements of the block density matrix $(\rho_B)_{b'b}$ can be calculated as the expectation $\langle K_b^\dagger K_{b'} \rangle$ of a product of referencing operators K_b and $K_{b'}$, which are themselves formed out of fermion operators c_j and $c_j^\dagger$ local to the block. By inspecting the matrix elements $(\rho_{B,1})_{ij}$ and G_{ij} of the 1-particle sector of ρ_B and the block Green function matrix G respectively, for block sizes up to $B=5$, we are led to a conjecture of the closed-form relation (2.20) between $\rho_{B,1}$ and G .

Adapting the technique that Chung and Peschel used to calculate the half-chain density matrix of a chain of spinless Bogoliubov fermions, we find that we can not only prove this conjecture, but also derive a closed-form relation (3.26) between the entire block density matrix ρ_B and G , which can also be written in (3.27) as the exponential of a pseudo-Hamiltonian $\tilde{H}$. The spectrum of $\tilde{H}$ is generated by the independent fermion operators $f_l^\dagger$, which also generate the eigenvectors of G , and hence can be determined by diagonalizing G . It is amusing to numerically compute the pseudo-Hamiltonian in real space. For $\bar{n} \neq \frac{1}{2}$, the generic form of $\tilde{H}$ (a bilinear in $\{c_j^\dagger\}$ and $\{c_j\}$) admits hopping to all other sites on the block, as well as an on-site potential. The symmetry at half filling ensures that the on-site potential is zero and hopping only connects to the other sublattice.

We identify three important implications of Eq. (3.27) in formulating truncation schemes based on ρ_B , for the purpose of performing a RG analysis. First, we note that the spectrum of ρ_B is completely determined by the block Green function matrix G . It suffices therefore to calculate the eigenvectors and eigenvalues in their 0- and 1-particle sectors. The eigenvectors and eigenvalues of the ($F > 1$)-particle sectors of ρ_B , if needed, can be systematically generated from the fermion operators $f_l^\dagger$ and their pseudoenergies φ_l , as illustrated in Sec. IV. This fact is evident in Ref. 14, but its significance was not emphasized. If one is studying the density matrix of a noninteracting toy model (as in this paper), we have an enormous saving in terms of computational time: instead of diagonalizing the entire ρ_B , which is of rank $O(e^B)$, we can diagonalize just the 1-particle sector $\rho_{B,1}$, which is of rank $O(B)$. Possible objects of such a study could be (i) the distribution of eigenvalues;¹⁸ (ii) errors in the dispersion relation due to truncation;¹⁸ and (iii) comparing the product basis of two blocks of length B with the basis of one block of length $2B$, to weigh the effects of the correlations, respectively, neglected or included.

Second, it is highly desirable in RG calculations to ensure that the truncation scheme preserves the symmetries of the target state. Using the specific example of particle-hole symmetry, we saw in Sec. IV that $\rho_{B,F}$ and $\rho_{B,B-F}$ have the same set of weights, and the eigenvectors of $\rho_{B,F}$ are related, up to a phase, to the eigenvectors of $\rho_{B,B-F}$ acted upon by $\mathcal{C}$. Naively, we might expect that to preserve particle-hole sym-

metry, all we have to do is to keep $\mathcal{C}|w_{B,F,k}\rangle$ in $\rho_{B,B-F}$ if $|w_{B,F,k}\rangle$ in $\rho_{B,F}$ is kept. However, there is more to particle-hole symmetry. Under the action of $\mathcal{C}$, the half-filled ground state $|\Psi_F\rangle$ goes (up to a phase) back to itself. Within the block, this global symmetry transformation brings the mixed state of the block back to the same mixed state. Because the mixed state of the block does not have a definite particle number, particle-hole symmetry is not merely a relation between $\rho_{B,F}$ and $\rho_{B,B-F}$. Rather, particle-hole symmetry imposes strict conditions on the spectra of $\rho_{B,F}$ and $\rho_{B,F'}$, for $F, F' = 0, \dots, B$. In fact, in Sec. III F, we elaborated on the condition that particle-hole symmetry imposes on the 1-particle sector. This condition is most intuitive when written in terms of the eigenvalues λ_l of G or the pseudoenergies φ_l , but not immediately apparent if we just stare at the 1-particle density matrix weights $w_{B,1,l}$. It is therefore dangerous to base symmetry-preserving truncation schemes on ρ_B and its eigenvalues alone.

This brings us to the last of the implications that we wish to highlight. While a toy noninteracting model is studied in this paper, our ultimate goal is to address interacting systems, particularly Fermi liquids. Since these (in their low-energy limit) have the same eigenstate structure as a noninteracting Fermi sea (after a unitary transformation), their density matrices also should have the same structure as a noninteracting system. The explicit form of the many-body density matrix, as exhibited in Sec. III of this paper, hints at the proper design of truncation schemes. Rather than independently truncating in each F -particle sector, we should define the truncated states using a set of “creation operators” which satisfy the usual anticommutation relations, and quite likely these are closely related to the approximate quasiparticle creation operators, which should be constructed as a product of the renormalization scheme. We will have more discussions on the implications of such a truncation scheme based on picking out a set of appropriate creation operators for the numerical study of interacting systems, the role of dimensionality, and comparisons with the conventional density matrix renormalization group, in a second paper.¹⁸

Based on our observations on the pattern of degeneracies within and between the F -particle sectors of ρ_B in Sec. IV, we realize that if the truncation is carried out naively, there is a very real danger of ending up with an inconsistent scheme of truncation. This problem occurs quite generally, at various filling fractions and block sizes, but can be most clearly illustrated using our example of $B=6$ at half filling. For example, let us say that as the result of a naive truncation, the states $f_{-a}^\dagger|0\rangle$, $f_{-b}^\dagger|0\rangle$, $f_{-c}^\dagger|0\rangle$, and $f_c^\dagger|0\rangle$ in the 1-particle sector are kept. Examining the 2-particle sector, we find the states $f_{-a}^\dagger f_a^\dagger|0\rangle$ and $f_{-c}^\dagger f_c^\dagger|0\rangle$, which are degenerate in their pseudoenergies. We can build up the latter, but not the former, using the 1-particle operators kept, and so we should keep the latter but not the former. If we truncate the 2-particle sector naively, then based on the density-matrix weights alone we would be probably end up keeping or throwing out both of these 2-particle states.

In fact, the situation for naive truncation is worse, since the state $f_{-a}^\dagger f_b^\dagger|0\rangle$ has lower pseudoenergy than $f_{-c}^\dagger f_c^\dagger|0\rangle$

and will be kept instead. We see therefore that naive truncation is likely to lead to inconsistencies: some many-particle states built up from the 1-particle states kept get thrown out, while other many-particle states that cannot be built up from the set of 1-particle states kept end up being retained. Hence, we find that as far as particle-conserving models are concerned, for any truncation scheme to be consistent, the truncation must be carried out on the 1-particle sector of ρ_B alone.

Finally, let us remark that everything done in this paper can be trivially extended to the case of spinfull fermions, so long as they are noninteracting. Every object in our calculations, in particular the Fermi sea wave function and the block density matrix, will merely in the spinfull case be replaced by the direct product of two such objects with spin-up and spin-down flavors.

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APPENDIX A: AUTOMATING THE NUMERICAL COMPUTATION OF ρ_B

As we saw in Sec. II, each of the 2^B basis configurations of the block corresponds to an operator K_b , so that $(\rho_B)_{b'b} = \langle K_b^\dagger K_{b'} \rangle$. Therefore, to obtain all matrix elements of ρ_B it sufficed to automate the calculation of expectations of an arbitrary string of creation/annihilation operators (each operator acting on one site).

First, this formal string of operators must be simplified. Through a systematic set of anticommutations, it is brought to a canonical form, such that (a) it is normal ordered, with one substring of all creation operators followed by one substring of all annihilation operators; and (b) within each substring the operators are ordered by the site. Of course, each site can appear at most once in each substring (otherwise it reduces to zero). A complication of this step is that the result is generally a sum of many terms in the canonical form, since every rearrangement of the form $c_1 c_1^\dagger \rightarrow 1 - c_1^\dagger c_1$ produces two terms from one.

Next, we note that within this sum, only terms containing a balanced number, say n , each of creation and annihilation operators will contribute to the expectation. By the Wick theorem, such $2n$ -point functions $G_{\bar{i}_1, \dots, \bar{i}_n, j_1, \dots, j_n}$ reduces to the determinant of an $n \times n$ matrix, as shown in Eq. (2.14).

For models in which fermion number F is conserved, we can further separate ρ_B into the various F -particle sectors $\rho_{B,F}$ before diagonalization. This is particularly important at

half filling, for there exist generic degeneracies between states in different sectors (see Sec. IV), and there is a danger that a naive diagonalization of the whole matrix ρ_B will produce eigenstates with mixed particle number.

The limiting consideration for the whole calculation is the diagonalization time, which is determined by the condition number of ρ_B , rather than array storage. In general, the condition number, which is the ratio of the largest weight to the smallest weight, grows exponentially with system size.¹⁸

APPENDIX B: BLOCK INVERSION FORMULA

Consider a square $N \times N$ symmetric matrix $\mathcal{M}$ written in matrix block form as

$$\mathcal{M} = \begin{bmatrix} A & B \\ B^T & C \end{bmatrix}, \quad (\text{B1})$$

where A is a square $N_1 \times N_1$ symmetric matrix, B is a $N_1 \times N_2$ nonsquare matrix, and C is a square $N_2 \times N_2$ symmetric matrix. Here $N_1 + N_2 = N$.

If we write the inverse matrix $\mathcal{M}^{-1}$ also in the matrix block form

$$\mathcal{M}^{-1} = \begin{bmatrix} D & E \\ E^T & F \end{bmatrix}, \quad (\text{B2})$$

where D is a square $N_1 \times N_1$ symmetric matrix, E is an $N_1 \times N_2$ nonsquare matrix, and F is a square $N_2 \times N_2$ symmetric matrix, how are D , E , and F related to the matrix blocks A , B , and C in $\mathcal{M}$?

Using the fact that $\mathcal{M}\mathcal{M}^{-1} = \mathbb{1}$, and thus

$$\begin{bmatrix} A & B \\ B^T & C \end{bmatrix} \begin{bmatrix} D & E \\ E^T & F \end{bmatrix} = \begin{bmatrix} \mathbb{1}_{N_1 \times N_1} & 0_{N_1 \times N_2} \\ 0_{N_2 \times N_1} & \mathbb{1}_{N_2 \times N_2} \end{bmatrix} \quad (\text{B3})$$

(where the subscripts, which will henceforth be dropped for notational clarity, following the 1's and 0's indicate the shape and size of the matrices) we find the following relations between the matrix blocks of $\mathcal{M}$ and $\mathcal{M}^{-1}$:

$$AD + BE^T = \mathbb{1}, \quad (\text{B4a})$$

$$AE + BF = 0, \quad (\text{B4b})$$

$$B^T D + CE^T = 0, \quad (\text{B4c})$$

$$B^T E + CF = \mathbb{1}. \quad (\text{B4d})$$

Solving for D , E , and F in terms of A , B and C , we find that

$$D = [A - BC^{-1}B^T]^{-1}, \quad (\text{B5a})$$

$$E = -A^{-1}B(C - B^T A^{-1}B)^{-1}, \quad (\text{B5b})$$

$$F = [C - B^T A^{-1}B]^{-1}. \quad (\text{B5c})$$

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¹⁹Reference 14 avoids the singularities by assuming a Hamiltonian with nonzero anomalous terms containing double creation or double annihilation operators. Alternatively, realizing that we have definite occupation numbers, i.e., $\langle \tilde{c}_k^\dagger \tilde{c}_k \rangle = 0, 1$ at $T=0$, the density matrix ρ_0 must be written as a product of projection operators, i.e., $\rho_0 = \prod_{|k| < k_F} \tilde{c}_k^\dagger \tilde{c}_k \prod_{|k| > k_F} \tilde{c}_k \tilde{c}_k^\dagger$. This is possible only if $\tilde{\Gamma}_{kk} = +\infty$ for $|k| < k_F$ and $\tilde{\Gamma}_{kk} = -\infty$ for $|k| > k_F$. For the purpose of algebraic manipulations, this choice of $\tilde{\Gamma}_{kk}$ must be regularized, i.e., take $\tilde{\Gamma}_{kk} = \Lambda \operatorname{sgn}(k_F - |k|)$, and take $\Lambda \rightarrow \infty$ at the end of the calculations. With this choice of regularization, e^Γ can then be written in terms of the zero-temperature Green function matrix $\mathcal{G}$, whose matrix elements in momentum space are $\mathcal{G}_{kk} = \theta(k_F - |k|)$ [where $\theta(x) = 0$ for $x < 0$ and $\theta(x) = 1$ when $x > 0$ is the step function] as $e^\Gamma = e^{-\Lambda} \mathbb{1} + (e^\Lambda - e^{-\Lambda}) \mathcal{G}$. It is then easy to show that $(\mathbb{1} + e^\Gamma)^{-1} = (\mathbb{1} + e^{-\Lambda})^{-1} \mathbb{1} + [(1 + e^\Lambda)^{-1} - (1 + e^{-\Lambda})^{-1}] \mathcal{G}$, which becomes $(\mathbb{1} - \mathcal{G})$ in the limit of $\Lambda \rightarrow \infty$.
²⁰One possible form for the charge-conjugation operator is $\mathcal{C} = \prod_j [i^{j+1} c_j^\dagger + (-i)^{j+1} c_j]$, where the product runs over all lattice sites.
²¹If the bipartite lattice is not a Bravais lattice, then wherever the wave vector k appears as an index, it must be replaced by the combination of k and a band index. All of the results—in particular those of Sec. III F—still go through in this generalized case, provided that all lattice sites are symmetry equivalent.