Fermion-boson transmutation and comparison of statistical ensembles in one dimension

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The theoretical description of interacting fermions in one spatial dimension is simplified by the fact that the low energy excitations can be described in terms of bosonic degrees of freedom. This fermion-boson transmutation (FBT) which lies at the heart of the Luttinger liquid concept is presented in a way which does not require a knowledge of quantum field theoretical methods. As the basic facts can already be introduced for noninteracting fermions they are mainly discussed. As an application we use the FBT to present exact results for the low temperature thermodynamics and the occupation numbers in the microcanonical and the canonical ensemble. They are compared with the standard grand canonical results.

1. INTRODUCTION

The low temperature thermodynamic properties of simple metals can be qualitatively understood in terms of the simple Sommerfeld model, which treats the conduction electrons as noninteracting fermions in a box. Typical results are a specific heat linear in temperature and a constant spin susceptibility in qualitative agreement with experiments. Landau’s Fermi liquid theory rests on the assumption of quasi-particles which are in a one-to-one correspondence to noninteracting fermions. This leads to a linear specific heat and a constant spin susceptibility but involves renormalized quantities like the effective mass and the quasi-particle interaction parameters, which are difficult to calculate microscopically. The consistency of the approach was shown using perturbation theory to infinite order and more recently by renormalization group techniques.

The problem of interacting fermions simplifies in one dimension. In a pioneering paper Tomonaga treated the case of a two-body interaction which is long ranged in real space. He showed that the low energy excitations of the noninteracting as well as the interacting system can be described in terms of noninteracting bosons. The important idea to solve the case of interacting fermions was the observation that a long range interaction in real space is short ranged in momentum space and therefore only particles and holes in the vicinity of the Fermi points are involved in the interacting ground state and states with a low excitation energy. To obtain his results, Tomonaga linearized the energy dispersion around the two Fermi points \( \pm k_F \). Luttinger later used a model with strictly linear energy dispersions which is closely related to the massless Thirring model. The exact solution for the Luttinger model was presented by Mattis and Lieb. A very elegant method to calculate correlation functions for the model is the bosonization of the fermion field operator. The exponents of the anomalous power law decay of various correlation functions are determined by the anomalous dimension, which can be calculated explicitly for the Tomonaga-Luttinger (TL-) model.

It was an important observation of Haldane that the low energy physics of the exactly solvable TL-model provides the generic scenario for one-dimensional fermions with repulsive interactions. Like in the Landau Fermi liquid picture a few parameters completely determine the low energy physics. Generally they are as difficult to calculate as the Landau parameters. In contrast to the higher dimensional case there are additional exactly solvable models for which Haldane’s Luttinger liquid scenario can be tested and the parameters determining the anomalous dimension can be calculated using the Bethe-ansatz technique.

Another important manifestation of Luttinger liquids is called spin charge separation, i.e. for low energy excitations the charge and spin degrees are completely decoupled. This shows up, for example, in the spectral function of the one-particle Green’s function, which largely determines the photoemission spectrum. Recent high resolution photoemission experiments on quasi one-dimensional organic conductors have been interpreted to show Luttinger liquid behaviour.

In the present paper we present the basic ideas behind the Luttinger liquid concept in very simple terms, involving only basic quantum mechanics and statistical mechanics. We therefore believe that our approach requires less theoretical knowledge than the field theory approach to FBT published in this journal some time ago.

In section II we present the fermion-boson transmutation in terms that should be accessible to anybody who has had an elementary course in solid state physics. Especially no use is made of the method of second quantization. The concepts introduced in section II are used in section III and IV to compare the different statistical ensembles for noninteracting fermions in a box. In the grand canonical ensemble the constraint of a fixed particle number which makes the calculation complicated in the canonical ensemble is relaxed and the determination of thermodynamical quantities is straightforward. The microcanonical ensemble is seldom used in this context. Our discussion of the basic ideas of the FBT allows us to present a comparison of the three ensembles. We show
explicitly how the results approach each other in the limit of infinite box size with constant density, i.e. the thermodynamic limit. For the calculation of the occupation numbers in the canonical ensemble the numerical effort increases quickly with the system size when the elementary approach of section IV is used. We take this as an opportunity to discuss the fermion-boson transmutation again on a more advanced level using the method of second quantization in section V. The techniques which allow the calculation of the properties of the TL-model of interacting fermions are introduced again in the context of noninteracting fermions. The power of this method is shown by presenting a closed expression for the occupation number of noninteracting fermions in the canonical ensemble, which allows to discuss the transition to the Fermi function in the thermodynamic limit.

The paper is written such that readers not familiar with the method of second quantization can understand fermion boson transmutation in its elementary form and the comparison of the statistical ensembles by reading sections I to IV only.

II. NONINTERACTING FERMIONS IN A BOX

We consider particles in one dimension in a box of length $L$ with fixed boundary conditions $\phi(0) = \phi(L) = 0$. The single particle eigenfunctions and energies are given by

$$\phi_n(x) = \sqrt{2/L} \sin \left( \frac{k_n x}{L} \right),$$

and

$$\epsilon_n \equiv \epsilon(k_n) = \frac{\hbar^2 k_n^2}{2m},$$

with $k_n = n\pi/L$ and $n \in \mathbb{N}$. Later we will also consider periodic boundary conditions. Then the spacing of the $k$-values is doubled and negative and positive values occur. In the following the spin of the fermions is neglected for simplicity, i.e. we consider spinless fermions as in [§]. The ground state of $N$ fermions is given by filling the lowest momentum states up to the Fermi wavevector $k_F = n_F\pi/L$ where $n_F = N$ and the excited states can be classified by giving the occupation numbers $n_{k_n}$, which are zero or one. For fixed particle number $N$ the sum of the occupation numbers has to be equal to $N$. This constraint makes the evaluation of the canonical partition function difficult. In the well known procedure of Darwin and Fowler an integral representation for the Kronecker delta describing the constraint is used. If the corresponding integral is evaluated by the method of steepest descent the result is equivalent to the grand canonical calculation, where only the average particle number is fixed as particle exchange with a bath is assumed. In the following we show that in the low temperature regime the canonical partition function can be expressed as the partition function of a photon gas, i.e. massless bosons.

We first summarize the well known grand canonical result [§]. The total energy $E_{gc}$ as a function of the temperature $T$ and the chemical potential $\mu$ is given by

$$E_{gc} = \sum_n \frac{\epsilon_n}{e^{\beta \epsilon_n - \mu} + 1},$$

where $\beta = 1/(k_B T)$ and $k_B$ is the Boltzmann constant. The chemical potential $\mu$ becomes a function of temperature if the average particle number is assumed to be given by the fixed value $N$

$$N = \sum_n \frac{1}{e^{\beta \epsilon_n - \mu} + 1}.$$  

In the thermodynamic limit $L \to \infty$, $N/L$ fixed, the low temperature result for the energy, the specific heat and other thermodynamic quantities can be explicitly evaluated using the Sommerfeld technique [§]. They are determined by the one-particle density of states per unit length $\rho_0(\epsilon) = 1/\pi \hbar v(\epsilon)$ in the vicinity of the Fermi energy $\epsilon_F \equiv \epsilon_{n_F}$, where $\hbar$ times the velocity $v(\epsilon)$ is given by $d\epsilon(k)/dk$ as a function of $\epsilon$. The low temperature specific heat, for example, is linear in temperature and determined by $\rho(\epsilon_F)$ [§]. This is an indication that in order to arrive at this result one is allowed to simplify the spectrum of eigenvalues in Eq. (2) in the vicinity of the Fermi energy.

For $n \gg 1$ the eigenvalue spectrum given by Eq. (2) becomes locally equidistant

$$\epsilon_{n+1} - \epsilon_n = \frac{2n + 1}{2n - 1} \rightarrow 1.$$  

![Specific heat for the quadratic (solid line) and the linearized (dashed line) electron dispersions.](image)

As in Refs. [§] and [§] we therefore linearize the spectrum $\epsilon_n$ around the Fermi point $n_F$. 

![Specific heat for the quadratic (solid line) and the linearized (dashed line) electron dispersions.](image)
\[
\epsilon_n^{(l)} = \epsilon_F + hv_F(n - n_F)\pi/L,
\]
where \(v_F = \hbar k_F/m = \hbar\pi(N/L)/m\) is the Fermi velocity. As we keep the density \((N/L)\) constant while increasing \(L\) the Fermi velocity is independent of the system size. In the following we consider this as the model for which we want to determine the low temperature thermodynamics. Fig. 1 shows the temperature regime \(k_B T \ll \epsilon_F\) for which the specific heats for both models agree. The results where obtained by numerical evaluation of Eqs. (3) and (4) in the thermodynamic limit. The linearization in Eq. (6) is the essential step to obtain the exact solution for the interacting TL-model. The constant energy separation of the linearized model is given by \(\Delta = \hbar v_F\pi/L\).

For the linearized model also the excitation spectrum of the \(N\)-electron system is equidistant

\[
E_M = E_0 + M\Delta,
\]
where \(E_0\) is the ground state energy of the filled Fermi sea. For large \(M\) the eigenvalues are highly degenerate. The determination of the degeneracy can be reduced to an old problem in combinatorics if we classify the corresponding states not by fermionic occupation numbers as discussed above, but in terms of the upward shifts of the occupied levels compared to the Fermi sea. This is exemplified in Fig. 2 where a special excited state for \(M = 20\) is shown. The highest occupied level is shifted by seven energy units, the second and third by four, the forth by three and the fifth and sixth highest by one unit. All deeper levels are unshifted. The excitation energy in units of \(\Delta\) is given by \(M = 7 + 4 + 4 + 3 + 1 + 1 = 20\). This is one of the possible partitions of \(M\) of the number \(M = 20\).

![Diagram showing the classification scheme for the excited states](image)

Each other of the 627 partitions of \(M = 20\), written in lexicographic order, as in our example, uniquely classifies an other possible excited state corresponding to this excitation energy. For small \(M\) it is easy to write down all partitions. For \(M = 4\) the five possible partitions are: \([4]\); \([3, 1]\); \([2, 2]\); \([2, 1, 1]\); \([1, 1, 1, 1]\). For a general \(M\) a partition is defined by a set of \(M\) numbers \(m_i \in \mathbb{N}_0\) such that

\[
M = m_1 + 2m_2 + 3m_3 + \ldots + Mm_M = \sum_{i=1}^{M} im_i \quad (8)
\]

Already more than two hundred years ago Euler proved important theorems about the number of partitions. His use of generating functions can be considered the earliest precursor of the methods of quantum statistical mechanics.

A formally simple expression for the number \(g_M\) of partitions of \(M\) can be given as a sum over a Kronecker delta using the defining Eq. (8)

\[
g_M = \sum_{m_1=0}^{\infty} \ldots \sum_{m_M=0}^{\infty} \sum_{m_{M+1}=0}^{\infty} \ldots \delta_{M,\sum_{i=1}^{M} im_i}. \quad (9)
\]

From Eq. (8) it is obvious that it is unnecessary to include more than \(M\) summations in Eq. (9), but the form with the additional infinite number of summations turns out to be useful to calculate the canonical partition function of the linearized model

\[
Z_c = \sum_{M=0}^{\infty} \tilde{g}_M e^{-\beta(E_0 + M\Delta)} . \quad (10)
\]

Here \(\tilde{g}_M\) is the degeneracy corresponding to the excitation energy \(M\Delta\). For excitation energies \(M\Delta\) smaller than \(n_F\Delta\) all partitions of \(M\) lead to a possible excited state of the \(N\)-particle system and \(\tilde{g}_M = g_M\). For \(M > n_F\) the degeneracy of excited states is smaller than the number of partitions \(\tilde{g}_M < g_M\). For \(M = n_F + 1\), e.g. there is no allowed excited \(N\)-particle state related to the partition \([1, 1, \ldots, 1]\), \(n_F + 1\) because in the groundstate there are only \(n_F\) fermions that can be shifted upwards. For \(M > n_F\) we have to take into account that one-particle states exist only for quantum numbers \(n \geq 1\). Two arguments can be given to use \(\tilde{g}_M\) as the degeneracy also for \(M > n_F\). The one in spirit of Tomonaga’s treatment of the interacting case is to argue that for \(n_F\Delta/(k_B T) \gg 1\) the contribution of these highly excited states is exponentially small in this large ratio and the replacement of \(\tilde{g}_M\) by \(g_M\) in Eq. (10) makes no relevant difference. The solution corresponding to Luttinger’s treatment of interacting fermions consists of adding an infinite Dirac sea of fermions in one-particle states with \(n \leq 0\). Then the replacement of \(\tilde{g}_M\) by \(g_M\)
is exact, but one has to be careful with the treatment of
an infinite number of electrons.\footnote{The integrals in the
thermodynamic limit. In this limit the sums can
be replaced by integrals and we obtain from Eq. (12)
\begin{equation}
e_{e}(T) \equiv \frac{(k_{B}T)^{2}}{\pi \hbar v_{F}} I_{-},
\end{equation}
where the integrals \(I_{\pm}\) are defined as
\begin{equation}
I_{\pm} \equiv \int_{0}^{\infty} \frac{x}{e^{x^{2} \pm 1}} dx.
\end{equation}
Eq. (13) is the one-dimensional version of the Stefan-
Boltzmann law of black body radiation which states
that in \(d\) dimensions the energy density is proportional
to \(T^{d-1}\), or to Debye’s theory of the low temperature
specific heat due to acoustical phonons.\footnote{For the calculation in the grand canonical ensemble us-
ing Eq. (3) the contribution of the states above \(e_{F}\) equals
the part below \(e_{F}\) for the linear dispersion and the
chemical potential is temperature \textit{independent}. This yields
\begin{equation}
e_{\text{ge}}(T) = \frac{(k_{B}T)^{2}}{\pi \hbar v_{F}} 2I_{+}.
\end{equation}
The integrals \(I_{\pm}\) can be found in every good table of
integrals or textbook on statistical mechanics.\footnote{The
results in Eqs. (13) and (15) agree can be shown
without actually calculating the integrals. Elementary
algebra yields
\begin{equation}
I_{-} - I_{+} = 2 \int_{0}^{\infty} \frac{x}{e^{2x} - 1} dx = I_{-}/2.
\end{equation}
and we obtain \(I_{-} = 2I_{+}\), which shows the equivalence
of the canonical and the grand canonical ensemble in the
thermodynamic limit. The numerical value is given by\footnote{In
the following section the specific heat for both ensem-les is discussed for finite systems. For a given density and
temperature there is a natural length scale (thermal
De Broglie wave length) given by \(a(T) \equiv \hbar v_{F}\pi/(k_{B}T)\).
The system size \(L\) is large compared to \(a(T)\) if \(k_{B}T\)
is large compared to the level spacing \(\Delta\).}
\begin{equation}
c_{\infty} \equiv \frac{\pi k_{B}^{2} T}{3 \hbar v_{F}}.
\end{equation}

\section{III. THERMODYNAMIC PROPERTIES FOR
FINITE SYSTEMS}

The Stefan-Boltzmann law Eq. (13) for the energy per
unit length is only correct in the thermodynamic limit. For
finite \(L\) the sum in Eq. (12) has to be performed nume-
rically. For \(L/a(T) \gg 1\) the Euler summation formula
in its most simple form\footnote{The microcanonical results approach those of the canonical
and the grand canonical ensemble for large \(L\).}
\begin{equation}
\sum_{j=0}^{j_{\pm}} f(j) \equiv \int_{j_{0}}^{j_{\pm}} f(x) dx + \left[ f(j_{0}) + f(j_{1}) \right]/2 \mp \ldots
\end{equation}
provides the leading finite size correction
\begin{equation}
\frac{c_{L,c}}{c_{\infty}} = 1 - \frac{3}{2 \pi^{2}} \frac{a(T)}{L} + O\left(\frac{a(T)}{L}\right)^{2}.
\end{equation}
Fig. 3 shows \(c_{L,c}/c_{\infty}\) as a function of \(L/a(T)\). As
\(L/a(T) \approx k_{B}T/\Delta\) this plot can be viewed as the specific
heat ratio as a function of system size for fixed temperature or as a function of temperature for a given length of the system. For small arguments the ratio is small due to the well known phenomenon of freezing of the excited states for temperatures small compared to the excitation energies. Fig. 3 also shows the corresponding results for the *grand canonical* specific heat following from the numerical evaluation of the result using Eq. (3). For small arguments the exponential suppression is weaker than in the canonical case as the chemical potential lies in the middle between the highest occupied and the lowest unoccupied state of the Fermi sea. The use of the Euler summation formula Eq. (19) shows that there is no finite size correction of order $a(T)/L$ as in the canonical result Eq. (20) and the asymptotic limit is reached very quickly.

$$\frac{1}{T_{\text{micro}}(E_M)} = \left[ \frac{\partial S_{\text{micro}}(E_M)}{\partial E_M} \right]_L = k_B \left[ \ln g_M \right]'.$$ (22)

Due to the discreteness of the energy the derivative in Eq. (22) has to be evaluated as a ratio of differences $f'_M = (f_{M+1} - f_{M-1})/2$. This definition produces smoother results than the definition involving differences of neighbouring numbers. The microcanonical definition of the heat capacity for constant $L$ is

$$C_{L,\text{micro}}(E_M) = \left[ \frac{\partial T_{\text{micro}}(E_M)}{\partial E_M} \right]_L^{-1}. \quad (23)$$

As discussed in the preceding section the number of partitions $g_M$ plays a central role for the thermodynamics of the linearized model. In the microcanonical ensemble the number enters explicitly in Eq. (18). The values of the $g_M$ for $M$ up to 500 can be found in a standard handbook. They increase very quickly with $M$ as can be seen from $g_{500} \approx 2.3 \cdot 10^{21}$, which leads to $S_{\text{micro}}(E_0 + 500\Delta)/k_B \approx 49.20$. For values of $M$ of the order fifty or larger already the crudest approximation of Ramanujan

$$(g_M)_R = e^{\pi \sqrt{2M/3}}/(4M \sqrt{3}), \quad (21)$$

provides a good approximation. One obtains, for example $\ln \{g_M(500)\}_R \approx 49.18$. In Fig. 4 we show $S_{\text{micro}}$ as a function of $M$ and compare the exact result using the recursion relation with the Ramanujan approximation Eq. (21), which smooths the number theoretical fluctuations. The inverse microcanonical temperature is defined as

![FIG. 3. Ratio of the grand canonical specific heat and the specific heat in the thermodynamic limit $c_\infty$ (solid line) and the canonical specific heat and $c_\infty$ (dashed line) as a function of $L/a(T)$.](image1)

![FIG. 4. Microcanonical entropy as a function of the energy calculated with help of the exact degeneracies (circles) and the Ramanujan approximation Eq. (18) (solid line).](image2)

![FIG. 5. Ratio of the exact microcanonical specific heat and the one calculated with the help of the Ramanujan approximation as a function of $[(E_M - E_0)/\Delta]^{1/2}$.](image3)
\[ C_{L,R}(E_M) = \pi k_B \sqrt{\frac{2(E_M - E_0)}{3\Delta}} + \mathcal{O}\left( \sqrt{\frac{\Delta}{E_M - E_0}} \right). \]  

This should be compared with the relation \( L c = \pi k_B \sqrt{2 L e(T)/(3\Delta)} \), where \( e(T) = e_c(T) = e_{ge}(T) \), which follows from Eqs. (13) or (15). As in the large energy limit \( E - E_0 \) in the microcanonical ensemble and \( E(T) - E_0 \) in the canonical (or grand canonical) ensemble can be identified, as discussed in the next section, \( C_{L,R}/L \) agrees with \( c_\infty \) in this limit. Fig. 5 shows how the exact microcanonical result Eq. (23) approaches the canonical result \( C_{L,R} \), as a function of \( \sqrt{(E_M - E_0)/\Delta} \), which takes the role of \( L/a(T) \) in Fig. 3. The ratio \( c_{\text{micro}}/c_{L,R} \) shows quite strong fluctuations for values \( \sqrt{(E_M - E_0)/\Delta} \) below 5.

As in the thermodynamic limit the entropy per unit length agrees for all three ensembles we can use the \textit{grand canonical entropy} to obtain an estimate for the \textit{number of partitions}. This yields the Ramanujan expression Eq. (21) with \( 4M \sqrt{3} \) replaced by 1.

\section*{IV. OCCUPATION NUMBERS}

For variable particle number the method of second quantization in Fock space is the appropriate mathematical framework. The Hamiltonian for noninteracting fermions considered in section II reads

\[ H_0 = \sum_m \epsilon_m \hat{n}_m = \sum_m \epsilon_m \hat{c}_m^\dagger \hat{c}_m, \]  

where the \( \hat{n}_m \) are the occupation number operators and \( \hat{c}_m^\dagger (\hat{c}_m) \) are fermionic creation (annihilation) operators, which obey canonical anticommutation relations

\[ [c_m, c_l^\dagger] = 0, \quad [c_m, c_l] = \delta_{m,l}. \]  

Explicit use of the method of second quantization is only made in the next section. Here we discuss the calculation of the expectation value of \( \hat{n}_m \) in the three ensembles. The calculation in the grand canonical ensemble is standard and for arbitrary system size yields the \textit{Fermi function}

\[ \langle \hat{n}_m \rangle_{\text{gc}, T} = \frac{1}{e^{\beta(\epsilon_m - \mu)} + 1} = f(\epsilon_m). \]  

We next consider the model with the linearized dispersion Eq. (6) in the \textit{microcanonical ensemble}. In section II we have labeled the states of excitation energy \( M \Delta \) in terms of the \textit{list of upward shifts} \( [\alpha]_M \)

\[ [\alpha]_M = [l_1, l_2, \ldots] \]  

with \( l_i \geq l_{i+1} \geq 0 \),

which corresponds to a partition in lexicographic order. The expectation value of the occupation number is given by

\[ \langle \hat{n}_m \rangle_{\text{micro}, E_M} = \frac{1}{g_M} \sum_{[\alpha]_M} \langle [\alpha]_M | \hat{n}_m | [\alpha]_M \rangle. \]  

The expectation value of \( \hat{n}_m \) in the state \( [\alpha]_M \) can easily be calculated due to the definition of the list \( [\alpha]_M \)

\[ \langle [\alpha]_M | \hat{n}_m | [\alpha]_M \rangle = 1 \quad \text{for} \quad m = n_F + l_i - i + 1, \]  

and zero otherwise. In order to perform the numerical calculations all partitions of \( M \) have to be \textit{explicitly} created, which leads to a drastic increase of computer time for increasing \( M \). The numerical results will be discussed below together with the \textit{canonical result}

\[ \langle \hat{n}_m \rangle_{c, T} = \frac{1}{Z_c} \sum_{M=0}^{\infty} g_M \langle \hat{n}_m \rangle_{\text{micro}, E_M} e^{-\beta(E_0 + M \Delta)}. \]  

The canonical result can therefore be obtained directly from the microcanonical one if the temperature is low enough that the probability distribution

\[ w_M(T) = g_M e^{-\beta(E_0 + M \Delta)} / Z_c, \]  

has decayed to “zero” for values of \( M \) for which the calculation of the microcanonical average is still feasible. Note that while the Fermi function can be obtained from the grand canonical potential by a derivative with respect to \( \epsilon_m \), such a procedure is not possible for the canonical free energy. In order to calculate the canonical average for higher temperatures the \textit{method of the bosonization of the field operator} \cite{[15]} can be used which is described in the next section. We therefore only consider results for quite low temperatures in this section.

Fig. 6 shows the average occupation numbers for the three ensembles \( \tau \equiv k_B T/\Delta = 3 \). The microcanonical curve is for \( M = 10 \), which roughly corresponds to the maximum of the probability distribution \( w_M(T) \) shown in Fig. 7. The overall agreement of the results is quite good already at this small value of \( \tau \). Note that the microcanonical result yields the ground state occupancies for \( |m - n_F| > M \), e.g. \( \langle \hat{n}_m \rangle_{\text{micro}, E_M} = 0 \) for \( m > M + n_F \), while the canonical and the grand canonical results go to zero continuously.
and holes at the bottom of the Fermi sea one can replace the \( l \) by \( \tilde{l} \) in the lowest \( \tilde{l} \) states at the bottom of the band divided by \( l \). For \( l \ll n_F \) and \( N \) fermion states which have no holes at the bottom of the Fermi sea one can replace the operator on the rhs of Eq. (34) by the unit operator. One can make this an exact statement if a Dirac sea is added, i.e. the sum in Eq. (33) runs not from 1 but from \(-m_0\) with \( m_0 \to \infty \). An analogous discussion for \( l \neq l' \) leads to

\[
[b_l, b_{l'}^\dagger] = \delta_{l,l'} \mathbb{1},
\]

e.g. the operators defined in Eq. (33) obey boson commutation relations.

With the help of these ladder operators we can create an orthonormal basis set of many fermion states labeled by bosonic quantum numbers \( \{\tilde{m}_l\} \) with \( \tilde{m}_l \in \mathbb{N}_0 \), if one treats the Fermi sea \( |F(N)\rangle \) as the harmonic oscillator ground state

\[
|\{\tilde{m}_l\}\rangle = \prod_l \frac{1}{\sqrt{\tilde{m}_l!}} (b_l^\dagger)^{\tilde{m}_l} |F(N)\rangle.
\]

All states with \( \sum_l l\tilde{m}_l = M \) provide a new basis of states corresponding to the excitation energy \( M\Delta \) of \( H_0 \). They are rather complicated linear combinations of the states discussed in section II which could be labeled either by fermionic occupation numbers or by the list \( [\alpha]_M \) of the upward shifts. If for \( M = 4 \) we label the \( [\alpha]_M \) by \( |i\rangle \) with \( i = 1, \ldots, 5 \), in the order in which the partitions of \( M = 4 \) were presented in section II, we obtain e.g.

\[
\begin{align*}
&b_4^\dagger |F\rangle = \frac{1}{2} (|1\rangle - |2\rangle + |4\rangle - |5\rangle) \\
&b_4^\dagger b_4^\dagger |F\rangle = \frac{1}{\sqrt{3}} (|1\rangle + |3\rangle + |5\rangle) \\
&\frac{1}{\sqrt{4!}} (b_4^\dagger)^4 |F\rangle = \frac{1}{\sqrt{24}} (|1\rangle + 3|2\rangle + 2|3\rangle + 3|4\rangle + |5\rangle).
\end{align*}
\]

As long as we consider only noninteracting fermions both types of basis sets are completely well suited for the description. It turns out that for fermions with a two-body interaction the interacting groundstate has a much simpler form in the bosonic basis set Eq. (36).

In Eq. (33) we have expressed the Bose operators \( b_l(b_l^\dagger) \) in terms of the fermionic operators. In order to take advantage of the bosonization one has to address the reverse problem: Can one express fermionic operators completely in terms of the Bose operators? Here one proceeds in two steps. It is possible to bosonize the operator \( H_0 \) with the help of the Kronig identity

\[
\sum_{l=1}^{\infty} b_l b_l^\dagger = \sum_{n=1}^{\infty} n c_n^\dagger c_n - \frac{1}{2} (\hat{N}^2 + \hat{\mathcal{N}}),
\]

where \( \hat{\mathcal{N}} \equiv \sum_n c_n^\dagger c_n \) is the fermionic particle number operator. For the proof of this relation the boson commutation relations of the \( b_l(b_l^\dagger) \) is not needed. As the lhs of Eq. (38) contains products of four fermion operators it might look surprising that one obtains a one-particle operator and only a term involving the particle number
operator on the right hand side. It is left as an exercise to the reader to show that the additional four fermion terms exactly vanish. If we subtract \( N \) and multiply by \( \hbar v_F \pi / L \) we obtain

\[
H_0 = \hbar v_F \sum_{l=1}^{\infty} \frac{l \pi}{L} b_l^\dagger b_l + h(\hat{N}),
\]

(39)

where the function \( h(\hat{N}) \) is irrelevant in the following.

It as also possible to bosonize a long range two-body interaction if periodic boundary conditions are used. Generalizing the procedure described above one linearizes around both Fermi points \( \pm k_F \). Then the Bose operators corresponding to Eq. (33) are the two contributions to \( \alpha \)

where the function \( h \) is defined as

\[
F \left[ \frac{l \pi}{L}, \frac{m \pi}{L} \right] = \sum_{l=-\infty}^{\infty} e^{ilv c_l},
\]

(45)

It is periodic in \( v \) with period \( 2 \pi \). Using the arguments presented following Eq. (41) the bosonized form of \( \psi^\dagger(u)\psi(v) \) reads

\[
\psi^\dagger(u)\psi(v) = G_N(u,v)e^{-i(\phi(u) - \phi(v))}e^{-i(\phi^0)};
\]

(46)

and the auxiliary field operator \( \phi(u) \) is given by

\[
\phi(u) = -i \sum_{n=1}^{\infty} \frac{e^{inu}}{\sqrt{n}} b_n,
\]

(47)

and \( G_N(u,v) \) is a so far undetermined function of the particle number operator. As the Fermi sea with \( N \) fermions in addition to the Dirac sea is the vacuum state for the bosons, i.e. \( b_l|F(N)\rangle = 0 \), the expectation value of the product of the exponentials in Eq. (46) in the Fermi sea equals one and yields

\[
G_N(u,v) = \langle F(N)|\psi^\dagger(u)\psi(v)|F(N)\rangle,
\]

(48)

which can be calculated in the fermionic picture using the definition Eq. (45) and \( \left< F(N)|c_l^\dagger c_l|F(N)\right> = \delta_{k,l}\Theta(N - l) \), where \( \Theta(x) \) is the step function (\( \Theta(0) = 1 \))

\[
G_N(u,v) = \sum_{l=-\infty}^{\infty} e^{il(u-v)},
\]

(49)

In the second equality we have added an infinitesimal imaginary shift in \( u - v \) in order to make the formal sum convergent. This is a typical example of the problems with the infinite Dirac sea.

After the bosonization of \( \psi^\dagger(u)\psi(v) \) is completed, which actually is simpler than the bosonization of a single field operator as no additional operators changing the fermion number have to be introduced, we can come to our application of calculating the canonical expectation value of \( c^\dagger_m c_m \). If we denote the canonical average of an
operator $A$ in a state with $N$ fermions in addition to the Dirac sea by $\langle A \rangle_{N,T}$ we obtain with the Bose function $b(x) = (e^x - 1)^{-1}$

$$\langle \psi^\dagger(u)\psi(v) \rangle_{N,T} = G_N(u, v) \times \exp \left\{ \sum_{n=1}^{\infty} \left( 2 \cos [n(u - v)] - 2 \right) \frac{b(n\Delta b)}{n} \right\}. \quad (50)$$

Here we have used the formula $\langle e^{A}e^{B} \rangle = e^{\frac{i}{2}B}e^{A^2+2AB+B^2}$ for a canonical expectation value for free bosons which was proved by Mermin in “one sentence”. It is valid for operators $A$ and $B$ which are linear in the boson creation and annihilation operators. To calculate the expectation value of the occupancies we need the inversion formula to Eq. (45)

$$c_{l} = \frac{1}{2\pi} \int_{0}^{2\pi} e^{-i\nu l} \psi(v) dv. \quad (51)$$

As the rhs of Eq. (50) is a function of $u - v$ only one integration can be performed and one obtains

$$\langle c_{N+m}c_{N+m} \rangle_{N,T} = \frac{1}{2\pi} \int_{0}^{2\pi} e^{-i\nu (m+N)} \times \langle \psi^\dagger(u)\psi(0) \rangle_{N,T}. \quad (52)$$

In order to analytically perform the remaining integration in Eq. (52) we expand $\langle \psi^\dagger(u)\psi(0) \rangle$ in a Laurent series in $z \equiv \exp{(iu)}$

$$\langle \psi^\dagger(u)\psi(0) \rangle_{N,T} = e^{iuN} \sum_{n=-\infty}^{\infty} d_{n} e^{iun}, \quad (53)$$

where the coefficients $d_{n}$ can be calculated recursively as discussed in the appendix. Using the notation of section IV we finally obtain

$$\langle \hat{n}_{N+F+m} \rangle_{c,T} = d_{m}. \quad (54)$$

For all values of $\tau$ for which the calculation of $\langle \hat{n}_{m} \rangle_{c,T}$ using Eq. (31) is numerically feasible (e.g. $\tau = 3$ in Fig. 6), the results using Eqs. (31) and (54) are identical. As mentioned in the introduction the result of the present section which used Eq. (46) as the essential ingredient is very close in spirit to the calculation of the occupancies of the interacting TL-model.

**SUMMARY**

This paper intended to serve a dual purpose. First to explain in terms as simple as possible the concept of bosonization which plays the essential role in the Luttinger liquid picture of interacting fermions in one dimension. We only shortly discussed interacting electrons, but every reader who followed the algebra of section V should have no problem understanding e.g. the calculation of the occupancies in the interacting case. As an application of the concepts we presented results for the microcanonical and the canonical ensemble for noninteracting fermions. The comparison of our results with the standard textbook grand canonical results can serve as a rare explicit example for the general arguments concerning the equivalence of the three ensembles in the thermodynamic limit.
APPENDIX A:

In this appendix we present the method to obtain the coefficients $d_m$ of the Laurent series in Eq. (53) which determine the canonical occupation numbers $\langle n_{nF+m} \rangle_{c,T}$. According to Eqs. (49) and (50) we can write

$$\langle \psi^\dagger (u)\psi (0) \rangle_{N,T} = e^{iN\mu} \left\{ \sum_{l=0}^{\infty} z^{-l} \right\}$$

$$\times \exp \{ f(z) + f(1/z) - 2f(1) \}, \quad (A1)$$

where $z = \exp (iu)$ and the function $f(z)$ is given by

$$f(z) = \sum_{n=1}^{\infty} \frac{b(n/\tau)}{n} z^n. \quad (A2)$$

The geometric series Eq. (A1) is considered as a formal power series. The first step is to determine the coefficients of the power series of the function

$$F(z) = e^{f(z)} = \sum_{m=0}^{\infty} c_m z^m. \quad (A3)$$

Using $F'(z) = f'(z)F(z)$ and $c_0 = 1$ one can obtain recursion relations for $m \geq 1$

$$c_m = \frac{1}{m} \sum_{l=1}^{m} b(l/\tau)c_{m-l}. \quad (A4)$$

The next step is to write the last factor in Eq. (A1) as a Laurent series

$$F(z)F(1/z)/[F(1)]^2 \equiv \sum_{l=-\infty}^{\infty} a_l z^l. \quad (A5)$$

By comparing coefficients one obtains using Eqs. (A2) and (A3)

$$a_l = \exp \left\{ -2 \sum_{n=0}^{\infty} \frac{b(n/\tau)}{n} \right\} \sum_{m=0}^{\infty} c_m c_{m+l} = a_{-l}. \quad (A6)$$

As for fixed $\tau$ the $c_m$ go to zero exponentially for large $m$ the infinite sum converges well. In the last step we have to multiply the Laurent series in Eq. (A5) with the geometric series in Eq. (A1). This yields with Eqs. (53) and (54)

$$d_m = \sum_{n=0}^{\infty} a_{n+m} = \langle n_{nF+m} \rangle_{c,T}. \quad (A7)$$

The numerical evaluation of the canonical occupation numbers with this method is possible for much higher temperatures than via Eq. (31).
called “Schur’s Lemma”, see e.g. M. Tinkham, *Group Theory and Quantum Mechanics* (MacGraw-Hill, New York, 1964)

24 N. D. Mermin, “A short simple evaluation of expressions of the Debye-Waller form,” J. Math. Phys. 7, 1038 (1966)