Grassmann Algebra and Fermions at Finite Temperature

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Abstract

For any \(d\)-dimensional self-interacting fermionic model, all coefficients in the high-temperature expansion of its grand canonical partition function can be put in terms of multivariable Grassmann integrals. A new approach to calculate such coefficients, based on direct exploitation of the grassmannian nature of fermionic operators, is presented. We apply the method to the soluble Hatsugai-Kohmoto model, reobtaining well-known results.

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1 Introduction

A quantum system at thermal equilibrium can be completely described provided that one knows its grand canonical partition function, which can be expressed as a path integral. For bosonic systems, an advantageous feature of the path integral approach is that of employing commuting functions instead of non-commuting operators. For fermionic systems, however, such an advantage is not obvious to hold, as the integration variables are also non-commuting.

In 1980, Kubo[1] used the path integral approach to calculate the grand canonical partition function of the Hubbard model, using the strong coupling limit and performing a perturbative expansion in the hopping constant ($t$). Even though his result is valid for any temperature, one does not have the exact coefficient of $\beta$ ($\beta = \frac{1}{kT}$) of the high temperature expansion of the partition function. Since then, improvements on the calculation of the high temperature expansion up to order $(\beta t)^9$ for the Hubbard model in two and three dimensions have been reported in the literature [2].

Recently, Grandati et al.[3] presented a method to calculate the grand canonical partition function of self-interacting fermions, by writing that function on a lattice and using the properties of the Grassmann algebra to calculate its expansion in powers of the coupling constant. They calculated the first two terms for the bi-dimensional chiral Gross-Neveu model, obtaining an analytical result; however, their approach is model-dependent. More recently, Creutz[4] used a numerical algorithm to calculate the generating functional of a fermionic model, rewritten on a lattice. He applied his algorithm to a unidimensional fermionic system involving a thousand grassmannian variables. He pointed out that this approach does not have the sign problems that generally hamper the application of the Monte Carlo method to fermionic models.

We do not write the grand canonical partition function of a self-interacting fermionic model on a lattice; instead, we present a new method to obtain the coefficients of its high temperature expansion in $d$-dimensions, where $d \geq 1$. But for the expansion in $\beta$, this method does not involve any other perturbative expansion (such as, say, in the coupling constant of the model). In section 2 we present the method, an extension to the one used to calculate the grand canonical partition function of the anharmonic fermionic oscillator[5], a quantum model in $d = 0$ space-dimension. In reference [6], the properties of the Grassmann algebra were used to calculate the moments of grassmannian gaussian integrals. This general result, together with the diagonalization of matrices $A^\sigma (\sigma = \uparrow, \downarrow)$ — matrices that appear when the trace of any fermionic operator is expressed in terms of a
multivariable Grassmann integral (see eq.(9)) — allows us to develop a general approach to obtain analytical expressions for the coefficients of the high temperature expansion of the grand canonical partition function of any self-interacting fermioning model in $d$-dimensions, even in the thermodynamical limit. In section 3 we apply the method to Hatsugai-Kohmoto model, a simple toy model that was used by Hatsugai and Kohmoto to explain the metal-insulator transition. The solution of this model is very simple, and does not require all of the features developed in section 2. In section 4 we present our conclusions and future applications of the present approach. In appendix A, the diagonalization of the matrices $A^{\sigma\sigma}$, for arbitrary lattice dimension and arbitrary number of points in the lattice, is described.

2 Expansion in the High Temperature Limit and the Grassmann Multivariable Integrals

The grand canonical partition function of any quantum system in the high temperature limit can be expanded in terms of $\beta$ as

\[
Z(\beta; \mu) = \text{Tr}(e^{-\beta K}) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \text{Tr}[K^n] \beta^n,
\]

where $K$ is given by

\[
K = H - \mu N,
\]

$H$ is the hamiltonian of the system, $\mu$ is the chemical potential and $N$ is the total number of particles operator.

The fermionic creation ($a_i^\dagger$) and destruction ($a_j$) operators can be mapped into generators of the Grassmann algebra $\{\bar{\eta}_i, \eta_j\}$ as follows:

\[
a_i^\dagger \rightarrow \bar{\eta}_i \quad \text{and} \quad a_j \rightarrow \frac{\partial}{\partial \bar{\eta}_j},
\]

where $i, j = 1, 2, \cdots, \mathcal{N}$. The generators of this Grassmann algebra of dimension $2^{2\mathcal{N}}$, written explicitly as $\{\bar{\eta}_1, \cdots, \bar{\eta}_{\mathcal{N}}; \eta_1, \cdots, \eta_{\mathcal{N}}\}$, satisfy the following anti-commutation relations:
The trace of any normal-ordered fermionic operator $O$ is
\[
\text{Tr}[O] = \int \prod_{i=1}^{N} d\eta_i d\bar{\eta}_i \ O^\circledast(\bar{\eta}, \eta) \ e^{\sum_{j=1}^{N} 2\bar{\eta}_j \eta_j},
\]
(5)
where we use the shorthand notation: $\bar{\eta} \equiv \{\bar{\eta}_1, \cdots, \bar{\eta}_N\}$ and $\eta \equiv \{\eta_1, \cdots, \eta_N\}$, and $O^\circledast(\bar{\eta}, \eta)$ is the kernel of the fermionic operator $O$ in the normal order. (By “normal ordered operator” we mean an operator in which all destruction operators are to placed to the right of all creation operators.) Naively, it can be said that the Grassmannian function $O^\circledast(\bar{\eta}, \eta)$ is obtained by replacing $a_i^\dagger \rightarrow \bar{\eta}_i$ and $a_i \rightarrow \eta_i$ in operator $O$. [5, 7, 10].

Let us consider from now on the case where the creation and destruction operators are characterized by the indices $(\vec{\ell}; \sigma)$, where $\vec{\ell}$ is a $d$-dimensional lattice vector $(d = 1, 2, 3, \cdots)$ and $\sigma$ is the spin component. The components of vector $\vec{\ell}$ need not to be orthogonal. This lattice vector could equally represent either the space vector $\vec{x}$ or the momentum vector $\vec{k}$. If the fermionic operator $O$ is a product of $n$ normal ordered fermionic operators $Q$, we have [5, 7, 10]

\[
\text{Tr}[Q^n] = \int \prod_{\vec{\ell}} \prod_{\sigma=\pm 1} \prod_{\alpha=0}^{n-1} d\eta_\sigma(\vec{\ell}; \alpha)d\bar{\eta}_\sigma(\vec{\ell}, \alpha) \ e^{\sum_{\nu=0}^{n-1} \bar{\eta}_\sigma(\vec{\ell}; \nu)[\eta_\sigma(\vec{\ell}; \nu) - \eta_\sigma(\vec{\ell}; \nu+1)]} \times
\]
\[
\times Q^\circledast(\bar{\eta}_\sigma(\vec{\ell}; 0), \eta_\sigma(\vec{\ell}; 0)) \ Q^\circledast(\bar{\eta}_\sigma(\vec{\ell}; 1), \eta_\sigma(\vec{\ell}; 1)) \times \cdots \times Q^\circledast(\bar{\eta}_\sigma(\vec{\ell}; n-1), \eta_\sigma(\vec{\ell}; n-1)).
\]
(6)
where we define $\sigma = \uparrow \equiv +1, \downarrow \equiv -1$. The Grassmann variables in eq.(6) satisfy the boundary conditions
\[
\eta_\sigma(\vec{\ell}; n) = -\eta_\sigma(\vec{\ell}; 0) \quad \text{and} \quad \eta_\sigma(\vec{\ell}; \nu) = 0, \quad \text{for} \quad \nu > n,
\]
(7)
with $\sigma = \pm 1$ and $\vec{\ell}$ stands for any vector on the lattice. Eq.(6) is still valid for a product of $n$ ordered ordered operators, not necessarily equal.

Relation (6) is used to write the terms of the expansion of the grand canonical partition function in the high temperature limit as multivariable Grassmann integrals. For a $d$-dimensional fermionic model, the coefficients of the expansion $Z(\beta, \mu)$ in eq.(1) become
\[
\text{Tr}[K^n] = \int \prod_{\vec{\ell}} \prod_{\sigma = \pm 1} \prod_{\alpha = 0}^{n-1} d\eta_\sigma(\vec{\ell}; \alpha) d\bar{\eta}_\sigma(\vec{\ell}; \alpha) e^{\sum_{\vec{\ell}} \sum_{\sigma = \pm 1} \sum_{\nu = 0}^{n-1} \eta_\sigma(\vec{\ell}; \nu)[\eta_\sigma(\vec{\ell}; \nu - \eta_\sigma(\vec{\ell}; \nu + 1)]}
\times
\times K^\oplus(\eta_\sigma(\vec{\ell}; 0), \eta_\sigma(\vec{\ell}; 0)) K^\oplus(\bar{\eta}_\sigma(\vec{\ell}; 1), \eta_\sigma(\vec{\ell}; 1)) \times \cdots \times K^\oplus(\eta_\sigma(\vec{\ell}; n-1), \eta_\sigma(\vec{\ell}; n-1)),
\]

(8)

the boundary conditions (7) still hold for the generators \(\eta_\sigma(\vec{\ell}; \nu)\).

It is much easier to handle generators with one index, then we map the generators \(\eta_\sigma(\vec{\ell}, \nu)\) and \(\bar{\eta}_\sigma(\vec{\ell}, \nu)\) into single-indexed anti-commuting variables. The sum in the exponential on the r.h.s. of eq.(8) can be written as

\[
\sum_{\vec{\ell}} \sum_{\sigma = \pm 1} \sum_{\nu = 0}^{n-1} \bar{\eta}_\sigma(\vec{\ell}; \nu)[\eta_\sigma(\vec{\ell}; \nu) - \eta_\sigma(\vec{\ell}; \nu + 1)] = \equiv \sum_{I,J=1}^{2nN^d} \bar{\eta}_I A_{IJ} \eta_J.
\]

(9)

Note that the argument of the exponential on the r.h.s. of eq.(8) is diagonal in the indices \(\vec{\ell}\) and \(\sigma\). Having the components of the column vector \(\eta_J\) (or the line vector \(\bar{\eta}\)) grouped according to the values of \(\sigma\), and then each subset ordered according to \(\nu\), and finally each subsubset ordered according to \(\vec{\ell}\), the matrix \(A\) will have the block-structure

\[
A = \begin{pmatrix} A^{\uparrow \uparrow} & 0 \\ 0 & A^{\downarrow \downarrow} \end{pmatrix},
\]

(10)

whose entries are matrices of dimension \(nN^d \times nN^d\) and \(d\) is the dimension of the vector \(\vec{\ell}\).

The indices \(I, J\) are such that \(I, J = 1, 2, \cdots, 2nN^d\), where \(N^d\) is the number of points in the lattice. The matrices \(A^{\uparrow \uparrow}\) and \(A^{\downarrow \downarrow}\) are identical. Taking into account the anti-periodic condition in temperature (7) in eq.(9), the matrices \(A^{\sigma \sigma}\), where \(\sigma = \uparrow, \downarrow\), are found to have the following block-structure:

\[
A^{\uparrow \uparrow} = A^{\downarrow \downarrow} = \begin{pmatrix} 1_{N^d \times N^d} & -1_{N^d \times N^d} & 0_{N^d \times N^d} & \cdots & 0_{N^d \times N^d} \\ 0_{N^d \times N^d} & 1_{N^d \times N^d} & -1_{N^d \times N^d} & \cdots & 0_{N^d \times N^d} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1_{N^d \times N^d} & 0_{N^d \times N^d} & 0_{N^d \times N^d} & \cdots & 1_{N^d \times N^d} \end{pmatrix},
\]

(11)
The symbols \( \mathbb{1}_{N^d \times N^d} \) and \( \mathbf{0}_{N^d \times N^d} \) stand for the identity and null matrices of dimension \( N^d \times N^d \), respectively. Any lattice vector \( \vec{\ell} \) can be written as
\[
\vec{\ell} = \ell_1 \vec{u}_1 + \ell_2 \vec{u}_2 + \cdots + \ell_d \vec{u}_d,
\]
where \( \ell_i = 1, 2, \ldots, N \) \((i = 1, 2, \ldots, d)\), and \( N \) is the number of points in the lattice in the direction of the \( d \)-dimensional basis vector \( \vec{u}_i \). A particular basis for which \( A^{\sigma \sigma} \) has the block-form shown in (11), yields the following mapping
\[
\eta_\sigma(\vec{\ell}; \nu) \longrightarrow \eta_{[\ell_1 + (\ell_2 - 2)N + \cdots + (\ell_d - 1)N^{(d-1)} + \nu]N^d}.
\]
The generators \( \bar{\eta}_\sigma(\vec{\ell}; \nu) \) have an analogous mapping. With the newly indexed generators, the expression of \( \text{Tr}[K^n] \) (eq.(8)) becomes,
\[
\text{Tr}[K^n] = \int \prod_{I=1}^{2nN^d} d\eta_I d\bar{\eta}_I e^{i \sum_{I,j=1}^{2nN^d} A_\sigma^{\upsilon \sigma} \eta_I \bar{\eta}_j} \times K^{\circ\circ}(\bar{\eta}, \eta; \nu = 0) K^{\circ\circ}(\bar{\eta}, \eta; \nu = 1) \cdots K^{\circ\circ}(\bar{\eta}, \eta; \nu = n - 1). \tag{14}
\]

Note that expression (14), up to the constant \( -\frac{1}{n!} \), is the coefficient at order \( \beta^n \) of the expansion in the high-temperature limit of the grand canonical partition function for any self-interacting fermionic model. The specific model to be studied is represented by the Grassmannian function \( K^{\circ\circ} \), but the matrix \( A \) is the same for all fermionic models. Once the sub-matrices \( A^{\uparrow \downarrow} \) and \( A^{\downarrow \uparrow} \) are null, the multivariable integral (14) is equal to the product of the contributions coming from the sectors: \( \sigma \sigma = \uparrow \uparrow \) and \( \sigma \sigma = \downarrow \downarrow \) separately. The Grassmann functions \( K^{\circ\circ} \) are polynomials in the generators of the algebra. Therefore, the r.h.s. of eq.(14) are moments of the multivariable Grassmann Gaussian integrals. In reference [6] it is shown that these integrals can be written as co-factors of the matrix \( A \).

The integrals in eq.(14), for sector \( \sigma \sigma = \uparrow \uparrow \), have the form:
\[
M(L, K) = \int \prod_{i=1}^{nN^d} d\eta_i d\bar{\eta}_i \eta_{l_1} \eta_{k_1} \cdots \eta_{l_m} \eta_{k_m} e^{i \sum_{j=1}^{nN^d} \bar{\eta}_j A_{\upsilon \sigma}^{\upsilon \sigma} \eta_j}, \tag{15}
\]
with \( L = \{l_1, \ldots, l_m\} \) and \( K = \{k_1, \ldots, k_m\} \). The products \( \bar{\eta}_j \eta_j \) are ordered in such a way that \( l_1 < l_2 < \cdots < l_m \) and \( k_1 < k_2 < \cdots < k_m \). From reference [6], the result of this type of integrals is equal to:
\[
M(L, K) = (-1)^{(l_1 + l_2 + \cdots + l_m) + (k_1 + k_2 + \cdots + k_m)} A(L, K), \tag{16}
\]
where \( A(L, K) \) is the determinant of the matrix obtained from matrix \( A^{\uparrow\uparrow} \) by deleting the lines \( \{l_1, \cdots, l_m\} \) and the columns \( \{k_1, \cdots, k_m\} \). \( M(L, K) \) is a co-factor of matrix \( A^{\uparrow\uparrow} \). The Grassmann integrals to be calculated in sector \( \downarrow\downarrow \) are the same type as eq. (15).

Evaluating determinants of non-diagonal matrices of dimension \( nN^d \times nN^d \) is still a hard task, even if we have restricted ourselves to multivariable integrals of a fixed sector \( \sigma\sigma \). Calculating such determinants is a suitable task for computers, and it obviously depends on hardware and software resources. Fixing \( n \), for instance, there is an upper practical limit for \( N \), so that the calculation of determinants is feasible. One possibility for evaluating eq. (14) is that of assigning different values for \( N \) and, from the results obtained, trying to extrapolate for an arbitrary value of \( N \). If we are lucky, some recursion expression for eq. (14) for all \( N \), could be recognized.

Our approach to calculate the integral (15) is, for fixed \( n \) and arbitrary \( N \), to explore the block-structure of matrices \( A^{\sigma\sigma} \), \( \sigma = \uparrow \) and \( \sigma = \downarrow \), diagonalizing it through a similarity transformation

\[
P^{-1} A^{\sigma\sigma} P = D,
\]

where the matrix \( D \) is,

\[
D = \begin{pmatrix}
\lambda_1 1_{N^d \times N^d} & \Phi_{N^d \times N^d} & \cdots & \Phi_{N^d \times N^d} \\
\Phi_{N^d \times N^d} & \lambda_2 1_{N^d \times N^d} & \cdots & \Phi_{N^d \times N^d} \\
\vdots & \vdots & \ddots & \vdots \\
\Phi_{N^d \times N^d} & \Phi_{N^d \times N^d} & \cdots & \lambda_n 1_{N^d \times N^d}
\end{pmatrix},
\]

\( \lambda_i, i = 1, 2, \cdots, n \), are the eigenvalues of matrices \( A^{\sigma\sigma} \), \( \sigma = \uparrow, \downarrow \), and calculate the co-factors of the matrix \( D \). The \( j^{th} \)-column of matrix \( P \) is the eigenvector of \( A^{\sigma\sigma} \) associated to the eigenvalue \( \lambda_j \). Each eigenvalue of matrix \( A^{\sigma\sigma} \) has degeneracy \( N^d \). The matrices are not hermitian, thus some eigenvalues are complex. In the following, we will be working on the \( \sigma\sigma = \uparrow\uparrow \) sector; however, the results for the \( \sigma\sigma = \downarrow\downarrow \) sector are analogous since \( A^{\uparrow\uparrow} = A^{\downarrow\downarrow} \).

We will apply the following transformation of variables,

\[
\eta' = P^{-1} \eta \quad \text{and} \quad \bar{\eta}' = \bar{\eta} P,
\]

where \( \eta' \equiv \{\eta_1', \cdots, \eta_{nN^d}'\} \) and \( \bar{\eta}' \equiv \{\bar{\eta}_1', \cdots, \bar{\eta}_{nN^d}'\} \). The jacobian of the transformation (19) is equal to one.

Due to the fact that \( A^{\uparrow\uparrow} \) is a block-matrix, the matrix \( P \) also has
a block structure. This fact implies that transformations (19) do not mix up lattice indices.

In a schematic way, the integrals $M(L, K)$ (eq.(15)) become:

$$M(L, K) = \int \prod_{i=1}^{nN^d} d\eta_i d\bar{\eta}_i \overline{(\eta P^{-1})_{i_1} (P \eta)_{k_1} \cdots (\bar{\eta} P^{-1})_{l_m} (P \eta)_{k_m}} \sum_{i,j=1}^{nN^d} \tilde{\eta}_i \tilde{D}_{ij} \eta_j,$$  \hspace{1cm} (20)

where $D_{ij}$ are the entries of the diagonal matrix $D$. The expression $M(L, K)$ fits into the form of eq.(13), and hence corresponds to some co-factor of the diagonalized matrix $D$ (eq.(16)). It is very simple to calculate these co-factors, and the matrix $P$ is the same for any self-interacting fermionic model.

In Appendix A we present the derivation of the eigenvalues and eigenvectors of matrix $D$ for arbitrary values of $n$ and $N$. From eqs. (65) and (66), for arbitrary value of $n$, we have that

$$p^{(n)}_{\nu\nu'} = \frac{1}{\sqrt{n}} e^{\frac{i\pi}{n}(2\nu'+1)(\nu+1)},$$ \hspace{1cm} (21)

and

$$q^{(n)}_{\nu\nu'} = \frac{1}{\sqrt{n}} e^{-\frac{i\pi}{n}(2\nu'+1)(\nu+1)},$$ \hspace{1cm} (22)

with $\nu, \nu' = 0, 1, \cdots, n-1$, and

$$P = \begin{pmatrix} p^{(n)}_{00} \mathbb{1}_{N^d \times N^d} & \cdots & p^{(n)}_{0,n-1} \mathbb{1}_{N^d \times N^d} \\ \vdots & \ddots & \vdots \\ p^{(n)}_{n-1,0} \mathbb{1}_{N^d \times N^d} & \cdots & p^{(n)}_{n-1,n-1} \mathbb{1}_{N^d \times N^d} \end{pmatrix},$$ \hspace{1cm} (23)

and

$$P^{-1} = \begin{pmatrix} q^{(n)}_{00} \mathbb{1}_{N^d \times N^d} & \cdots & q^{(n)}_{0,n-1} \mathbb{1}_{N^d \times N^d} \\ \vdots & \ddots & \vdots \\ q^{(n)}_{n-1,0} \mathbb{1}_{N^d \times N^d} & \cdots & q^{(n)}_{n-1,n-1} \mathbb{1}_{N^d \times N^d} \end{pmatrix}.$$ \hspace{1cm} (24)

The diagonal elements of matrix $D$ are:

$$\lambda^{(n)}_\nu = 1 - e^{\frac{i\pi}{n}(2\nu'+1)}, \hspace{1cm} \nu = 0, 1, \cdots, n-1.$$ \hspace{1cm} (25)

where the eigenvalues are $N^d$-fold degenerated, $N^d$ being the number of lattice sites. Due to lattice translation symmetry, we should note that the elements $p^{(n)}_{\nu\nu'}$ and $q^{(n)}_{\nu\nu'}$ do not carry any lattice site index.
This is a general approach, and it can be applied to any self-interacting fermionic model. The important point here is that the relations (21)-(25) are valid for any self-interacting fermionic model with space translation symmetry.

3 Application to Hatsugai-Kohmoto Model

The calculation of an exactly soluble model is a nice way to test a new approach. Hatsugai and Kohmoto\cite{10} proposed a toy model (HK model) that shares the atomic and band limits of the Hubbard model\cite{11}. Using the Green function and path integral approaches, Nogueira and Anda\cite{12} established the equivalence of this model (with unrestricted hopping) and the Hubbard model (with infinite-range hopping).

In this section we derive the grand canonical partition function of the HK model using the results presented in section 2. The Hamiltonian of the HK model in momentum space is\cite{12}

\[
H = \sum_{\vec{k}} \sum_{\sigma=\uparrow,\downarrow} \varepsilon(\vec{k}) n_{\sigma}(\vec{k}) + U \sum_{\vec{k}} n_{\uparrow}(\vec{k}) n_{\downarrow}(\vec{k})
\equiv \sum_{\vec{k}} H(\vec{k}), \quad (26)
\]

where \(n_{\sigma}(\vec{k}) \equiv a_{\sigma}^{\dagger}(\vec{k}) a_{\sigma}(\vec{k})\) and \(a_{\sigma}^{\dagger}(\vec{k})\) (\(a_{\sigma}(\vec{k})\)) is the creation (destruction) operator of an electron with momentum \(\vec{k}\) and spin \(\sigma\). The function \(\varepsilon(\vec{k}) = -2t \sum_{i=1}^{3} \cos k_i\), \(\vec{k} = (k_1, k_2, k_3)\), corresponds to the nearest hopping of the electrons in the dual-space lattice. \(U\) is the strength of the repulsion between electrons with the same momentum \(\vec{k}\) but opposite spin components.

From eqs. (1) and (26), the grand canonical partition function of the HK model is

\[
Z(\beta; \mu) = Tr \left[ \prod_{\vec{k}} e^{-\beta K(\vec{k})} \right] = \prod_{\vec{k}} \left[ Tr_{\vec{k}} e^{-\beta K(\vec{k})} \right]. \quad (27)
\]

We have

\[
K(\vec{k}) = \sum_{\sigma=\uparrow,\downarrow} \Delta(\vec{k}) n_{\sigma}(\vec{k}) + U n_{\uparrow}(\vec{k}) n_{\downarrow}(\vec{k}), \quad (28)
\]
where we define: $\Delta(\vec{k}) \equiv \varepsilon(\vec{k}) - \mu$, and $\mu$ is the chemical potential. In eq.(27), the symbol $Tr_{\vec{k}}$ stands for the trace for a fixed vector $\vec{k}$, whereas $Tr$ represents the trace for all $\vec{k}$'s.

The high temperature expansion for the grand canonical partition function $Z(\beta; \mu)$ is

$$Tr_{\vec{k}}[e^{-\beta \mathbf{K}(\vec{k})}] = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \beta^n Tr_{\vec{k}}[\mathbf{K}^n(\vec{k})].$$

(29)

Since all the operators on the r.h.s. of eq.(28) commute, we can apply the Newton’s multinomial expression to write $Tr_{\vec{k}}[\mathbf{K}^n(\vec{k})]$ as

$$Tr_{\vec{k}}[\mathbf{K}^n(\vec{k})] = \sum_{n_1,n_2,n_3=0}^{n} \frac{n!}{n_1!n_2!n_3!} \Delta^{n_1+n_2+n_3}(\vec{k}) U^{n_3} Tr_{\vec{k}}[\mathbf{n}^{n_1+n_3}(\vec{k}) \mathbf{n}^{n_2+n_3}(\vec{k})].$$

(30)

The symbol $\sum'$ means that the summation indices satisfy the condition $n_1 + n_2 + n_3 = n$.

Let $l_1$, $l_2$ and $l_3$ be the integers that determine the lattice vector $\vec{k}$. The mapping (13) takes the index $\vec{k}$ into the index $L \equiv l_1 + (l_2 - 1)N + (l_3 - 1)N^2$, where $N$ is the number of points in the momentum lattice in each direction. In the sum on the r.h.s. of eq.(30), we calculate the trace for a fixed $\vec{k}$, which means that in eq.(6) we take a single point in the momentum lattice ($N = 1$). Then,

$$Tr_{\vec{k}}[\mathbf{n}^{n_1+n_3}(\vec{k}) \mathbf{n}^{n_2+n_3}(\vec{k})] = T_{n_1,n_3}^{\uparrow \uparrow} \times T_{n_2,n_3}^{\downarrow \downarrow},$$

(31)

where

$$T_{n_1,n_3}^{\uparrow \uparrow} \equiv \int \prod_{I=1}^{n} d\eta_I(L) d\bar{\eta}_I(L) \sum_{J=1}^{n} \bar{\eta}_I(L) A_{ij}^{\uparrow \uparrow} J \eta_J(L) \times \bar{\eta}_0(L) \bar{\eta}_0(L) \cdots \bar{\eta}_{n_1-1}(L) \bar{\eta}_{n_1-1}(L) \bar{\eta}_{n_1+n_2}(L) \eta_{n_1+n_2}(L) \cdots \bar{\eta}_{n-1}(L) \eta_{n-1}(L),$$

(32)

and

$$T_{n_2,n_3}^{\downarrow \downarrow} \equiv \int \prod_{J=n+1}^{2n} d\eta_J(L) d\bar{\eta}_J(L) \sum_{J=1}^{2n} \bar{\eta}_J(L) A_{ij}^{\downarrow \downarrow} J \eta_J(L) \times \bar{\eta}_{n+n_1}(L) \eta_{n+n_1}(L) \cdots \bar{\eta}_{n+n_1+n_2-1}(L) \eta_{n+n_1+n_2-1}(L) \times \bar{\eta}_{n+n_1+n_2}(L) \eta_{n+n_1+n_2}(L) \cdots \bar{\eta}_{2n-1}(L) \eta_{2n-1}(L).$$

(33)

The matrices $\mathbf{A}^{\sigma \sigma}$, $\sigma = \uparrow, \downarrow$, are given by eq.(11) with $N = 1$. According to eqs. (13) and (14), the presence of $\bar{\eta}$’s (and $\eta$’s) in the integrand on the r.h.s. of eqs. (32) and (33) allows one to evaluate the integrals as the determinants of matrices obtained after deletion of lines (and columns) of the matrices $\mathbf{A}^{\sigma \sigma}$, $\sigma = \uparrow, \downarrow$. For this particular model, it
turns out easier to apply eq. (14) directly, rather than using the similarity transformation (17), since the lattice is unidimensional. We should mention that for $N = 1$, we recover the case of the anharmonic fermionic oscillator, which has been considered in a previous work [5]. Now we discuss the values of $I^{↑↑}_{n_1,n_3}$ (eq. (32)), in view of the possible values of the indices $(n_1, n_2, n_3)$.

i) $n_1 = n$, $n_2 = 0$ and $n_3 = 0$.

In this case the first $n$ lines and the first $n$ columns of matrix $A^{↑↑}$ are deleted; hence,

$$I^{↑↑}_{n,0} = 1.$$  \hspace{1cm} (34)

ii) $n_1 = 0$, $n_2 = n$ and $n_3 = 0$.

In this case no lines or columns are deleted in $A^{↑↑}$; so,

$$I^{↑↑}_{0,n} = \det(A^{↑↑}) = 2.$$  \hspace{1cm} (35)

iii) $n_1 = 0$, $n_2 = 0$ and $n_3 = n$.

This case is equal to case i and therefore

$$I^{↑↑}_{0,n} = 1.$$  \hspace{1cm} (36)

iv) $n_1 \neq 0$, $n_2 \neq 0$ and $n_3 \neq 0$.

In this case, the first $n_1$ lines and columns are deleted, as well as the last $n_3$ lines and columns of matrix $A^{↑↑}$. The triangular matrix thus obtained has its determinant equal to 1, for any value of $n$. Then,

$$I^{↑↑}_{n_1,n_3} = 1.$$  \hspace{1cm} (37)

Equivalent results are valid for $I^{↑↓}_{n_2,n_3}$.

From the results (34)-(37) and the equivalent results for $I^{↑↓}_{n_2,n_3}$, we have

$$Tr_{\vec{k}}[\sum_{n=0}^{n_1+n_3} (\vec{k}) n^{n_2+n_3}(\vec{k})] = (1 + \delta_{n_1+n_3,0})(1 + \delta_{n_2+n_3,0}),$$  \hspace{1cm} (38)

that substituted in eq. (30) gives

$$Tr_{\vec{k}}[\sum_{n=0}^{n_1+n_3} (\vec{k}) n^{n_2+n_3}(\vec{k})] = [2\Delta(\vec{k}) + U]^n + 2\Delta^n(\vec{k}).$$  \hspace{1cm} (39)

Returning to eqs. (27) and (29), we finally get
\( \mathcal{Z}(\beta; \mu) = \prod_{\vec{k}} \left[ 1 + e^{-\beta(2\Delta(\vec{k})+U)} + 2e^{-\beta\Delta(\vec{k})} \right], \)  

that gives the same free energy density found in reference [12].

4 Conclusions

Calculations involving fermionic fields do demand some extra care, in comparison to the manipulation of bosonic fields. For this reason, fermionic models are usually bosonized, in a strategy designed to avoid the “annoying” fermionic features. However, moments of grassmannian multivariable integrals can be easily calculated, as shown in eqs. (15) and (16). In this paper we have presented a new approach, based on the explicit use of Grassmann algebra properties, to the problem of calculating the coefficients of the high temperature expansion of the grand canonical partition function for any \( d \)-dimensional self-interacting fermionic model \((d = 1, 2, 3, \cdots)\). We have explored the results (15) and (16) and the possibility of performing the similarity transformation (17) for a system with arbitrary dimension \( d \) and arbitrary number of lattice points \( N^d \). It is important to point out that the matrices \( \mathbf{A}^\sigma \) \((\sigma = \uparrow, \downarrow)\) are model-independent; they are solely related to kinetical aspects of the approach. To simplify the notation, we considered that the number of points in each direction of the lattice is the same, but the results derived are still valid if this is not true. The fact that our results are analytical allows us to obtain the thermodynamical limit for any self-interacting fermionic model.

As a simple example of application of the method (that does not explore all of its features, though), we have considered the Hatsugai-Kohmoto model, which is diagonal in momentum space and had been solved by other approaches. We have derived its grand canonical partition function, and obtained the same free energy density found in the literature [12].

The most important features of this method appear when the hamiltonian has non-commuting terms and, consequently, Newton’s multinomial expansion does not apply. Equations (15)-(16) and the similarity transformation (17) then become the keystone of our analytical results. That is the case of the Hubbard model [11]; the grand canonical partition function for the unidimensional version of this model is known in integral form [13]. A closed expression for this function was obtained by Takahashi [13], within certain limits only. By the application of the approach we have presented here, we are currently calculating the coefficients of that partition function, up to order \( \beta^5 \) and for
any value of the parameters of the model, as well for any value of the chemical potential. These calculations will soon be submitted to publication.

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Appendix

A Calculation of Eigenvalues and Eigenvectors of Matrix $A^{\sigma\sigma}$

This appendix is devoted to calculating the eigenvalues and eigenvectors of the matrix $A^{\sigma\sigma}$, defined in eq.(11), as well as determining the matrices $P$ and $P^{-1}$ that diagonalize it (see eq.(17)).

The characteristic equation for $A^{\sigma\sigma}$ is

$$
\text{det}
\begin{pmatrix}
(1 - \lambda) \mathbb{1}_{N^d \times N^d} & -\mathbb{1}_{N^d \times N^d} & \mathbb{O}_{N^d \times N^d} & \cdots & \mathbb{O}_{N^d \times N^d} & \mathbb{O}_{N^d \times N^d} \\
\mathbb{O}_{N^d \times N^d} & (1 - \lambda) \mathbb{1}_{N^d \times N^d} & -\mathbb{1}_{N^d \times N^d} & \cdots & \mathbb{O}_{N^d \times N^d} & \mathbb{O}_{N^d \times N^d} \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
\mathbb{O}_{N^d \times N^d} & \mathbb{O}_{N^d \times N^d} & \mathbb{O}_{N^d \times N^d} & \cdots & (1 - \lambda) \mathbb{1}_{N^d \times N^d} & -\mathbb{1}_{N^d \times N^d} \\
\mathbb{1}_{N^d \times N^d} & \mathbb{O}_{N^d \times N^d} & \mathbb{O}_{N^d \times N^d} & \cdots & \mathbb{O}_{N^d \times N^d} & (1 - \lambda) \mathbb{1}_{N^d \times N^d}
\end{pmatrix} = 0.
$$

(41)

Observe that this matrix (of total dimension $nN^d \times nN^d$), consists of a $n \times n$ block matrix, each block having dimension $N^d \times N^d$. Moreover, these blocks are either null matrices $\mathbb{O}_{N^d \times N^d}$ or proportional to the identity matrix $\mathbb{1}_{N^d \times N^d}$.

We will demonstrate a useful property of the determinant of a block matrix in which all blocks are diagonal, such as the previous matrix. Take a block-matrix $\mathbf{M}$ composed of blocks $\mathbf{B}^{[i,j]}$, namely
\[
M = \begin{pmatrix}
B^{[1,1]} & B^{[1,2]} & \cdots & B^{[1,n]} \\
B^{[2,1]} & B^{[2,2]} & \cdots & B^{[2,n]} \\
\vdots & \vdots & \ddots & \vdots \\
B^{[n,1]} & B^{[n,2]} & \cdots & B^{[n,n]}
\end{pmatrix}
\]

(42)

where each block \(B^{[i,j]}\) is diagonal:

\[
(B^{[i,j]})_{\alpha\beta} = \delta_{\alpha\beta} b^{[i,j]}_{\alpha},
\]

(43)

where \(\alpha, \beta = 1, 2, \ldots, N^d\). (No summation over repeated indices is implied). We define a “determinant-like” matrix function \(F\) upon the blocks \(B^{[i,j]}\) as

\[
F \equiv \sum_{\theta_1, \theta_2, \ldots, \theta_n=1}^{n} \varepsilon_{\theta_1, \theta_2, \ldots, \theta_n} B^{[1,\theta_1]} B^{[2,\theta_2]} \cdots B^{[n,\theta_n]},
\]

(44)

where \(\varepsilon_{\theta_1, \theta_2, \ldots, \theta_n}\) is the Levi-Civita symbol in \(n\)-dimension. Obviously, \(F\) and the blocks \(B^{[i,j]}\) have all the same dimensions, \(N^d \times N^d\). Using eq.(43), we have

\[
F_{ab} = \delta_{a,b} \sum_{\theta_1, \theta_2, \ldots, \theta_n=1}^{n} \varepsilon_{\theta_1, \theta_2, \ldots, \theta_n} (b^{[1,\theta_1]}_a b^{[2,\theta_2]}_a \cdots b^{[n-1,\theta_{n-1}]}_a b^{[n,\theta_n]}_a).
\]

(45)

From eq.(45) and the definition of the determinant, we obtain

\[
det F = det \Gamma_1 \ det \Gamma_2 \ldots det \Gamma_n,
\]

(46)

where we have defined \(n\) matrices \(\Gamma_p\) of dimension \(N^d \times N^d\) as

\[
(\Gamma_p)_{uv} \equiv b^{[u,v]}_p
\]

(47)

so that

\[
det \Gamma_p = \sum_{\omega_1, \omega_2, \ldots, \omega_N=1}^{N} \varepsilon_{\omega_1, \omega_2, \ldots, \omega_N} (b^{[1,\omega_1]}_p b^{[2,\omega_2]}_p \cdots b^{[n-1,\omega_{n-1}]}_p b^{[n,\omega_n]}_p).
\]

(48)

Thus, the evaluation of \(det F\) is equivalent to the evaluation of the determinant of a block matrix \(\Gamma\), defined as

\[
\Gamma \equiv \begin{pmatrix}
\Gamma_1 & \Phi_{N^d \times N^d} & \cdots & \Phi_{N^d \times N^d} \\
\Phi_{N^d \times N^d} & \Gamma_2 & \cdots & \Phi_{N^d \times N^d} \\
\vdots & \vdots & \ddots & \vdots \\
\Phi_{N^d \times N^d} & \Phi_{N^d \times N^d} & \cdots & \Gamma_n
\end{pmatrix}
\]

(49)
However, $\Gamma$ and $M$ only differ by an even number of permutations of lines and columns! More specifically, $M$ can be recovered from $\Gamma$ if we reorder the lines of the latter according to the pattern

$$(1, 2, \ldots, nN^d) \rightarrow (1, N^d + 1, 2N^d + 1, \ldots, (n - 1)N^d + 1,$$

$$2, N^d + 2, 2N^d + 2, \ldots, (n - 1)N^d + 2, \ldots,$$

$$\ldots, N^d - 1, 2N^d - 1, 3N^d - 2, \ldots, nN^d - 1,$$

$$N^d, 2N^d, 3N^d, \ldots, nN^d)$$

(50)

- i.e., the 1st line is left untouched, the 2nd line is replaced by the $(N^d + 1)^{th}$ line, etc.- and then have the columns of the resulting matrix reordered in the same fashion. (The same result is obtained if we reorder columns before lines.) As the total number of permutations is even, we have $\det M = \det \Gamma$. Combining (51), (46) and (44), we finally obtain

$$\det M = \det F = \det\left( \sum_{\theta_1, \theta_2, \ldots, \theta_n = 1}^{n} \varepsilon_{\theta_1, \theta_2, \ldots, \theta_n} B^{[1, \theta_1]} B^{[2, \theta_2]} \ldots B^{[n, \theta_n]} \right)$$

(52)

In conclusion, if the matrix $M$ is composed of diagonal blocks $B^{[i,j]}$, the determinant of $M$ is equal to the determinant of the matrix $F$, defined as a “determinant-like” function upon the blocks $B^{[i,j]}$.

Turning our attention back to eq.(41), we expand the determinant in terms of “cofactors”, based on the last “line” of blocks:

$$\det \left( (-1)^{1+n} I_{N^d \times N^d} (-I_{N^d \times N^d})^{n-1} + (-1)^{n+n} (1 - \lambda) I_{N^d \times N^d} (1 - \lambda)^{n-1} I_{N^d \times N^d}^{-1} \right) = 0$$

(53)

which yields the characteristic equation

$$(1 + (1 - \lambda)^{n}) = 0.$$
where \( k = 0, 1, 2, \ldots, n - 1 \). Observe that if \( \lambda_k \) is an eigenvalue, so is its complex conjugate: \( \lambda_k^* = \lambda_{n-k-1} \). Let us denote by \( V_k \) an eigenvector of \( A^{\sigma \sigma} \) associated to \( \lambda_k \). It has the structure

\[
V_k = \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{pmatrix}
\]

(56)

where each \( v_i, i = 1, 2, \ldots, n \) is a \( 1 \times N^d \) matrix. We obtain

\[
v_i = -(1 - \lambda_k)i \xi, \text{ where } i = 1, \ldots, n - 1
\]

(57)

and \( \xi = v_n \) is an arbitrary column vector of dimension \( N^d \). There are \( N^d \) possible linearly independent choices for \( \xi \), corresponding to \( N^d \) distinct eigenvectors associated to the same eigenvalue \( \lambda_k \). We choose them to be

\[
\xi^{(1)}_k = \begin{pmatrix} -1 \\ 0 \\ \vdots \\ 0 \\ 0 \end{pmatrix}, \quad \xi^{(2)}_k = \begin{pmatrix} 0 \\ -1 \\ \vdots \\ 0 \\ 0 \end{pmatrix}, \quad \ldots, \quad \xi^{(N^d-1)}_k = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ -1 \\ 0 \end{pmatrix}, \quad \xi^{(N^d)}_k = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ -1 \end{pmatrix}
\]

(58)

so that each \( \xi^{(l)}_k \) corresponds to an eigenvector \( V^{(l)}_k \), where \( l = 1, 2, \ldots, N^d \), associated to the eigenvalue \( \lambda_k \).

The matrix \( P \) that diagonalizes \( A^{\sigma \sigma} \) can be obtained by concatenating all eigenvectors \( V^{(l)}_k \) for all eigenvalues \( \lambda_k, k = 0, 1, \ldots, n - 1 \), up to a normalizing factor \( R \):

\[
P = \begin{pmatrix} p^{(n)}_{00} \mathbb{I}_{N^d \times N^d} & \ldots & p^{(n)}_{0,n-1} \mathbb{I}_{N^d \times N^d} \\ \vdots & \ddots & \vdots \\ p^{(n)}_{n-1,0} \mathbb{I}_{N^d \times N^d} & \ldots & p^{(n)}_{n-1,n-1} \mathbb{I}_{N^d \times N^d} \end{pmatrix},
\]

(59)

where

\[
p^{(n)}_{\nu \nu'} = R e^{\frac{c}{N} (2 \nu' + 1) (\nu + 1)},
\]

(60)

with \( \nu, \nu' = 0, 1, \ldots, n - 1 \). The matrix

\[
P^{-1} = \begin{pmatrix} q^{(n)}_{00} \mathbb{I}_{N \times N} & \ldots & q^{(n)}_{0,n-1} \mathbb{I}_{N \times N} \\ \vdots & \ddots & \vdots \\ q^{(n)}_{n-1,0} \mathbb{I}_{N \times N} & \ldots & q^{(n)}_{n-1,n-1} \mathbb{I}_{N \times N} \end{pmatrix},
\]

(61)
where

\[ q^{(n)}_{\nu'\nu} = R' e^{-\frac{i\pi}{n}(2\nu'+1)(\nu+1)}, \]  

is the inverse of \( \mathbf{P} \), upon a suitable choice of \( R \) and \( R' \); i.e,

\[ R = R' = 1/\sqrt{n}, \]  

so that they satisfy the relation

\[ \sum_{\nu=0}^{n-1} p^{(n)}_{\nu\nu'} q^{(n)}_{\nu'\nu} = \delta_{\nu\nu'}. \]  

Hence,

\[ p^{(n)}_{\nu\nu'} = \frac{1}{\sqrt{n}} e^{\frac{i\pi}{n}(2\nu'+1)(\nu+1)} \]  

\[ q^{(n)}_{\nu'\nu} = \frac{1}{\sqrt{n}} e^{-\frac{i\pi}{n}(2\nu'+1)(\nu+1)}. \]

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