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Grassmann variable analysis for dimer problems in two dimensions

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Abstract. We present a new non-combinatorial interpretation for the fermionic nature of the 2D dimer problem. The partition functions of the closed-packed dimer models settled on the most general inhomogeneous rectangular, triangular, and hexagonal lattice nets are obtained as fermionic Gaussian integrals. These Gaussian representations provide the analytic results for the partition functions and dimer–dimer correlations for a variety of regular lattices, and can also be applied to analyse defects, boundary influences, effects of disorder etc, in dimer models.

The dimer model is the archetype for many interesting problems in statistical mechanics and condensed matter physics. The closed-packed dimer model on a proper rectangular lattice was first solved by Kasteleyn [1] and Temperley and Fisher [2]. Besides its importance for the dimer combinatorics itself, this remarkable solution has contributed much to the mathematics of the 2D Ising model and other lattice problems in statistical mechanics [3–5]. The dimer model has found many physical applications. We mention here the connection of the dimer problem on the hexagonal lattice [6] to the commensurate–incommensurate phase transitions due to a domain-wall analogy [7, 8]. This in turn provides us with a solvable model for the Pokrovsky–Talapov transition [9]. A new line of interest arises currently from the RVB theory for high- T_c superconductivity [10], where the dimer model is a structural ingredient used to construct the wavefunction of the antiferromagnetic RVB state [11]. The important feature of the 2D dimer problem is its fermionic nature. In retrospect, the appearance of a Pfaffian in Kasteleyn's [1, 6] combinatorial analysis already suggests the fermionic nature of the problem. The quantum fermion calculus has been applied by Fisher [2] in his version of the combinatorial matrix solution. More recently, the combinatorial analysis of the dimer problem in terms of fermionic fields (Grassmann variables) has been performed by Samuel [12] and Abanov [13]. The traditional approaches of this kind, however, are somewhat complicated even in a purely mathematical aspect, and differ significantly, in their spirit, from the methods commonly accepted in quantum field theory and condensed matter physics.

In this paper we present a very simple non-combinatorial interpretation for the fermionic nature of the 2D dimer problem based on the integration over Grassmann variables (non-quantum fermionic fields) and factorization principles for the density matrix. The approach is straightforward, the traditional combinatorial or transfer-matrix considerations will not be used. The factorization ideas resemble, in general, the idea of the insertion of Dirac's unity

$\Sigma |a\rangle\langle a| = 1$ in transformations in quantum mechanics. The principal point, related to the 2D nature of the problem, is the construction of the mirror-ordered factorized representation for the dimer density matrix (equation (12)). At this stage we apply the ideas first developed in the context of the 2D Ising model [14]. Within this new interpretation, we derive, for the first time, the Gaussian fermionic representations for the partition functions for the most general inhomogeneous rectangular, hexagonal, and triangular dimer lattices (equations (15), (18) and (19)). By a suitable specification of the distribution of the dimer weights, these representations provide the exact analytic solutions for the partition functions and the dimer-dimer correlations, in all orders, for a variety of regular homogeneous lattices, and may also be a good starting point for further studies.

We present the basic steps of fermionization by an example of a rectangular inhomogeneous lattice with a free boundary. Let the lattice sites be numbered by pairs of integers mn , with $m = 1, 2, \dots, M$ and $n = 1, 2, \dots, N$ running in horizontal and vertical directions, respectively. The dimers are objects living on lattice bonds. The given bond may be either free or covered by a dimer together with the two adjacent sites. The closed-packing restriction means that each lattice site must be covered by one and only one dimer; see figure 1(a). Let $t_{mn}^{(1)}$ and $t_{mn}^{(2)}$ be the dimer weights (activities) for horizontal and vertical bonds, respectively, as is shown in figure 1(b). The weight of a free bond is 1. For the whole lattice, the Boltzmann weight of a configuration is the product of the bond weights. The partition function, Q , arises by summing over the allowed configurations. This combinatorial definition for Q can be formalized as follows. With each lattice site mn we associate the commuting nil-potent variable η_{mn} , with $\eta_{mn}^2 = 0$, and write

$$Q = \text{Sp}_{(\eta)} \prod_{m=1}^M \prod_{n=1}^N (1 + t_{mn}^{(1)} \eta_{mn} \eta_{m+1n}) (1 + t_{mn}^{(2)} \eta_{mn} \eta_{mn+1}) \quad (1)$$

where we assume the free-boundary conditions for the variables: $\eta_{M+1n} = \eta_{mN+1} = 0$. The averaging rules for one variable are

$$\text{Sp}_{(\eta_{mn})} (1 | \eta_{mn} | \eta_{mn}^2 | \eta_{mn}^3 | \eta_{mn}^4 | \dots) = (0 | 1 | 0 | 0 | 0 | \dots) \quad (2)$$

with the global η -averaging in (1) being a superposition of the local averagings (2) taken over all the sites of a lattice. Evidently, the product of factors $1 + t\eta\eta'$ forming the 'density matrix' in (1) produces all possible coverings of a lattice by 'dimer molecules' $\eta t \eta'$. The averaging according to the rule (2) just selects the closed-packed configurations. Our goal is now to pass from the commuting nil-potent η -variables to the anticommuting Grassmann variables. The point is that the Grassmann variables are 'good' variables with many plausible properties and we know how to extract numbers from the Grassmann-variable expressions, which is not the case for the η -variables.

We remember that the Grassmann variables are non-quantum fermionic numbers purely anticommuting to zero. Given a set of Grassmann variables a_1, \dots, a_N , we have $a_i a_j + a_j a_i = 0$, $a_j^2 = 0$. The Berezin's rules of integration over one variable are [15]

$$\int da_j a_j = 1 \quad \int da_j 1 = 0. \quad (3)$$

In the multidimensional integral, the differential symbols da_1, \dots, da_N are again anticommuting with each other and with the variables. The basic formulae of the Grassmann-variable analysis concern the Gaussian fermionic integrals [15,16]. The

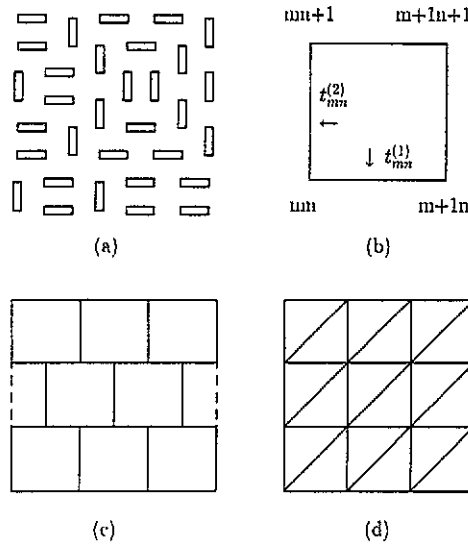


Figure 1. (a) A particular closed-packed dimer covering on a rectangular lattice. (b) Local enumeration of sites and bonds on a rectangular cell. (c) A fragment of the brick lattice, such a lattice is topologically equivalent to the hexagonal lattice. (d) The triangular lattice as a generalization of the rectangular one.

Gaussian integral of the first kind is related to the determinant

$$\int \prod_{j=1}^N da_j^* da_j \exp \left(\sum_{i=1}^N \sum_{j=1}^N a_i A_{ij} a_j^* \right) = \det \hat{A} \quad (4)$$

where $\{a_j, a_j^*\}$ is a set of completely anticommuting Grassmann variables, the matrix in the exponential is arbitrary. The Gaussian integral of the second kind is related to the Pfaffian of the associated skew-symmetric matrix:

$$\int da_N \dots da_2 da_1 \exp \left(\frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N a_i A_{ij} a_j \right) = \text{Pfaff } \hat{A} \quad A_{ij} = -A_{ji}. \quad (5)$$

The Pfaffian form is some combinatorial polynomial in elements A_{ij} known in mathematics for a long time. The Pfaffian and determinant of the associated skew-symmetric matrix are algebraically related: $\det \hat{A} = (\text{Pfaff } \hat{A})^2$. This relation can be most easily proved in terms of the fermionic integrals like (4) and (5) [12]. The linear superpositions of the Grassmann variables are again Grassmann variables and it is possible to make a linear change of variables in the fermionic integrals. As compared with the rules of the common analysis, the only difference is that the Jacobian will now appear in the inverse power [15]. New variables of integration can be introduced, in particular, by means of the Fourier substitution (transformation to the momentum space).

Let it be given only two Grassmann variables a and a^* . The elementary Gaussian exponential is $e^{\lambda aa^*} = 1 + \lambda aa^*$, the series terminates since $(aa^*)^2 = 0$. Making use of the basic rules (3), the typical weight factor from (1) can be factorized as follows:

$$1 + t\eta\eta' = \int da^* da e^{aa^*} (1 + t\eta) (1 + a^*\eta). \quad (6)$$

We intend to apply factorization (6) to pass in (1) from the commuting η -variables to the anticommuting Grassmann variables.

Introducing, for the whole lattice, a set of completely anticommuting Grassmann variables $\{a_{mn}, a_{mn}^*, b_{mn}, b_{mn}^*\}$, a pair per bond, we write

$$1 + t_{mn}^{(1)} \eta_{mn} \eta_{m+1n} = \int da_{mn}^* da_{mn} e^{a_{mn} a_{mn}^*} (1 + t_{mn}^{(1)} a_{mn} \eta_{mn}) (1 + a_{mn}^* \eta_{m+1n})$$

$$= \underset{(a_{mn})}{\text{Sp}} \{A_{mn} A_{m+1n}^*\} \quad (7a)$$

$$1 + t_{mn}^{(2)} \eta_{mn} \eta_{m n+1} = \int db_{mn}^* db_{mn} e^{b_{mn} b_{mn}^*} (1 + t_{mn}^{(2)} b_{mn} \eta_{mn}) (1 + b_{mn}^* \eta_{m n+1})$$

$$= \underset{(b_{mn})}{\text{Sp}} \{B_{mn} B_{m n+1}^*\} \quad (7b)$$

where in the last lines we introduce the abbreviated notation for the arising Grassmann factors:

$$A_{mn} = 1 + t_{mn}^{(1)} a_{mn} \eta_{mn} \quad A_{m+1n}^* = 1 + a_{mn}^* \eta_{m+1n}$$

$$B_{mn} = 1 + t_{mn}^{(2)} b_{mn} \eta_{mn} \quad B_{m n+1}^* = 1 + b_{mn}^* \eta_{m n+1} \quad (7c)$$

while $\text{Sp}(\dots)$ stand for the Gaussian averagings $\int da^* da e^{aa^*}(\dots)$ and $\int db^* db e^{bb^*}(\dots)$. The totally commuting local averaging symbols can be gathered in one place, forming the global Gaussian averaging. The indices mn in the above Grassmann factors are chosen to be equal to the indices of the variables η_{mn} involved in these factors. The idea is to place nearby, in the process of fermionization, the four factors $A_{mn}, A_{mn}^*, B_{mn}, B_{mn}^*$ with the same variable η_{mn} and to average over η_{mn} in each group of factors independently, thus producing a purely fermionic representation for Q . The obstacle to this method is that the individual Grassmann factors are neither commuting nor anticommuting with each other. It might, therefore, be difficult, in general, to find the four relevant factors nearby. The problem of a suitable ordering of the non-commuting Grassmann factors thus arises. In fact, though the Grassmann factors themselves are neither commuting nor anticommuting, what can really be used in the ordering arrangements is that the doublets presenting the bond weights, $A_{mn} A_{m+1n}^*, B_{mn} B_{m n+1}^*$, can be treated as totally commuting objects, if taken as a whole, since the non-commuting linear fermionic terms involved in these doublets are effectively equal to zero under the sign of the Gaussian averaging. Alternatively, we can first place the weight $1 + t\eta\eta'$ into any suitable position among the other Grassmann factors, and then we pass to the factorized representation (7). The doublets $A_{mn} A_{m+1n}^*$ and $B_{mn} B_{m n+1}^*$ can thus be moved through any product of other Grassmann factors as if they were purely commuting.

In the fermionization process, we will also apply the two ordering principles illustrated below by tutorial examples:

$$(x_0 \bar{x}_1) (x_1 \bar{x}_2) (x_2 \bar{x}_3) (x_3 \bar{x}_4) = x_0 (\bar{x}_1 x_1) (\bar{x}_2 x_2) (\bar{x}_3 x_3) \bar{x}_4 \quad (8)$$

$$(x_1 \bar{x}_1) (x_2 \bar{x}_2) (x_3 \bar{x}_3) = (x_1 (x_2 (x_3 \bar{x}_3) \bar{x}_2) \bar{x}_1) = x_1 x_2 x_3 \bar{x}_3 \bar{x}_2 \bar{x}_1. \quad (9)$$

In equation (8) we simply re-read the product by joining together the neighbouring symbols with the same indices. In (9) we assume that the doublets $(x_j \bar{x}_j)$ are totally commuting with the individual x -factors, while the separable factors themselves may be non-commuting, and separate proper and bar factors.

With this notes, we proceed to the global factorization of the density matrix. In transformations from (10) to (12) we omit, for brevity, the sign of the Gaussian averaging

arising by factorization. First, we put one commuting weight (7) between the two Grassmann factors of another, also cf (9), and write

$$(1 + t_{mn}^{(1)} \eta_{mn} \eta_{m+1n}) (1 + t_{mn}^{(2)} \eta_{mn} \eta_{mn+1}) = B_{mn} A_{mn} A_{m+1n}^* B_{m+1n}^* \quad (10)$$

Next, we multiply the weights (10) over m , for a given fixed n , applying the rules (9) and (8), respectively:

$$\prod_{m=1}^M B_{mn} A_{mn} \xrightarrow{m} A_{m+1n}^* \prod_{m=1}^M B_{m+1n}^* \xleftarrow{m} = \prod_{m=1}^M A_{mn}^* \xrightarrow{m} B_{mn} A_{mn} \prod_{m=1}^M B_{mn}^* \xleftarrow{m} \quad (11)$$

where the arrows indicate the direction of increasing m in the ordered products. In the final expression we put $A_{M+1n}^* = 1$, since $\eta_{M+1n} = 0$, and introduced, formally, the lacking symbols $A_{1n}^* = 1 + a_{0n}^* \eta_{1n}$ with $a_{0n}^* = 0$, cf (7), so that in fact $A_{1n}^* = 1$. Now we multiply the products (11) over n , with n increasing from left to right, applying the rule (8) with respect to index n :

$$\prod_{n=1}^N \left\{ \prod_{m=1}^M A_{mn}^* \xrightarrow{m} B_{mn} A_{mn} \prod_{m=1}^M B_{m+1n}^* \right\} = \prod_{n=1}^N \left\{ \prod_{m=1}^M B_{mn}^* \prod_{m=1}^M A_{mn}^* \xrightarrow{m} B_{mn} A_{mn} \right\} \quad (12)$$

In the final expression we again annihilate the factors $B_{mN+1}^* = 1$, since $\eta_{mN+1} = 0$, and create the lacking factors $B_{m1}^* = 1$, where $b_{m0}^* = 0$. Being forced in (11) to separate the mn and $m n + 1$ factors in order to apply the linear arrangement (8) with respect to m , in (12) we try to restore, whenever possible, the normal situation by combining the factors with equal mn . All the local weights (6) are already involved in (12). For the ‘density matrix’ from (1) we thus obtained a special ‘mirror-factorized’ representation (12). In this representation the η -variables can be easily eliminated.

The η -averaging reduces to the averaging over individual variables η_{mn} at the junction of the m -products in (12) and yields, finally, the product of the linear forms in Grassmann variables:

$$L_{mn} = t_{mn}^{(1)} a_{mn} + t_{mn}^{(2)} b_{mn} + a_{m-1n}^* + (-1)^{m+1} b_{mn-1}^* \quad (13)$$

First, we fix n and average at the junction the complete product $B_{mn}^* A_{mn}^* B_{mn} A_{mn} = 1 + \eta_{mn} (t_{mn}^{(1)} a_{mn} + t_{mn}^{(2)} b_{mn} + a_{m-1n}^* + b_{mn-1}^*) + \dots$ with $m = 1$, given n , with the result correctly presented by (13) at $m = 1$. Then we move the L_{mn} -form from the junction to the left through the remaining product of B_{mn}^* factors with given n . At the junction we then find again the complete product of four neighbouring factors with equal index mn , $m = 2$ and repeat the procedure for $m = 2$, and then for $m = 3, 4, 5, \dots, M$, for given n , and all over again for other values of n . The translation of the linear fermionic form L_{mn} to the left is just responsible for the factor $(-1)^{m+1}$ occurring in (13). This sign factor arises because the variables b_{mn}^* , involved in the B_{mn}^* factors, change their sign each time we move L_{mn} from the junction to the left.

The η -variables being completely eliminated, we find the dimer partition function as a product of the L_{mn} forms under the sign of the Gaussian averaging coming from factorization. In this already purely fermionic expression, we can exponentiate L_{mn} making use of the identity $L_{mn} = \int dc_{mn} \exp \{c_{mn} L_{mn}\}$, where c_{mn} are some auxiliary Grassmann

variables. The partition function then appears as a Gaussian integral:

$$Q = \int \prod_{n=1}^N \prod_{m=1}^M da_{mn}^* da_{mn} db_{mn}^* db_{mn} \overset{m}{dc}_{mn} \exp \left\{ \sum_{m=1}^M \sum_{n=1}^N [a_{mn} a_{mn}^* + b_{mn} b_{mn}^* + (t_{mn}^{(1)} a_{mn} + t_{mn}^{(2)} b_{mn} + a_{m-1n}^* + (-1)^{m+1} b_{mn-1}^*) c_{mn}] \right\} \quad a_{0n}^* = b_{m0}^* = 0. \quad (14)$$

The above integral can in turn be simplified by integrating out the a -, b -fields by means of identities like $\int da^* da \exp\{aa^* + aL' + a^*L''\} = \exp\{L''L'\}$, where L' , L'' are some linear forms in c -variables. Eliminating the a -, b -fields, we come to the final expression:

$$Q = \int \prod_{n=1}^N \prod_{m=1}^M \overset{m}{dc}_{mn} \exp \left\{ \sum_{m=1}^M \sum_{n=1}^N [t_{mn}^{(1)} c_{m+1n} c_{mn} + (-1)^{m+1} t_{mn}^{(2)} c_{mn+1} c_{mn}] \right\} \quad (15)$$

with the free-boundary conditions for fermions: $c_{M+1n} = 0$, $c_{mN+1} = 0$. The partition function is now expressed as a simple fermionic Gaussian integral. This representation is exact and completely equivalent to that of (1). In field-theoretical language, the fermionic form in the exponential is called the fermionic action. The action in (15) is quadratic, we thus deal with a free-fermion field theory on a lattice. As is well known from the quantum field theory and solid state physics, the free-fermion representation of a model is in essence equivalent to its exact solution. In the given case, if we assume that or another regular distribution of the dimer weights, the integral can be performed analytically (also see (4) and (5)). The key point in the above derivation is the mirror-ordered factorized representation for the density matrix (12) which makes possible the elimination of the η -variables. However, despite a simple solution in the 2D case exposed above, the ordering problem for Grassmann factors is, in general, a non-trivial one. In particular, this problem can hardly be solved for the 3D dimer lattice, the 3D dimer problem remains unsolved, the same holds for the 3D Ising model. The gap between two and three dimensions is in fact large.

It is important that the free-fermion representation for the partition function (15) is derived for the most general inhomogeneous distribution of the dimer weights. This can be used for at least three purposes: (i) one can deduce the fermionic expressions for the dimer-dimer correlation functions of any order and orientation simply by differentiating (15) with respect to the activities $t_{mn}^{(1)}$, $t_{mn}^{(2)}$, (ii) one can analyse the disordered problem, the influence of defects and impurities, and (iii) one can study the dimer problem on regular lattices by specifying the appropriate periodic distribution of the activities in (15). As the simplest illustration for the last point, we note that (15) contains all the information about the brick lattice (see figure 1(c)) which is equivalent to the hexagonal lattice neglecting the boundary effects. The fermionic representation for Q for the inhomogeneous brick-hexagonal lattice arises by making some of the vertical weights $t_{mn}^{(2)}$ zero in accordance with figure 1(c). It is interesting that the homogeneous hexagonal lattice exhibits an exotic phase transition [6, 8], as distinct from the homogeneous rectangular lattice with no phase transition [1, 2]. The fermionic representations for a variety of more complicated regular lattices also follow from (15).

For actual calculations for homogeneous lattices, the standard device is to pass to the momentum space (Fourier substitution for fermions). For instance, for the homogeneous rectangular lattice, $t_{mn}^{(1)} = t_1$, $t_{mn}^{(2)} = t_2$, the fermionic action in (15) is put into block-diagonal

form by the substitution:

$$c_{mn} = \frac{2^{1+m+n}}{\sqrt{(M+1)(N+1)}} \sum_{p=1}^M \sum_{q=1}^N c_{pq} \sin\left(\frac{\pi pm}{M+1}\right) \sin\left(\frac{\pi qn}{N+1}\right). \tag{16}$$

The partition function then factorizes into the product of similar integrals over the groups of variables: c_{pq} , $c_{M+1-p,q}$, $c_{p,N+1-q}$, $c_{M+1-p,N+1-q}$. For both M and N even, the evaluation of the integral gives

$$Q = \prod_{p=1}^{M/2} \prod_{q=1}^{N/2} \left[4t_1^2 \cos^2 \frac{\pi p}{M+1} + 4t_2^2 \cos^2 \frac{\pi q}{N+1} \right] \tag{17}$$

in accordance with the combinatorial result [1, 2]. (Also see the analogous momentum-space calculations for the 2D Ising models in [12, 16, 18].)

The fermionization can also be performed for the toroidal (periodic in both directions) boundary conditions. We refer here to the experience with the 2D Ising model on a torus [17]. The final result is

$$Q|_{\text{torus}} = \frac{1}{2} [G|_{--} + G|_{-+} + G|_{+-} - G|_{++}] \tag{18}$$

where G is the fermionic integral given in (15), but now with the four combinations of the periodic–aperiodic closing conditions for fermions:

$$(\pm|\pm) = (c_{M+1n} = \pm c_{1n} | c_{mN+1} = \pm c_{m1}).$$

The original partition function Q in (18) is that of (1) with $\eta_{M+1n} = \eta_{1n}$ and $\eta_{mN+1} = \eta_{m1}$. The characteristic expansion of Q into the sum of four integrals, also known for the 2D Ising model, is in fact a purely fermionic effect due to the transposition of the products of the boundary Grassmann factors necessary in this case, cf [17]. The analytic result [1] for the homogeneous rectangular torus follows from (18) by Fourier substitution. In the given case one has to expand c_{mn} over the Fourier exponentials with integer momenta for periodic directions and with half-integer momenta for aperiodic directions. The Fourier transformation is in general simpler for the toroidal integrals (18) than for the free boundary case (15). (We have also checked that the solution for the hexagonal lattice with Kasteleyn’s transition follows from (18), and calculated some other partition functions, and some correlations.)

The Gaussian fermionic representations can also be derived for the triangular inhomogeneous lattice. The triangular lattice can be viewed as a rectangular one with a diagonal added in each lattice cell; see figure 1(d). Respectively, we must add diagonal factors $1 + t_{mn}^{(3)} \eta_{mn} \eta_{m+1n+1}$ in (1). For the free boundary, the partition function is then given by an integral like (15), but now with an extended fermionic action in the exponential

$$S(c) = \sum_{m=1}^M \sum_{n=1}^N \left[t_{mn}^{(1)} c_{m+1n} c_{mn} + (-1)^{m+1} t_{mn}^{(2)} c_{mn+1} c_{mn} + (-1)^m t_{mn}^{(3)} c_{m+1n+1} c_{mn} \right]. \tag{19}$$

Respectively, for the toroidal conditions the triangular partition function for an inhomogeneous lattice is given by (18) where the integrals are to be taken with the extended action (19).

In conclusion, we have reformulated the closed-packed dimer problem on inhomogeneous 2D lattices as free-fermion field theories. The generalized inhomogeneous partition functions are obtained in the form of Gaussian integrals over Grassmann variables. This puts the dimer model, which is originally a combinatorial problem, closer to the typical models of quantum statistics and solid state physics. The approach is flexible enough to

deal with non-standard and complicated lattices, different boundary conditions, local defects and perturbations, etc. For regular lattices, the Gaussian representations of this kind provide the analytic results for thermodynamic functions and correlations.

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