Grassmannian representation of the two-dimensional monomer-dimer model

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We present an application of the Grassmann algebra to the problem of the monomer-dimer statistics on a two-dimensional square lattice. The exact partition function, or total number of possible configurations, of a system of dimers with a finite set of \( n \) monomers at fixed positions can be expressed via a quadratic fermionic theory. We give an answer in terms of a product of two pfaffians and the solution is closely related to the Kasteleyn result of the pure dimer problem. Correlation functions are in agreement with previous results, both for monomers on the boundary, where a simple exact expression is available in the discrete and continuous case, and in the bulk where the expression is evaluated numerically.

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The study of the classical dimer model has a very long history in physics and mathematics. This model is interesting as a direct physical representation, e.g. diatomic molecules on a two-dimensional substrate\(^1\). From the mathematical point of view, this model on bipartite lattice - known as a special case of perfect matching problem\(^2\), is a famous and active problem of combinatorics and graph theory\(^3\). The partition function of the 2D dimer model was solved independently using Pfaffian methods\(^4\)-\(^6\), resulting in the exact calculation of correlation functions\(^7\)-\(^9\) using Toeplitz determinant.

For the general dimer problem where monomers are present - the lattice sites that are not covered by the dimers are regarded as occupied by monomers- there is no exact solution except in 1D where the solution can be expressed in terms of Chebyshev polynomials\(^10\), on the complete graph and on locally tree-like graphs\(^11\). For 3D lattices, no exact solution exists for the pure close-packed dimer problem. Recent advances concern the analytic solution of the problem where there is a single monomer on the boundary of a 2D lattice\(^12\)-\(^13\), correlation functions for monomers located on the boundary\(^14\)-\(^15\), and localization phenomena of a monomer in the bulk\(^16\)-\(^17\).

The field of analytical solutions in the monomer-dimer model is still uncharted, but many rigorous results exist, e.g. location of the zeroes of the partition function\(^18\)-\(^19\), monomer-monomer and dimer-dimer correlation functions\(^7\)-\(^8\), series expansions of the partition function\(^20\) and exact recursion relation\(^21\). This lack of exact solution has been formalized in the context of computer science\(^22\). The importance of the dimer model in theoretical physics and combinatorics also comes from the direct mapping between the Ising model without magnetic field and the dimer model on a decorated lattice\(^4\)-\(^6\),\(^23\). Furthermore the Ising model in a magnetic field can be mapped to the general monomer-dimer model\(^19\).

Here we present a Grassmannian or fermionic formulation of the monomer-dimer model, which possesses an exact solution in term of the product of two explicit pfaffians. We study the close-packed model, where an allowed dimer configuration has the property that each site of the lattice is paired with exactly one of its nearest neighbors, creating a dimer. In the simplest form, the number of dimers is the same in all the configurations, the partition function is given by the equally-weighted average over all possible dimer configurations. In the following, we will include unequal fugacities, so that the average to be taken then includes non-trivial weighting factors.

We first review a very simple non-combinatorial interpretation of the 2D dimer model based on the integration over Grassmann variables\(^24\) and factorization principles for the density matrix\(^25\)-\(^26\). A dimer model can be described with Boltzmann weights \( t_x \) and \( t_y \) of some coupling energy along the two directions. For example a magnetic field along one direction implies non-identical weight values. The partition function for a lattice of size \((L \times L)\) with \( L \) even can directly be written as

\[
Q_0 = \int \prod_{m,n} \text{d} \eta_{mn} (1 + t_x \eta_{mn} \eta_{m+1,n})(1 + t_y \eta_{mn} \eta_{mn+1})(1)
\]

where \( \eta_{mn} \) are nilpotent and commuting variables satisfying\(^27\) \( \eta_{mn}^2 = 0, \int \text{d} \eta_{mn} \eta_{mn} = 1 \), and \( \int \text{d} \eta_{mn} = 0 \). The integrals can be performed if we introduce, following

![FIG. 1: Typical dimer configuration for a square lattice of size 6x6 without monomer (right) and with 6 monomers (left, red dots).](image)

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closely Hayn and Plechko\textsuperscript{25}, a set of Grassmann variables \(\{a_{mn}, \bar{a}_{mn}, b_{mn}, \bar{b}_{mn}\}\) such that

\[
1 + t_x \eta_{mn} \eta_{m+1n} = \int \! d\bar{a}_{mn} d\bar{a}_{m+1n} e^{a_{mn} \bar{a}_{mn}} (1 + a_{mn} \eta_{mn})(1 + t_x \bar{a}_{mn} \eta_{m+1n}),
\]

\[
1 + t_y \eta_{mn} \eta_{mn+1} = \int \! d\bar{b}_{mn} d\bar{b}_{mn+1} e^{b_{mn} \bar{b}_{mn}} (1 + b_{mn} \eta_{mn})(1 + t_y \bar{b}_{mn} \eta_{mn+1}).
\]

(2)

This decomposition allows for an integration over the Grassmann variables \(\eta_{mn}\), after rearranging the different link variables \(A_{mn} = 1 + a_{mn} \eta_{mn}, \bar{A}_{m+1n} = 1 + t_x \bar{a}_{mn} \eta_{m+1n}, B_{mn} = 1 + b_{mn} \eta_{mn}\) and \(\bar{B}_{mn+1} = 1 + t_y \bar{b}_{mn} \eta_{mn+1}\). Then the partition function becomes

\[
Q_0 = \text{Tr}_{\{a, \bar{a}, b, \bar{b}, \eta\}} \prod_{m,n} (A_{mn} \bar{A}_{m+1n})(B_{mn} \bar{B}_{mn+1}),
\]

(3)

where we use the integration measure \(\text{Tr}_{\{\}}\) for the different Grassmannian and nilpotent variables with the adequate weights. The non-commuting link variables are then moved through the product in such a way that each \(\eta_{mn}\) is isolated and can be integrated directly. This rearrangement is possible in two dimensions thanks to the

boundary conditions are now \(c_{0,n} = c_{m,0} = c_{L+1,n} = c_{m,L+1} = 0\). We consider a Fourier transformation satisfying open boundary conditions\textsuperscript{25}, \(c_{mn} = \frac{1}{\sqrt{2L+1}} \sum_{p=-L}^{L} f_p(q) \exp(iq_m)\), where \(f_p(q) = \sin(q_p)\). This leads to a block representation of the action in the momentum space, for momenta inside the reduced sector \(1 \leq p, q \leq L/2\). We note vectors \(c_\alpha = \{c_{pq}, c_{-pq}, c_{p-q}, c_{-p-q}\}\) where \(-p\) is meant for \(L + 1 - p\) and label \(\alpha = \{p, q\}\). The 4 components of these vectors will be written \(c_\mu\) with \(\mu = 1 \cdots 4\). Then \(S_0 = \frac{1}{2} \sum_\alpha \bar{c}_\alpha M \bar{c}_\alpha\), where the antisymmetric matrix \(M\) is defined by

\[
M_\alpha = \begin{pmatrix}
0 & 0 & -a_y(q) & -a_x(p) \\
0 & 0 & a_x(p) & -a_y(q) \\
a_y(q) & a_x(p) & 0 & 0 \\
a_x(p) & a_y(q) & 0 & 0
\end{pmatrix}
\]

with \(a_x(p) = 2t_x \cos(p)\) and \(a_y(q) = 2t_y \cos(q)\). The factor \(i\) can be absorbed in a redefinition of the \(c\)'s variables. One simply obtains a product of cosine functions\textsuperscript{25} as found by Kasteleyn\textsuperscript{4,5} since the pfaffian of \(\prod_\alpha M_\alpha\) is the product \(\prod_{p,q} \det(a_x(p) + a_y(q))\)

in the reduced sector of momenta, or

\[
Q_0 = \prod_{p,q=1}^{L/2} \left[ 4t_x^2 \cos^2\frac{p}{L} + 4t_y^2 \cos^2\frac{q}{L} \right] = \int \prod_{m,n} \! d\eta_{mn} \exp S_0.
\]

(5)

The matrix \(M_\alpha\) is deeply related to the Kasteleyn\textsuperscript{4} orientation matrix \(K\) since \(Q_0 = \text{Pf}(\prod_\alpha M_\alpha) = \text{Pf}(K)\). We consider now the case where an even number \(n\) of monomers are present in the lattice at different fixed positions \(r_i = (m_i, n_i)\) with \(i = 1, \cdots, n\), see Fig. 1. The partition function \(Q_n(\{r_i\})\), we define as a correlation function between monomers after summing up over all dimer configurations, is the number of all possible dimer configurations with the constraint imposed by fixing the given monomer positions. This quantity is evaluated by inserting \(\eta_{m,n}\) in Eq. (1) at each monomer location, which prevents dimers from occupying these sites. It is useful to introduce additional Grassmann variables \(h_i\) such that \(\eta_{m,n} = \int \! dh_i \exp(h_i \eta_{m,n})\). These insertions are performed at point \(r_i\) in Eq. (4), and the integration over \(\eta_{m,n}\) modifies \(L_{m,n_i} \rightarrow L_{m,n_i} + h_i\). However, by moving the anti-commuting variables \(dh_i\) to the left of the remaining ordered product, a minus sign is introduced in front of each \(b_{mn,-1}\) or \(t_y\) coupling in \(\bar{B}_{mn}\).
FIG. 2: Typical configuration of the system with four monomers. The sign of the couplings $t_y$ are reversed (red links) along the black-dashed line that arises from moving the Grassmann fields conjugated to the defects towards the right boundary.

for all $m > m_l$. We can replace more generally $\tilde{b}_{mn-1}$ by $\tilde{e}_{mn}b_{mn-1}$ such that $\epsilon_{mn} = -1$ for $m > m_l$, and $\epsilon_{mn} = 1$ otherwise. The integration is then performed on the remaining $\{a, \tilde{a}, b, \tilde{b}\}$ variables as usual, so that $Q_n(\{r_i\})$ can be expressed as a Gaussian form, with a sum of counter terms corresponding to the monomer insertions, or

$$Q_n(\{r_i\}) = \text{Tr}_{\{c,h\}} e^{S_0 + \sum_{\{r_i\}} \epsilon_{mn} n_i h_i + S_f},$$

$$S_f = 2t_y \sum_{\{r_i\}} \sum_{m=m_l+1}^L (-1)^{m+1} c_{mn} c_{m+1,n},$$

The contribution $S_f$ corresponds to a line of defects, as shown in Fig. 2. The addition of monomers is therefore equivalent to inserting a magnetic field $h_i$ at points $r_i$, as well as a line of defect $c_{mn} c_{m+1,n}$ running from the monomer position to the right boundary $m = L$. If two monomers have the same ordinate $n_i = n_j$, the line of defects will only run between the two monomers and will not reach the boundary. The part of the field interaction can be Fourier transformed such that $\sum_{\{r_i\}} c_{mn} n_i h_i = \sum_{p,q=1}^L c_{pq} H_{pq} = \sum_{\alpha,\beta} c_{\alpha\beta} H_{\alpha\beta}$. The term $S_f$ in the action can be written as $\frac{i}{2} c_{\alpha\beta} V_{\alpha\beta} c_{\alpha\beta}$, with the perturbative matrix $V_{\alpha\beta}$ given by

$$V_{\alpha\beta} = V_{pq,p'q'} = \sum_{\{r_i\}} 2t_y (-1)^{n_i} \left\{ \sum_{m=m_l+1}^L f_m(p) f_m(p') \right\} \left( f_{n_i-1}(q) f_{n_i}(q') - f_{n_i-1}(q') f_{n_i}(q) \right).$$

The different components $V^{\mu\nu}_{\alpha\beta}$ are given explicitly, for the first terms, by $V^{11}_{\alpha\beta} = V_{pq,p'q'}$, $V^{12}_{\alpha\beta} = V_{pq,-p'q'}$, $V^{21}_{\alpha\beta} = V_{-pq,p'q'}$, and so on. Then the full fermionic action is $S = \frac{i}{2} c_{\alpha\beta} W^{\mu\nu}_{\alpha\beta} c_{\alpha\beta} + c_{\alpha\beta} H_{\mu\nu}^{\alpha\beta}$ with antisymmetric matrix $W^{\mu\nu}_{\alpha\beta} = \delta_{\alpha\beta} M^{\mu\nu} + V_{\mu\nu}^{\alpha\beta}$ satisfying $W^{\mu\nu}_{\alpha\beta} = -W^{\nu\mu}_{\beta\alpha}$. By construction, this matrix can be represented as a block matrix of global size $(L^2 \times L^2)$

$$W = \begin{pmatrix}
M_{\alpha=(1,1)} & V_{(1,1),(1,2)} & V_{(1,1),(1,3)} & \cdots \\
-V_{(1,1),(1,2)} & M_{(1,2)} & V_{(1,2),(1,3)} & \cdots \\
-V_{(1,1),(1,3)} & -V_{(1,2),(1,3)} & M_{(1,3)} & \cdots \\
\vdots & \vdots & \vdots & \ddots
\end{pmatrix},$$

where each of the $(L^2/4) \times (L^2/4)$ blocks is a $(4 \times 4)$ matrix. Labels $\alpha$ are ordered with increasing momentum $(1, 1), (1, 2) \cdots (1, L/2), (2, 1) \cdots$. Then $Q_n(\{r_i\})$ can formally be written using $Q_n(\{r_i\}) = \text{Tr}_{\{c,h\}} \exp \left( \frac{i}{2} c_{\alpha\beta} W^{\mu\nu}_{\alpha\beta} c_{\alpha\beta} + c_{\alpha\beta} H_{\mu\nu}^{\alpha\beta} \right)$. The linear terms in $c_{\alpha\beta} c_{\alpha\beta}$ can be removed using a translation $c_{\alpha\beta} \rightarrow c_{\alpha\beta} + g_{\mu\nu}$, with $g_{\mu\nu} = i(W^{-1})^{\mu\nu}_{\alpha\beta} H_{\alpha\beta}^{\mu\nu}$. After a further rescaling of variables $c_{\alpha} \rightarrow i^{-1/2} c_{\alpha}$, one obtains

$$Q_n(\{r_i\}) = \text{Pf}(W) \text{Tr}_{\{h\}} \exp \left[ -\frac{i}{2} (W^{-1})^{\mu\nu}_{\alpha\beta} H_{\alpha\beta}^{\mu\nu} \right].$$

The fields $H_{\mu\nu}^{\alpha\beta}$ depend on $h_i$ through the identity $H_{\mu\nu}^{\alpha\beta} = \sum_{i=1}^n \Lambda_{i,\alpha,\beta} h_i$, where coefficients $\Lambda_{i,\alpha,\beta}$ are expressed using a 4-dimensional vector $\Lambda_{i,\alpha} = \bar{f}_{mn}(p) f_{n_i}(q) \Lambda_{i,\alpha}$. The components of momentum-independent vector $\Lambda_{i,\alpha}$ are $(i m_i - n_i, i m_i + n_i, -i m_i - n_i, -i m_i + n_i$). Its role is to fix whether the configuration of the monomers is allowed or not (in this case the correlator is zero). The final and compact expression for $Q_n(\{r_i\})$ is then

$$Q_n(\{r_i\}) = \text{Pf}(W) \text{Pf}(C),$$

where $C$ is a real $(n \times n)$ antisymmetric matrix with elements $C_{ij} = -i \Lambda_{i,\alpha,\beta} (W^{-1})^{\mu\nu}_{\alpha\beta} \Lambda_{j,\alpha,\beta}$. The antisymmetry can be easily verified using the antisymmetry property of $W$ or $W^{-1}$. $Q_n$ is therefore a product of two pfaffians where the positions of the monomers are specified in both matrices $W$ and $C$. It is worth noting that such general factorization was found for the correlation function between two monomers in term of the product of two spin-spin correlation functions of the Ising model at criticality, due to the analogy of the dimer model with a dual Ising model. It is however not obvious here to have such a direct identification with this result since the two pfaffians in Eq. (9) are of different nature. We can also mention that factorization of the correlation function exists in other models such as the one-dimensional
Functions $u$ and $v$ are specified by

$$u_k^{\alpha,\beta} = \sum_{m=m_0+1}^{L} (-1)^{s+1} f_m(p) f_m(p'), \quad \text{(10)}$$

$$v_k^{\alpha,\beta} = \sum_{m=m_0+1}^{L} (-1)^{s+1} f_m(q) f_{m-1}(q') + (-1)^{s} f_m(q') f_{m-1}(q).$$

It is also worth noting that we have a similar structure in the real space, where the total action Eq. (7) is expressed by $S = \frac{1}{2} \sum_{m,n} W_{m,n,m',n'} + \sum_{i} c_{m,n} h_i$, with $W$ containing both the connectivity matrix $M$ and the contribution of the line of defects $V$. A direct computation also leads to the factorization $Q_n([r_i]) = Pf(W)Pf(C)$, where $C_{ij} = (W^{-1})_{m,n,m,n_j}$ is a $(n \times n)$ antisymmetric matrix.

Exact dimers enumeration algorithms\textsuperscript{31} up to size of $10 \times 10$ has been widely used to compared with the theoretical prediction. For instance there are 1,903,752 different configurations of dimers with two monomers at coordinates $r_1 = (2,3)$ and $r_2 = (7,5)$ on a 8 $\times$ 8 lattice, in accordance with the computation of $Q_2(r_1, r_2)$ taking $t_x = t_y = 1$. As possible other application, we could obtain the full partition function of the monomer-dimer model by summing up over all the possible number of monomers and over all the possible positions. The result for the 8 $\times$ 8 lattice is 179,788,343,101,980,135\textsuperscript{21}, compared with the 12,988,816 configurations without monomer. In Fig. 3, we have solved numerically for a size $L = 96$ the modified correlation function $Q_2([r_1, r_2])Q_0^{-1} = Pf(M^{-1}W)Pf(C)$, for two monomers at positions $r_1 = (m, L/2-k)$ and $r_2 = (m, L/2+k+1)$, $k = 0 \cdots L/2$, distant of $d = 2k + 1$. Due to finite size effects, a curve for a given $m$ is distinguished depending on the parity of $k$. In the large size limit, this difference is indiscernible. Fig. 3 shows the crossover between a behavior in $d^{-1}$ near the boundary ($m = 96$) to a bulk behavior in $d^{-1/2}$ ($m = 48$). Interestingly, when the monomers are located exactly on the boundary ($m = L$), $V = 0$, and $W = M$, in this case $Q_n([r_i]) = Q_n Pf(C)$, and it is straightforward to compute exactly the elements of matrix $C$. In the discrete case one obtains

$$C_{ij} = \frac{4}{(L+1)^2} \sum_{p,q=0}^{L/2} \left[ \left( \delta_{ij} + n_i n_j \right) \pi_p \cos \frac{\pi_p}{L+1} \sin^2 \frac{\pi_q}{L+1} + \left( \delta_{ij} + n_i n_j \right) \pi_q \sin \frac{\pi_p}{L+1} \sin \frac{\pi_q}{L+1} \right] f_y \cos \frac{\pi_p}{L+1} \sin^2 \frac{\pi_p}{L+1}$$

$$f_y \sin \frac{\pi_p}{L+1} \sin \frac{\pi_q}{L+1}. \quad \text{(11)}$$

$C_{ij}$ are zero if $n_i$ and $n_j > n_i$ have the same parity. For example, fixing one monomer on the first site $n_1 = 1$ and taking $n_2 = 2k$, we have, for $t_x = t_y = 1$ in the asymptotic limit $L \to \infty$ and large $k$, the following
expansion $C_{12} \simeq \frac{2}{d} k^{-1} - \frac{1}{d} k^{-5}$. In the case $n_1 = L/2 - k$ and $n_2 = L/2 + k + 1$, as shown in inset of Fig. 3, $C_{12} \simeq \frac{2}{d} d^{-1} - \frac{1}{d} d^{-3}$ instead, with $d = 2k + 1$. This result is in agreement with the work of Priezzhev and Ruelle on the scaling limit of the correlation functions of boundary monomers in a system of a close packed dimers in term of a 1D chiral free fermion theory.

In summary, we presented a practical fermionic solution of the 2D monomer-dimer model on the square lattice, which allows for expressing the correlation functions between monomers in term of two pfaffians, and gave an explicit formula for boundary correlations. This can also be used for studying more general $n$-point correlation functions, thermodynamical quantities or transport phenomena of monomers. Other lattice types, such as hexagonal, can be considered as well.

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