Tetramers with vacancies on the square lattice

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I. INTRODUCTION

Two-dimensional dimer models were introduced in statistical mechanics in the 1930s to study the adsorption of diatomic molecules on a surface [1]. In its basic formulation, a dimer on a two-dimensional lattice is an object that lives on a bond b between two nearest-neighbour sites with some associated activity $z_b = \exp -\varepsilon_b/kT$ where ε_b may be thought of as the adsorption energy of the dimer. The general monomer-dimer problem, which allows dimers of some finite density to coexist with unoccupied sites on the lattice, has not been solved exactly, although some rigorous results on the nature of these systems, as well as numerical, series expansion and Monte Carlo studies, are available in the literature (see [2] for a review). In comparison, the problem of completely covering a lattice with dimers so that every site has exactly one dimer residing on it has been solved exactly for a variety of two-dimensional lattices. Henceforth, we will refer to this specific situation as the close-packed dimer model.

Interest in the dimer problem was renewed by the introduction of the quantum dimer model (QDM) [3], and with the recent work on resonating valence bond states (cite) in models of magnetism. In the limit when kinetic terms vanish, the QDM reduces to a classical dimer model with interactions that favour neighbouring dimers being aligned parallel to each other. The focus of this paper will be the work by Alet et al on the interacting dimer model on the square lattice reported in [4] and [5], which overlaps with the study of doped QDMs by Papanikolau et al in [6]. In particular, several features of the model can be explained in the context of the two-dimensional Coulomb gas within the framework of renormalization group.

II. CLASSICAL INTERACTING DIMERS ON THE SQUARE LATTICE

A. Setup

Interactions are added to the dimer model described above by considering the partition function with modified weights that favour parallel dimers via

$$Z = \sum_{\{c\}} \exp\left(-\frac{v}{T}(N^c(=) + N^c(||))\right) \tag{1}$$

where T is the temperature, $N^c(=)$ and $N^c(||)$ count the number of plaquettes with horizontal and vertical parallel dimers respectively in configuration c, and the sum is over all possible configurations. The interaction v favours alignment when $v < 0$. The partition function corresponds to the diagonal part of the QDM Hamiltonian, while in the $T \to \infty$ limit, it reduces to the noninteracting dimer model. When aligning interactions are present, there are four degenerate columnar ground states in the close-packed phase, as illustrated in figure 1. For the following few sections, the close-packed dimer problem is considered except in section II E where the behaviour of the model when doped with monomers is considered.

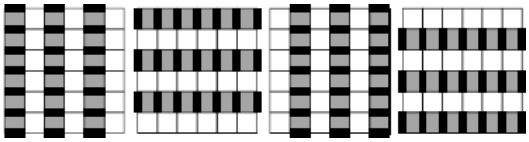

FIG. 1: The four possible columnar ground states under aligning interactions. Every shaded plaquette has an energy $v < 0$. (from ref. [4])

B. Mapping to the Coulomb gas

1. Two-component Coulomb gas

In this section we summarize the main features of the two-component Coulomb gas (CG). The results quoted here have been derived in the lecture notes and assigned problems of MIT course 8.334 [7, 8] and are also presented in [9].

We begin with the Sine-Gordon model in two dimensions which includes symmetry breaking fields:

$$Z = \int D\theta(\mathbf{x}) \exp\left\{-\int \mathrm{d}^2\mathbf{x}\left[\frac{K}{2}(\nabla\theta)^2 + \lambda_p \cos(p\theta)\right]\right\} \tag{2}$$

where p is an integer and θ takes on values from 0 to 2π. In the absence of vortices, the model is equivalent to a roughening model with electric charges with fugacity $y_p = \lambda_p a^2/2$ that interact with a Coulomb interaction. Only charges that are integer multiples of p are allowed. When vortices are introduced, they interact like vortices in the XY model. The Sine-Gordon model thus maps to a two-component Coulomb Gas (CG) with electric charges and magnetic charges (vortices). Near zero particle fugacity, the recursion relations of the electric charge and magnetic charge fugacities, y_p and y respectively, and the coupling K are [7]

$$\begin{aligned}\frac{\mathrm{d}y_p}{\mathrm{d}l} &= \left(2 - \frac{p^2}{4\pi K}\right) y + p \\ \frac{\mathrm{d}y}{\mathrm{d}l} &= (2 - \pi K) y \\ \frac{\mathrm{d}K^{-1}}{\mathrm{d}l} &= 4\pi^3 y^2 - \frac{\pi p^2 y_p^2}{2} K^{-2}\end{aligned} \tag{3}$$

A distinct feature of the CG is that the vacuum (no charges) is a line of fixed points on the K axis [9]. The above recursion relations are exact in the linear deviations y and y_p from this line. When only magnetic charges are present, the fugacity y is relevant when $K < 2/\pi$ and grows under renormalization, pushing K^{-1} to larger and larger values. This is the limit of a free gas of magnetic monopoles with a very weak interaction due to the high screening effect of nearby monopoles. When $K > 2/\pi$, y is irrelevant and the system renormalizes to a finite value of K on the line of fixed points $y = 0, 0 < K^{-1} < \pi/2$. In this case the interactions between monopoles binds them tightly into pairs or higher multipoles as a result of which their screening effect is diluted.

If electric charges alone are considered, a similar picture arises: the fugacity y_p is relevant when $K > p^2/8\pi$ and the system renormalizes to one of free electric charges; it is irrelevant when $K < p^2/8\pi$ and the charges exist as tightly bound multipoles. The above recursion relations are strictly valid only for $2/\pi < K < p^2/8\pi$, when both the vortices y and the cosine perturbation y_p are irrelevant and the assumption of low fugacities is preserved under renormalization.

2. Mapping

The dimer problem may be mapped onto a height model, for which a Sine-Gordon description exists. We follow the description in [6] and match it to the Sine-Gordon description in the previous section. The mapping involves the definition of a height variable h on each plaquette of the square lattice (or equivalently, on the dual lattice) according to the following rule: upon traversing the four plaquettes around a site on the even (odd) sublattice in the counterclockwise sense, the height changes by +3 (-3) if a dimer is present on the common plaquette edge being crossed, and by -1 (+1) if the edge is vacant. In the close-packed situation where exactly one dimer is present on every site, there are only four unique dimer configurations surrounding a plaquette. The height field can thus only take on values dictated by the periodicity $h \equiv h + 4$. Furthermore, if every dimer in a close-packed configuration is shifted by one bond, the heights are transformed via $h \to h + 1$ but (in the limit of large system size) the state is equivalent in energy. If we now coarse-grain the height variable to a rescaled field $\theta(\mathbf{x}) = \pi h(\mathbf{x})/2$, the periodicity constraint becomes $\theta \equiv \theta + 2\pi$, and the translational invariance is satisfied by an energy that does not change under $\theta \to \theta + \pi/2$. we may assign an energy to fluctuations of the height field via a stiffness K and interactions which must satisfy the two invariances; the most general form of such an action is then identical to the Sine-Gordon Hamiltonian above, with the constraint of translational invariance satisfied by $p = 4$ [5, 6]. The height field corresponds to the electric charge density in the CG picture. We have two terms, an entropic term dictated by the stiffness K and the interaction. The stiffness term favours height fields with minimum variation; in the context of the dimer model, this is because dimers in a region of constant coarse-grained height may make shifts around a closed loop that contribute to the entropy. In the continuum limit, The interaction term for $p = 4$, $\lambda_p \cos(4\theta)$ has four minima at $\theta = \{\pi/4, 3\pi/4, 5\pi/4, 7\pi/4\}$ which correspond to the average heights of the four columnar ground states of the interacting dimer model (as shown in figure 2). Vortices (θ changing by 2π around a site) are not allowed in the close-packed case (where as we have seen the allowed values of θ must satisfy $\theta = \theta + 2\pi$). The rules for assigning heights to plaquettes dictate that upon going around a monomer, i.e. a site with no dimers on it, the order parameter must change by $-4 \times \pi/2 = -2\pi$ if the monomer is on the even sublattice, and 2π if it is on the odd sublattice. Hence a monomer corresponds to

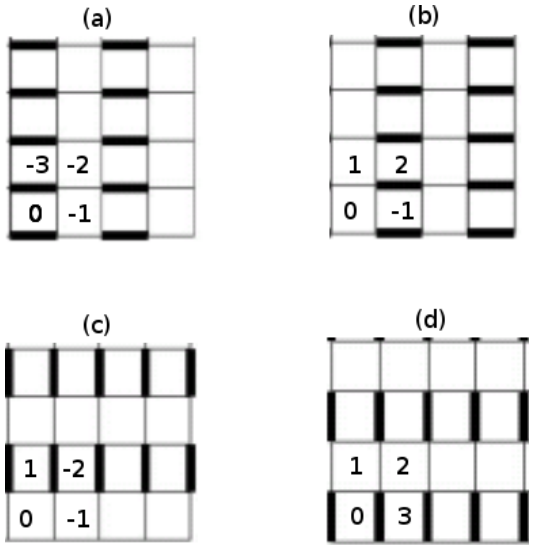

FIG. 2: The height variables for the four columnar ground states. The plaquette at the origin is assigned $h = 0$, and the remaining values follow from the rules for assigning height (see section II B 2). The displayed height configurations tile themselves across the entire lattice for each configuration. We see that the average coarse-grained height fields are $h = -3/2, 1/2, -1/2, 3/2$ for (a), (b), (c), and (d) respectively. The corresponding coarse-grained order parameter $\theta = (\pi h/2) \mod 2\pi$ takes on the values $5\pi/4, \pi/4, 7\pi/4, 3\pi/4$ respectively.

a magnetic particle (a vortex) with a charge of ± 1 in the CG picture.

C. CG predictions of the dimer model: Noninteracting case

Consider first the noninteracting case; the cosine term is absent. We have a height field with the possibility of vortices (i.e. monomer vacancies). A single electric charge $e = 1$ corresponds to a dimer, while a magnetic monopole with charge $m = \pm 1$ corresponds to a vortex. Treatment of the 2D CG gives the exponent corresponding to the magnetic and electric charge density correlation functions as [5, 9]:

$$\begin{aligned} \langle \rho_{e,m}(\mathbf{x}) \rho_{e,m}(\mathbf{x}') \rangle &\sim |\mathbf{x} - \mathbf{x}'|^{-\alpha(e,m)}; \\ \alpha(e,m) &= \frac{e^2}{2\pi K} + 2\pi K m^2 \end{aligned} \tag{4}$$

However, the exponents $\alpha(1,0) \equiv \alpha_d$, corresponding to the dimer-dimer correlation, and $\alpha(0,1) \equiv \alpha_m$, corresponding to the monomer-monomer correlation function[11], are known exactly in the close-packed case to be 2 and 1/2 respectively [10]. This allows the determination of the coupling constant K in the noninteracting case to be $K = 1/4\pi$ (note that the CG correctly predicts $\alpha_d = 1/\alpha_m$). Hence $K < 2/\pi$; i.e. the monomer fugacity is a relevant parameter. We noted in section II B 1 that the vacuum is a *critical phase* in the CG; this is reflected in the power-law correlations of the exact solution even though there is no long-range order to the dimer arrangements in the absence of interactions. The relevance of y implies that any finite density of monomers (vortices) immediately destroys the critical nature of the close-packed phase. Although the recursion relations become invalid very quickly for finite monomer density, the following qualitative picture survives: renormalization makes the interactions between particles weaker and weaker due to the screening effect of the monomers, giving rise to a finite correlation length.

D. Interacting dimers in the CG description

We now consider the case of close-packed interacting dimers, following [5]. In the Sine-Gordon formulation, the interaction was shown to correspond to a non-zero fugacity of particles with electric charge p. The noninteracting limit corresponds to $T = \infty$; we saw in the previous section that the value of K in this limit is $1/4\pi$ which is below $K_c = p^2/8\pi = 2/\pi$. Although we do not know the exact form for $K(T)$, we qualitatively expect $K(T)$ to rise as T is decreased. Turning on interactions corresponds to reducing T and correspondingly increasing $K(T)$ from $K(\infty) = 1/4\pi$. As long as $K(T) < p^2/8\pi$, y_p is irrelevant, and the system is renormalized to the vacuum which is simply the critical phase encountered in the noninteracting limit. There is a critical point at $K(T) = K_c$, beyond which y_p is renormalized to larger and larger values; i.e. the interaction proportional to y_p becomes relevant and the system settles into an *ordered phase* in which the order parameter takes on one of the four minima of the cosine potential, corresponding to the four columnar ground states which maximize the favourable parallel interactions. Hence under renormalization for $K > K_c$, the Sine-Gordon model is effectively a clock model that forces the order parameter θ into one of four values for the entire system. The system undergoes a phase transition from a disordered (albeit critical) phase to a highly ordered columnar phase.

E. Monomers in the interacting case

For the square lattice, the value $p = 4$ determined by height restrictions in the dimer picture turns out to be the special case of the Sine-Gordon model in which the the vortex fugacity y becomes marginal exactly at the critical interaction $K_c = p^2/8\pi = 2/\pi$ which marks the transition to the columnar ordered phase. This has several implications. First, as interactions are turned on, the system is unstable towards the introduction of monomers as long as it is in the critical phase ($1/4\pi < K < K_c$) since y is relevant thoughout the range. In this regard it remains similar to the noninteracting case.

The more interesting feature is that the fact that y is marginal exactly at K_c and irrelevant in the ordered phase. This suggests a critical line in the y–K plane that separates an ordered dimer phase with a low density of monomers (on the low temperature side) from a dimer-monomer liquid [4, 6]. Hence the ordered phase is robust to monomer doping compared to the critical phase.

III. CONCLUSION

We have summarized the renormalization group description of the dimer problem and the related monomer-dimer problem by mapping to the 2D Coulomb gas, presented in [4–6]. The CG matches the behaviour of the solved noninteracting close-packed dimer problem and allows a description of the more complicated monomer problem and the interacting case, which have not been exactly solved. The predictions of the CG description have been verified by a numerical transfer matrix method in [5] and Monte Carlo simulations in [6]. The problem illustrates the power of a coarse-grained renormalization group description to derive features of an unsolved system. Simultaneously, the interest in dimer problems, which has generated optimized transfer matrix and Monte Carlo techniques that are appropriate to it, provides a framework within which to numerically verify the renormalization group predictions of the Coulomb gas.

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[11] In the close-packed case, the monomer-monomer correlation function is defined in terms of the separation of exactly two vacancies in a lattice otherwise covered with dimers; hence the monomer density remains zero in the macroscopic system.