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FINITE-SIZE EFFECTS IN A DIMER MODEL OF CRYSTALLIZATION

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1. Introduction

A main problem of crystallization theory is the study of crystal growth in a fluid phase. Recently, several two-dimensional models have been proposed[1,2], in which captures and escapes of single atoms from the crystal surface have been identified with the transitions of a Markov process and the shape of the crystal edge - with its states. In such models the growth process takes place by a sequential addition of hard discs to the edge of the closely packed phase representing the crystal, see fig.1. The fluid phase in these models is treated as uncorrelated medium, so that the additions of atoms to different sites of the crystal edge could be considered as a sequence of independent random events.

A completely different picture may appear in melts or solutions with strong interparticle correlations not only in the crystal phase but in the fluid one too. For example, in the case of liquid crystals one should take into account orientational correlations in both phases. A simple model of such a situation is given by a dimer system completely covering the sites of a square lattice, as shown in fig.2. In this model the crystal may be represented by a region of regularly packed vertical dimers bordering with orientationally disordered fluid phase. In fig.2 the crystal edge is shown by a wavy line. It is easily seen that the addition of a single dimer to the crystal phase causes the rearrangement of a certain number of neighbouring dimers in the fluid phase. This illustrates the fact that crystal growth processes in correlated media may depend not only on simple kinetic properties, as in models[1,2], but on the global state of the sample as well. In this aspect the study of the equilibrium states of such systems becomes important too.

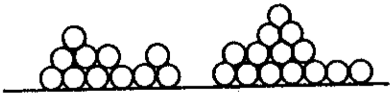


Fig. 1. Edge of crystal in a Markov rate model.

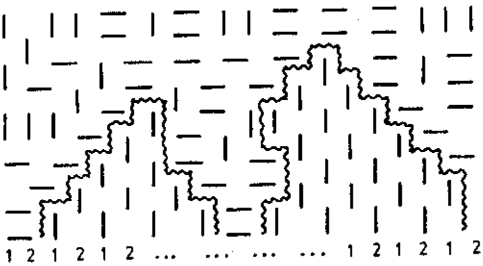


Fig. 2. Edge of crystal in the dimer model of crystallisation.

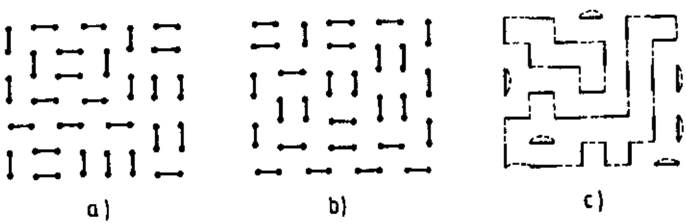
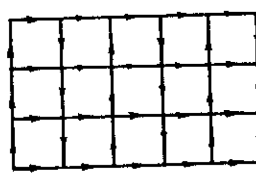


Fig. 3. Two dimer configurations and their syperposition.

Fig. 4. Arrow arrangements ensuring positivity of superpositional polygons.



Different configurations of the liquid - crystal interface can be created by fixing the number and position of vertical

dimers in a particular layer and requiring then close packing (if possible) of the dimers on the remaining lattice bonds. In fig.2 the bonds of the selected layer are labelled alternatively by 1 and 2. If all bonds with label 2 were occupied by dimers and all bonds with label 1 were vacant, then the ordered crystal phase should spread over the whole lattice. The difference $\Delta = \rho_1 - \rho_2$ of the average occupation numbers ρ_1 and ρ_2 of odd and even bonds, respectively, plays the role of an ordering parameter in the model. It is easily seen that a value $|\Delta| < 1$ is connected with the appearance of in-phase or out-of-phase crystal domains, which co-exist with orientationally disordered fluid phase. We may introduce an "external staggered field" acting on the selected layer of bonds by ascribing special activities ξ and η to the bonds labeled by 1 and 2, respectively. When $\xi/\eta \to 0$ or $\xi/\eta \to \infty$, a unique crystal phase is expected to spread over the lattice, characterized by the values -1 or +1 of the ordering parameter Δ.

It is the purpose of this paper to study the dependence of the ordering parameter Δ on the bond activities ξ and η, as well as on the lattice size. In order to obtain exact results, we simplify somewhat the problem by considering a lattice with the geometry of an infinite in the horizontal dimension cylinder.

The paper is organized as follows. In section 2 we describe the method of investigation, which reduces the problem to a random walk one. The solution of the obtained inhomogeneous equation for the corresponding generating function is derived in section 3. Section 4 contains the results and a discussion.

2. The method

There are many equivalent methods of calculation of the partition function and correlation functions in the dimer problem[3-5]. All of them exploit somehow the planarity of the lattice and lead to the evaluation of determinants of diagonizable matrices. This means that the dimer model is equivalent to a certain free-fermion problem, which in turn reduces to the solution of the discrete Laplace equation. The latter equation naturally arises in the theory of random walks. Thus the partition function of the dimer problem may be expressed in terms of the generating function of random walks. The use of the random walk theory is especially convenient in the study of correlation functions, since then various methods developed for dealing with lattice inhomogeneities can be applied.

We consider a square lattice Λ containing L rows and M columns, wrapped on a torus for the creation of periodic boundary conditions. We select the vertical lattice bonds between the $(L-1)$th and 0th row: to each dimer covering such a bond we assign a weight ξ if the column number is odd and a weight η if the column number is even. All the remaining vertical dimers have equal weights y and all the horizontal dimers have equal weights x. Define $Z_\Lambda(x,y,\xi,\eta)$ as the partition function of all dimer configurations, in which the lattice Λ is completely covered by dimers.

To reduce our problem to a random walk one, it is convenient to consider the square of the partition function, Z_Λ^2, rather than Z_Λ itself. Consider the superposition of any two dimer configurations entering into the product of the partition functions. It contains closed superpositional polygons, along which the dimers originating from the different partition functions alternate, and pairs of coinciding dimers. Both the former and the latter will be depicted as closed loops. Each lattice site belonging to a loop will be met just once at completing a run along the loop. This means that the loops are not self-intersecting. An example of a superposition of two dimer configurations and the corresponding set of loops is shown in fig.3. The loops containing more than two bonds have two orientations which distinguish between the two ways of alternating the bonds from the first and the second co-factor in the product $Z_\Lambda Z_\Lambda$; otherwise the choice of the orientation is arbitrary. In an elementary loop containing two bonds both orientations are considered as equivalent. Thus the square of the partition function, Z_Λ^2 , represents a weighted sum over all configurations of oriented loops completely covering the lattice.

Consider now a random walk on the lattice Λ . Each oriented loop of length $n \geq 2$ (n - even) is represented by a closed path running along n bonds without self-intersection. Let us assign a weight

$$\mathcal{X}(p) = \prod_{i=1}^{n} \omega(b_i) \qquad (2.1)$$

to any closed path, possibly self-intersecting, which runs along the bonds $b_1, b_2, \ldots, b_n$ (there may be coinciding bonds among them). In (2.1) the weight $\omega(b_i)$ of the step along the bond b_i takes the value xt , yt , ξt or ηt if the weight of the dimer covering that bond is x , y , ξ or η , respectively. Denote by $\{p\}_\Lambda$ the set of paths <u>without self-intersections</u>, such that no two paths from this set have a common lattice site. Introduce the partition function

$$Z_\Lambda^{(t)}(xt, yt, \xi t, \eta t) = \sum_{\{p\}_\Lambda} \prod_{p \in \{p\}_\Lambda} \mathcal{X}(p) , \qquad (2.2)$$

where the summation is over all possible sets $\{p\}_\Lambda$. The limit $t \to \infty$ corresponds to close packing of the paths and may be written as

$$\lim_{t \to \infty} t^{-ML} Z_\Lambda^{(t)}(xt, yt, \xi t, \eta t) = Z_\Lambda^2(x, y, \xi, \eta) . \qquad (2.3)$$

This means that all the thermodynamic functions, calculated with the aid of $Z_\Lambda^{(t)}$, yield in the limit $t \to \infty$ the corresponding thermodynamic functions of the dimer problem.

The enumeration of all configurations of closed paths, which enter into the partition function $Z_\Lambda^{(t)}$, is based on the equality

$$\prod_p{}' [1-\chi(p)] = \sum_{\{p\}_\Lambda} \prod_{p\in\{p\}_\Lambda} [-\chi(p)] , \tag{2.4}$$

where the prime in the left-hand side means that the product is taken over all non-periodic closed paths, i.e. over paths for which the sequence of bonds passed, $b_1, b_2, \ldots, b_n$, cannot be represented in the form $(b_1,\ldots,b_k),(b_1,\ldots,b_k),\ldots,(b_1,\ldots b_k)$ with some $k<n$. The identity (2.4) with a more general weight function χ is known in the context of the Ising model as Feynman's conjecture; its proof is given by Sherman[6]). In our case (2.4) has a rather simple meaning. A correspondence can be established between each term in the expansion of the left-hand side of (2.4) and a set of paths on the lattice. Consider a set in which two paths, p_1 and p_2, have a site in common, say $s\in\Lambda$. In the expansion of the left-hand side of the identity, a term can be found which completely reproduces the above set but with one exception: instead of the two intersecting paths, p_1 and p_2, there is just one self-intersecting at the site s path. The numbers of paths in the two sets differ by one while all the weights ω coincide. Since each path enters into (2.4) with minus sign, the contributions of the two intersecting and the one self-intersecting paths cancel out. Similar considerations hold true also in the case when p_1 and p_2 have several sites in common. The only exception is the case of periodic paths, when the random walking particle passes two or more times the same trajectory. Due to the fact that in the product in the left-hand side of (2.4) all paths are different, the expansion of that product does not contain terms which could cancel out periodic paths. That is why the periodic paths are excluded from the product.

As a result of the cancellation of all intersecting paths, in the right-hand side of (2.4) there remains a sum over all sets $\{p\}_\Lambda$ of paths without intersections. Thus the right-hand side of (2.4) coincides with the partition function (2.2) up to the factor -1 of each closed path in (2.4). In order to compensate for the wrong sign, we replace (2.1) by new weights of the random walk. Let us attach arrows to the bonds, as shown in fig.4. To each step traversed in the direction of the bond b_i we assign now a weight $\omega(b_i)$, and to a step traversed in the opposite direction we assign weight $-\omega(b_i)$. This change of weights does not ensure by itself the proper sign of each path p. But in the limit of close packing, see (2.3), there are only superpositional polygons left which completely cover the lattice. For such polygons a theorem due to Kasteleyn[7]) holds, which ensures the necessary change of sign.

Define instead of (2.1) a new weight function $\tilde{\chi}$, which on a path p consisting of the steps $s_1, s_2, \dots, s_n$ takes the value

$$\tilde{\chi}(p) = \prod_{i=1}^{n} \omega(b_i)\, \mathrm{sign}(s_i) \;, \tag{2.5}$$

where sign(s_i) = +1 if the step s_i is in the direction of the oriented bond b_i, and sign(s_i) = -1 in the opposite case. Then from equations (2.2) - (2.4) and Kasteleyn's theorem we obtain for $t \to \infty$

$$Z_\Lambda^{(t)}(xt, yt, \xi t, \eta t) = \prod_p{}' \left[1 - \tilde{\chi}(p)\right] \;. \tag{2.6}$$

There is still one defect remaining in the close-packing limit of expression (2.6): Kasteleyn's theorem ensures positivity of all superpositional <u>planar</u> polygons. But in the representation of $Z_\Lambda^{(t)}$ there are also polygons looping the torus once or several times either in horizontal or in vertical direction, or in both directions. The sign of these polygons does not change under the above replacement. In the remainder we confine ourselves to the finite-size effects in one dimension only, namely we keep L finite and pass to the limit $M \to \infty$. In this limit the lattice Λ has the geometry of an infinite cylinder. Any closed path looping the cylinder crosses any row an odd number of times. Therefore, each such path contains an odd power of ξ or η and hence the change $\xi \to -\xi$, $\eta \to -\eta$ in the right-hand side of (2.6) ensures its positivity.

Taking logarithm of both sides of eq.(2.6) we obtain

$$\ln Z_\Lambda^{(t)}(xt, yt, \xi t, \eta t) = \ln \prod_p{}' [1 - \tilde{X}(p)] . \qquad (2.7)$$

By expanding the logarithm in the right-hand side of (2.7) we obtain

$$\ln \prod_p{}' [1-\tilde{X}(p)] = -\sum_p{}' \sum_{j=1}^{\infty} \frac{1}{j} [\tilde{X}(p)]^j = -\sum_{i\in\Lambda} \sum_{n=1}^{\infty} \frac{1}{n} S_n(i) , \qquad (2.8)$$

where $S_n(i)$ is a sum over paths weighed according to the above described rules. This sum contains <u>all possible</u> closed paths starting and ending at site $i\in\Lambda$. Note that in the last equation (2.8) we have relaxed the condition for non-periodicity of the paths by interpreting $[\tilde{X}(p)]^j$ as a periodic path consisting of j cycles. The relaxation of all constraints on the paths allows us to use generating functions of simple random walks.

Note that the introduction of oriented lattice Λ breaks the translational invariance in horizontal direction. The invariance can be restored by introducing an elementary cell of two sites which are nearest neighbours in the same row. We label the sites in the elementary cell by σ , $\sigma = 1,2$.

Denote by $W_n^{\sigma\sigma'}(\ell,m|\ell',m')$ the weighed sum over all paths consisting of n steps, starting from site σ' in the cell $\underset{\sim}{r}' = (\ell', m')$ and ending at site σ in the cell $\underset{\sim}{r} = (\ell, m)$. The weight function of steps takes values $\pm xt, \pm yt, \pm \xi t, \pm \eta t$ similarly to the weight function for closed paths (2.5). The sum over the lattice sites in the right-hand side of (2.8) may be expressed in terms of $W_n^{\sigma\sigma'}$ as follows:

$$\sum_{i\in\Lambda} S_n(i) = \sum_{\sigma=1}^{2}\sum_{\ell=0}^{L-1}\sum_{m=1}^{M/2} W_n^{\sigma\sigma}(\ell,m|\ell,m) . \qquad (2.9)$$

Correspondingly, expression (2.7) takes the form

$$\ln Z_\Lambda^{(t)}(xt,yt,\xi t,\eta t) = -\sum_{\sigma=1}^{2}\sum_{\ell=0}^{L-1}\sum_{m=1}^{M/2}\sum_{n=1}^{\infty}\frac{1}{n}W_n^{\sigma\sigma}(\ell,m|\ell,m) . \qquad (2.10)$$

The function $W_n^{\sigma\sigma'}$ obeys the recurrence relation

$$W_{n+1}^{\sigma\sigma_0}(\underset{\sim}{r}|\underset{\sim}{r}_0) = \sum_{\underset{\sim}{r}',\sigma'} \gamma^{\sigma\sigma'}(\underset{\sim}{r}|\underset{\sim}{r}')W_n^{\sigma'\sigma_0}(\underset{\sim}{r}'|\underset{\sim}{r}_0) . \qquad (2.11)$$

The transition matrix $\gamma^{\sigma\sigma'}$ can be conveniently represented as a sum of two terms,

$$\gamma^{\sigma\sigma'} = p^{\sigma\sigma'} + q^{\sigma\sigma'}, \qquad (2.12)$$

where $p^{\sigma\sigma'}$ is the translationally invariant part and $q^{\sigma\sigma'}$ is connected with the presence of "defect" bonds ξ and η .

According to eq.(2.5) we have

$$p^{\sigma\sigma'}(\underset{\sim}{r}|\underset{\sim}{r}') = \begin{pmatrix} ty\delta_{m,m'}(\delta_{\ell,\ell'+1}-\delta_{\ell,\ell'-1}) & tx\delta_{\ell,\ell'}(-\delta_{m,m'-1}+\delta_{m,m'}) \\ tx\delta_{\ell,\ell'}(\delta_{m,m'+1}-\delta_{m,m'}) & ty\delta_{m,m'}(-\delta_{\ell,\ell'+1}+\delta_{\ell,\ell'-1}) \end{pmatrix} \qquad (2.13)$$

and

$$q^{\sigma\sigma'}(\underset{\sim}{r}|\underset{\sim}{r}') = \begin{pmatrix} -t(\xi+y)\delta_{m,m'}(-\delta_{\ell,L-1}\delta_{\ell',0}+\delta_{\ell,0}\delta_{\ell',L-1}) & 0 \\ 0 & t(\eta+y)\delta_{m,m'}(\delta_{\ell,L-1}\delta_{\ell',0}-\delta_{\ell,0}\delta_{\ell',L-1}) \end{pmatrix} . \qquad (2.14)$$

Introduce now the generating function

$$W^{\sigma\sigma'}(\ell,m|\ell',m') = \sum_{n=0}^{\infty} W_n^{\sigma\sigma'}(\ell,m|\ell',m') \qquad (2.15)$$

and sum up both sides of eq.(2.11) over n. Taking into account (2.12) and the initial condition

$$W_0^{\sigma\sigma'}(\ell,m|\ell',m') = \delta_{\sigma,\sigma'}\,\delta_{\ell,\ell'}\,\delta_{m,m'} \quad , \tag{2.16}$$

we obtain

$$\begin{aligned} W^{\sigma\sigma_0}(\underset{\sim}{r}|\underset{\sim}{r}_0) - \sum_{\underset{\sim}{r}',\sigma'} p^{\sigma\sigma'}(\underset{\sim}{r}|\underset{\sim}{r}')\,W^{\sigma'\sigma_0}(\underset{\sim}{r}'|\underset{\sim}{r}_0) = \\ = \delta_{\underset{\sim}{r},\underset{\sim}{r}_0}\,\delta_{\sigma,\sigma_0} + \sum_{\underset{\sim}{r}',\sigma'} q^{\sigma\sigma'}(\underset{\sim}{r}|\underset{\sim}{r}')\,W^{\sigma'\sigma_0}(\underset{\sim}{r}'|\underset{\sim}{r}_0) \; . \end{aligned} \tag{2.17}$$

From (2.10) it follows that in order to evaluate the partition function Z_Λ, we need the solution of the inhomogeneous equation (2.17) $W^{\sigma\sigma}(\underset{\sim}{r}|\underset{\sim}{r})$ for all $\underset{\sim}{r}\in\Lambda$. However, the problem can be significantly simplified if we take into account that the ordering parameter, mentioned in the Introduction, is the difference in the densities ρ_ξ and ρ_η of the dimers with activities ξ and η. Let us introduce

$$\rho_\xi(t) = \frac{1}{2M}\,\xi\,\frac{\partial}{\partial\xi}\,\ln Z_\Lambda^{(t)}(xt,yt,\xi t,\eta t) \; . \tag{2.18}$$

In view of relation (2.3) we have

$$\lim_{t\to\infty}\rho_\xi(t) = \rho_\xi \; . \tag{2.19}$$

The differentiation with respect to ξ in (2.18) selects from the sum (2.10) only those paths which pass a bond ξ at least once. If a path passes along ξ-bonds ν times, then its weight will contain a factor ξ^ν. The action of the operator $\xi\partial/\partial\xi$ leads to the appearance of a factor ν in front of its weight. A non-periodic clcsed path of length n may have as many as n starting points. With account of the factor n^{-1} each such path enters into the sum (2.10) with a coefficient ν. A path of length n containing j cycles has again n starting points and, therefore, enters into the sum (2.10) with a coefficient ν/j.

Consider now the sum

$$\sum_{m=1}^{M/2} \sum_{n=1}^{\infty} \overline{W}_n^{11}(0,m|0,m) , \tag{2.20}$$

where the bar means that only paths traversing a ξ-bond at the first or final step enter into $\overline{W}_n^{\sigma\sigma}$. It is easily seen that each non-periodic path passing along ξ-bonds ν times enters into the sum (2.19) ν times, since it may start or end at each of the ξ-bonds. A periodic path of j cycles enters into (2.19) with a coefficient ν/j which equals to all the possible starting points of the path in this case.

From the above considerations it follows that

$$\rho_\xi(t) = -\frac{1}{2M} \sum_{m=1}^{M/2} \sum_{n=1}^{\infty} \overline{W}_n^{11}(0,m|0,m) . \tag{2.21}$$

In order to introduce the generating function $W^{\sigma\sigma}$, we notice that

$$\overline{W}_n^{11}(0,m|0,m) = -\xi t\, W_{n-1}^{11}(L-1,m|0,m) + \xi t\, W_{n-1}^{11}(0,m|L-1,m), \tag{2.22}$$

and, with account of the lattice symmetry,

$$\overline{W}_n^{11}(0,m|0,m) = -2\xi t\, W_{n-1}^{11}(L-1,m|0,m) . \tag{2.23}$$

From equations (2.15), (2.19) - (2.23) and the translational invariance in the horizontal direction we obtain for ρ_ξ the final expression

$$\rho_\xi = \lim_{t\to\infty} \tfrac{1}{2}\xi t\, W^{11}(L-1,0|0,0) \tag{2.24}$$

and an analogous expression for ρ_η:

$$\rho_\eta = \lim_{t\to\infty} \tfrac{1}{2}\eta t\, W^{22}(L-1,0|0,0) . \tag{2.25}$$

Thus we have reduced the initial problem to the standard task of finding the generating functions of simple random walks on the lattice.

3. Solution of the equation for the generating function

Here we describe in short the method of solving the system of equations (2.17) which in expanded form reads:

$$W_{11}(\ell,m)+yt\left[W_{11}(\ell+1,m)-W_{11}(\ell-1,m)\right]+xt\left[W_{21}(\ell,m+1)-W_{21}(\ell,m)\right]=$$
$$=\delta_{\ell,0}\delta_{m,0}+(\xi+y)t\left[\delta_{\ell,L-1}W_{11}(0,m)-\delta_{\ell,0}W_{11}(L-1,m)\right], \tag{3.1a}$$

$$W_{12}(\ell,m)+yt\left[W_{12}(\ell+1,m)-W_{12}(\ell-1,m)\right]+xt\left[W_{22}(\ell,m+1)-W_{22}(\ell,m)\right]=$$
$$=(\xi+y)t\left[\delta_{\ell,L-1}W_{12}(0,m)-\delta_{\ell,0}W_{12}(L-1,m)\right], \tag{3.1b}$$

$$W_{21}(\ell,m)-yt\left[W_{21}(\ell+1,m)-W_{21}(\ell-1,m)\right]+xt\left[W_{11}(\ell,m)-W_{11}(\ell,m-1)\right]=$$
$$=-(\eta+y)t\left[\delta_{\ell,L-1}W_{21}(0,m)-\delta_{\ell,0}W_{21}(L-1,m)\right], \tag{3.1c}$$

$$W_{22}(\ell,m)-yt\left[W_{22}(\ell+1,m)-W_{22}(\ell-1,m)\right]+xt\left[W_{12}(\ell,m)-W_{12}(\ell,m-1)\right]=$$
$$=\delta_{\ell,0}\delta_{m,0}-(\eta+y)t\left[\delta_{\ell,L-1}W_{22}(0,m)-\delta_{\ell,0}W_{22}(L-1,m)\right]. \tag{3.1d}$$

Here for the sake of brevity we have set

$$W_{\sigma\sigma'}(\ell,m)=W^{\sigma\sigma'}(\ell,m\,|\,0,0;xt,yt,\xi t,\eta t)\ , \quad \sigma,\sigma'=1,2,$$

with (ℓ,m) , respectively $(0,0)$, being the coordinates of the final point $\underset{\sim}{r}$ and the initial point $\underset{\sim}{r}_0$.

It is readily seen that (3.1a) and (3.1c) comprise a set of coupled equations for the functions $W_{11}(\ell,m)$ and $W_{21}(\ell,m)$, while (3.1b) and (3.1d) comprise another set of coupled equations for the functions $W_{22}(\ell,m)$ and $W_{12}(\ell,m)$. Due to the symmetry relation

$$W^{22}(\ell,m\,|\,0,0;x,y,\xi,\eta) = W^{11}(\ell,m\,|\,0,0;x,y,\eta,\xi), \tag{3.2}$$

we need to solve the first set of coupled equations, (3.1a) and (3.1c), only, which after the Fourier transformation

$$\begin{aligned}\hat{W}_{\sigma\sigma'}(a_1,a_2) &= \frac{2}{LM}\sum_{\ell=0}^{L-1}\sum_{m=1}^{M/2} W_{\sigma\sigma'}(\ell,m)\exp\left(-2\pi i a_1\ell/L - 4\pi i a_2 m/M\right)\\ W_{\sigma\sigma'}(\ell,m) &= \sum_{a_1=0}^{L-1}\sum_{a_2=0}^{M/2}\hat{W}_{\sigma\sigma'}(a_1,a_2)\exp\left(2\pi i a_1\ell/L + 4\pi i a_2 m/M\right),\end{aligned} \tag{3.3}$$

takes the form

$$\begin{aligned}&\left[1+2iyt\sin\frac{2\pi a_1}{L}\right]\hat{W}_{11}(a_1,a_2) + xt\left(e^{4\pi i a_2/M}-1\right)\hat{W}_{21}(a_1,a_2) =\\ &\quad = \frac{2}{LM} + \frac{(\xi+y)t}{L}\left[e^{2\pi i a_1/L}\,\tilde{W}_{11}(0,a_2) - \tilde{W}_{11}(L-1,a_2)\right],\end{aligned} \tag{3.4a}$$

$$\begin{aligned}&\left[1-2iyt\sin\frac{2\pi a_1}{L}\right]\hat{W}_{21}(a_1,a_2) - xt\left(e^{-4\pi i a_2/M}-1\right)\hat{W}_{11}(a_1,a_2) =\\ &\quad = -\frac{(\eta+y)t}{L}\left[e^{2\pi i a_1/L}\,\tilde{W}_{21}(0,a_2) - \tilde{W}_{21}(L-1,a_2)\right].\end{aligned} \tag{3.4b}$$

Here $\tilde{W}_{\sigma\sigma'}$ denotes the Fourier transform of $W_{\sigma\sigma'}$ with respect to the second coordinate only,

$$\begin{aligned}\tilde{W}_{\sigma\sigma'}(\ell,a_2) &= \frac{2}{M}\sum_{m=1}^{M/2} W_{\sigma\sigma'}(\ell,m)\exp\left(-4\pi i a_2 m/M\right)\\ W_{\sigma\sigma'}(\ell,m) &= \sum_{a_2=1}^{M/2}\tilde{W}_{\sigma\sigma'}(\ell,a_2)\exp\left(4\pi i a_2 m/M\right).\end{aligned} \tag{3.5}$$

Now we consider (3.4a) and (3.4b) as a system of linear equations for $\hat{W}_{11}(a_1,a_2)$ and $\hat{W}_{21}(a_1,a_2)$. Its solution reads:

$$\hat{W}_{11}(a_1,a_2) = \frac{2}{tLM} B_{11}(a_1,a_2) + \frac{(\xi+y)}{L} B_{11}(a_1,a_2)\left[e^{2\pi i a_1/L}\tilde{W}_{11}(0,a_2) - \tilde{W}_{11}(L-1,a_2)\right] - \tag{3.6a}$$
$$- \frac{(\eta+y)}{L} B_{12}(a_1,a_2)\left[e^{2\pi i a_1/L}\tilde{W}_{21}(0,a_2) - \tilde{W}_{21}(L-1,a_2)\right],$$

$$\hat{W}_{21}(a_1,a_2) = -\frac{2}{tLM} B^*_{12}(a_1,a_2) - \frac{(\xi+y)}{L} B^*_{12}(a_1,a_2)\left[e^{2\pi i a_1/L}\tilde{W}_{11}(0,a_2) - \tilde{W}_{11}(L-1,a_2)\right] - \tag{3.6b}$$
$$- \frac{(\eta+y)}{L} B^*_{11}(a_1,a_2)\left[e^{2\pi i a_1/L}\tilde{W}_{21}(0,a_2) - \tilde{W}_{21}(L-1,a_2)\right],$$

where $B^*_{\sigma\sigma'}$ is the complex conjugate of $B_{\sigma\sigma'}$, and

$$B_{11}(a_1,a_2) = \frac{1}{\mathcal{D}(a_1,a_2)}\left[t^{-1} - 2iy\sin\frac{2\pi a_1}{L}\right]$$
$$B_{12}(a_1,a_2) = \frac{x}{\mathcal{D}(a_1,a_2)}\left[1 - \exp(4\pi i a_2/M)\right] \tag{3.7}$$

with

$$\mathcal{D}(a_1,a_2) = 4y^2\sin^2\frac{2\pi a_1}{L} + 4x^2\sin^2\frac{2\pi a_2}{M} + t^{-2}. \tag{3.8}$$

Next we have to determine the four quantities $\tilde{W}_{11}(0,a_2)$, $\tilde{W}_{21}(0,a_2)$, $\tilde{W}_{11}(L-1,a_2)$ and $\tilde{W}_{21}(L-1,a_2)$ which enter into equations (3.6). To this end we notice that

$$\sum_{a_1=0}^{L-1} \hat{W}_{\sigma\sigma'}(a_1,a_2) = \tilde{W}_{\sigma\sigma'}(0,a_2)$$
$$\sum_{a_1=0}^{L-1} e^{-2\pi i a_1/L}\hat{W}_{\sigma\sigma'}(a_1,a_2) = \tilde{W}_{\sigma\sigma'}(L-1,a_2), \tag{3.9}$$

and, therefore, the summation of equations (3.6a) and (3.6b) over a_1 , from 0 to $L-1$, and the summation of the same equations multiplied beforehand by $\exp(-2\pi i a_1/L)$, yields the required closed set of coupled linear equations:

$$\widetilde{W}_{11}(0,a_2) = \frac{2}{tM} A_{11}(0,a_2) + (\xi+y)\left[A_{11}(L-1,a_2)\widetilde{W}_{11}(0,a_2) - A_{11}(0,a_2)\widetilde{W}_{11}(L-1,a_2)\right] -$$

$$- (\eta+y)\left[A_{12}(L-1,a_2)\widetilde{W}_{21}(0,a_2) - A_{12}(0,a_2)\widetilde{W}_{21}(L-1,a_2)\right],$$

$$\widetilde{W}_{21}(0,a_2) = \frac{2}{tM} A_{21}(0,a_2) + (\xi+y)\left[A_{21}(L-1,a_2)\widetilde{W}_{11}(0,a_2) - A_{21}(0,a_2)\widetilde{W}_{11}(L-1,a_2)\right] -$$

$$- (\eta+y)\left[A_{22}(L-1,a_2)\widetilde{W}_{21}(0,a_2) - A_{22}(0,a_2)\widetilde{W}_{21}(L-1,a_2)\right],$$

$$(3.10)$$

$$\widetilde{W}_{11}(L-1,a_2) = \frac{2}{tM} A_{11}(1,a_2) + (\xi+y)\left[A_{11}(0,a_2)\widetilde{W}_{11}(0,a_2) - A_{11}(1,a_2)\widetilde{W}_{11}(L-1,a_2)\right] -$$

$$- (\eta+y)\left[A_{12}(0,a_2)\widetilde{W}_{21}(0,a_2) - A_{12}(1,a_2)\widetilde{W}_{21}(L-1,a_2)\right],$$

$$\widetilde{W}_{21}(L-1,a_2) = \frac{2}{tM} A_{21}(1,a_2) + (\xi+y)\left[A_{21}(0,a_2)\widetilde{W}_{11}(0,a_2) - A_{21}(1,a_2)\widetilde{W}_{11}(L-1,a_2)\right] -$$

$$- (\eta+y)\left[A_{22}(0,a_2)\widetilde{W}_{21}(0,a_2) - A_{22}(1,a_2)\widetilde{W}_{21}(L-1,a_2)\right].$$

Here we have introduced the notation

$$A_{\sigma\sigma'}(\ell,a_2) = \frac{1}{L}\sum_{a_1=0}^{L-1} e^{-2\pi i a_1 \ell/L} \begin{pmatrix} B_{11}(a_1,a_2) & B_{12}(a_1,a_2) \\ -B_{12}^{*}(a_1,a_2) & B_{11}^{*}(a_1,a_2) \end{pmatrix}. \qquad (3.11)$$

There are specific relationships between coefficients (3.11) at $\ell = L-1,\ 0,\ 1$ which greatly simplify the solution of eqs.(3.10). Namely, we notice that for L even and any a_2 ,

$$A_{11}(0,a_2) = A_{22}(0,a_2),$$

$$A_{12}(0,a_2) = -A_{21}^{*}(0,a_2) = x\left(1 - e^{4\pi i a_2/M}\right)A_{11}(0,a_2),$$

$$A_{11}(1,a_2) = -A_{22}(1,a_2) = -A_{11}(L-1,a_2) = A_{22}(L-1,a_2), \qquad (3.12)$$

$$A_{12}(1,a_2) = A_{21}(1,a_2) = A_{12}(L-1,a_2) = A_{21}(L-1,a_2) = 0,$$

$$A_{11}(1,a_2) = -\frac{1}{2y}\left\{1 - \left[4x^2\sin^2\frac{2\pi a_2}{M} + t^{-2}\right]A_{11}(0,a_2)\right\}.$$

Therefore, all the coefficients $A_{\sigma\sigma'}(\ell, a_2)$ with $\ell = L-1, 0, 1$ can be expressed in terms of just one sum,

$$A_{11}(0,a_2) = \frac{2}{L}\sum_{a_1=0}^{L/2-1}\left[4y^2\sin^2\frac{2\pi a_1}{L} + 4x^2\sin^2\frac{2\pi a_2}{M} + t^{-2}\right]^{-1}. \tag{3.13}$$

The next essential simplification arises in the close-packing limit. At the present stage of analysis this limit amounts to keeping just the leading order terms in t. Thus one finds (the complete solutions of eqs.(3.10) are given in the Appendix)

$$\tilde{W}_{11}(0,a_2) = \frac{2}{tM}\left\{\left[\frac{y^2+\eta^2}{2y^2} + \frac{y^2-\eta^2}{2y^2}4x^2\sin^2\frac{2\pi a_2}{M}A_{11}(0,a_2) + \frac{(\eta+y)^2}{y^2}\delta_L(a_2)(1+\delta_L(a_2))\right]\frac{A_{11}(0,a_2)}{d^2(a_2)} + O(t^{-2})\right\}, \tag{3.14a}$$

$$\tilde{W}_{21}(0,a_2) = -\frac{2}{tM}\left\{x(1-e^{-4\pi i a_2/M})\frac{A_{11}(0,a_2)}{d(a_2)} + O(t^{-2})\right\}, \tag{3.14b}$$

$$\tilde{W}_{11}(L-1,a_2) = \frac{2}{tM}\left\{\frac{1}{\xi+y} - \frac{1}{\xi+y}\left[\frac{y-\eta}{2y} + \frac{y+\eta}{2y}4x^2\sin^2\frac{2\pi a_2}{M}A_{11}(0,a_2)\right]\frac{1}{d(a_2)} + O(t^{-2})\right\}, \tag{3.14c}$$

$$\tilde{W}_{21}(L-1,a_2) = -\frac{2}{tM}\left\{(\xi-\eta)x(1-e^{-4\pi i a_2/M})\frac{A_{11}^2(0,a_2)}{d^2(a_2)} + O(t^{-2})\right\}, \tag{3.14d}$$

where

$$d(a_2) = \frac{y^2+\xi\eta}{2y^2} + \frac{y^2-\xi\eta}{2y^2}4x^2\sin^2\frac{2\pi a_2}{M}A_{11}(0,a_2) + \frac{(\xi+y)(\eta+y)}{y^2}\delta_L(a_2)\left[1+\delta_L(a_2)\right] + O(t^{-2}) \tag{3.15}$$

and

$$\delta_L(a_2)=\frac{1}{2}\left\{4x\left|\sin\frac{2\pi a_2}{M}\right|\left[y^2+x^2\sin^2\frac{2\pi a_2}{M}\right]^{1/2}A_{11}(0,a_2)-1\right\}. \qquad (3.16)$$

Notice that $\delta_L(a_2)\to 0$ when $L\to\infty$, since

$$\lim_{L\to\infty} A_{11}(0,a_2)=\left[4x^2\sin^2\frac{2\pi a_2}{M}+t^{-2}\right]^{-1/2}\left[4y^2+4x^2\sin^2\frac{2\pi a_2}{M}+t^{-2}\right]^{-1/2}=$$

$$=\frac{1}{4x}\left|\sin\frac{2\pi a_2}{M}\right|^{-1}\left[y^2+x^2\sin^2\frac{2\pi a_2}{M}\right]^{-1/2}+O(t^{-2}). \qquad (3.17)$$

Now we turn our attention to equation (3.14c). Obviously, from (3.3) and (3.9) we have

$$W_{11}(L-1,0)=\sum_{a_2=1}^{M/2}\tilde{W}_{11}(L-1,a_2). \qquad (3.18)$$

Thus, by summation of (3.14c) over a_2 from 1 to $M/2$, and subsequently passing to the limit $M\to\infty$, we obtain the desired result

$$\lim_{M\to\infty} W^{11}(L-1,0|0,0;x,y,\xi,\eta)=$$

$$=\frac{1}{(\xi+y)t}\left\{1-\frac{1}{\pi}\int_0^{\pi}d\varphi\,\frac{y(y-\eta)+y(y+\eta)R(\varphi)[1+2\delta_L(\varphi)]}{y^2+\xi\eta+(y^2-\xi\eta)R(\varphi)[1+2\delta_L(\varphi)]+2(\xi+y)(\eta+y)\delta_L(\varphi)[1+\delta_L(\varphi)]}\right\}, \qquad (3.19)$$

where, in the close-packing limit ($t\to\infty$),

$$R(\varphi)=x\,|\sin\varphi|\,(y^2+x^2\sin^2\varphi)^{-1/2}, \qquad (3.20)$$

$$\delta_L(\varphi)=y^L\left\{\left[x|\sin\varphi|+(y^2+x^2\sin^2\varphi)^{1/2}\right]^L-y^L\right\}^{-1}. \qquad (3.21)$$

The result for $\delta_L(\varphi)$ in (3.21) is exact. It can be easily obtained by using the identity[3])

$$\prod_{k=1}^{L/2} 2\left[u^2+\sin^2\frac{2\pi k}{L}\right]^{1/2} = \left[(1+u^2)^{1/2}+|u|\right]^{L/2} - \left[(1+u^2)^{1/2}-|u|\right]^{L/2} . \tag{3.22}$$

Indeed, by differentiation with respect to u of the logarithm of both sides of eq.(3.22), one finds

$$\begin{aligned} &\frac{2}{L}\sum_{k=1}^{L/2}\left[1+u^{-2}\sin^2\frac{2\pi k}{L}\right]^{-1} = \\ &\quad = (1+u^{-2})^{-1/2}\left\{1+2\,\frac{|u|^{-L}}{\left[1+(1+u^{-2})^{1/2}\right]^{L}-|u|^{-L}}\right\} . \end{aligned} \tag{3.23}$$

The expression for $\delta_L(\varphi)$ now follows by setting here

$$u = x\,|\sin\varphi|/y$$

and taking the definition (3.13) of $A_{11}(0,a_2)$ in the close-packing limit.

In the limit of large L we may separate in expression (3.19) the bulk term,

$$\begin{aligned} &W^{11}_{bulk}(L-1,0|0,0;x,y,\xi,\eta) = \\ &= \frac{1}{(\xi+y)t}\left\{1-\frac{1}{\pi}\int_0^{\pi} d\varphi\,\frac{y(y-\eta)+y(y+\eta)R(\varphi)}{y^2+\xi\eta+(y^2-\xi\eta)R(\varphi)}\right\} = \\ &= \eta t^{-1}\frac{1}{\pi}\int_0^{\pi} d\varphi\,\frac{1-R(\varphi)}{y^2+\xi\eta+(y^2-\xi\eta)R(\varphi)} , \end{aligned} \tag{3.24}$$

and the finite-size correction term,

$$\begin{aligned} &W^{11}_{corr}(L-1,0|0,0;x,y,\xi,\eta) = \\ &= 2yt^{-1}\frac{1}{\pi}\int_0^{\pi} d\varphi\,\frac{P(\varphi)[1+\delta_L(\varphi)]+2\eta y R(\varphi)\delta_L(\varphi)}{Q(\varphi)[Q(\varphi)+2\delta_L(\varphi)S(\varphi)]}\,\delta_L(\varphi) , \end{aligned} \tag{3.25}$$

where

$$
\begin{aligned}
P(\varphi) &= y^2-\eta^2+(y^2+\eta^2)R(\varphi) \\
Q(\varphi) &= y^2+\xi\eta+(y^2-\xi\eta)R(\varphi) \qquad\qquad (3.26) \\
S(\varphi) &= (y^2-\xi\eta)R(\varphi)+(\xi+y)(\eta+y)[1+\delta_L(\varphi)] \,.
\end{aligned}
$$

When $L\to\infty$, $\delta_L(\varphi)$ is essentially different from zero in the neighbourhood of the points $\varphi=k\pi$, $k=0,\pm1,\pm2,\cdots$, where

$$\delta_L(\varphi)\sim\left[\exp\left(L\frac{x}{y}|\sin\varphi|\right)+1\right]^{-1} \quad (L\to\infty\,,\ |\varphi-k\pi|\to 0). \qquad (3.27)$$

Since in the neighbourhood of these points $R(\varphi)\sim x|\sin\varphi|/y$, the leading-order finite-size correction becomes

$$W_{corr}^{11}(L-1,0|0,0;x,y,\xi,\eta)\simeq\frac{2}{\pi L}\,\frac{y^2(y^2-\eta^2)}{tx(y^2+\xi\eta)^2}\int_0^\infty dz\left[\cosh z+\frac{y(\xi+\eta)}{y^2+\xi\eta}\right]^{-1}. \qquad (3.28)$$

Evidently, at $y=\eta$ the $O(L^{-1})$ correction vanishes. In the case $\xi=\eta=y$ we obtain from (3.25), (3.26)

$$W_{corr}^{11}(L-1,0|0,0;x,y,y,y)=\frac{1}{yt}\,\frac{1}{\pi}\int_0^\pi d\varphi\,R(\varphi)\,\frac{\delta_L(\varphi)}{1+2\delta_L(\varphi)}\,. \qquad (3.29)$$

In the limit $L\to\infty$ equation (3.29) yields

$$W_{corr}^{11}(L-1,0|0,0;x,y,y,y)\simeq\frac{1}{xt}\,\frac{\pi}{6L^2} \quad (Lx/y\to\infty)\,. \qquad (3.30)$$

We emphasize that expression (3.19) is an exact result, valid for any even number L. In the special case of translationally invariant infinite cylinder, i.e. when $\xi=\eta=y$, it gives for the average density of horizontal dimers, see eqs.(2.24),(2.25)

$$\rho_y=\rho_\xi+\rho_\eta=\frac{1}{2}\left\{1-\frac{1}{\pi}\int_0^\pi d\varphi\,\frac{x|\sin\varphi|}{[y^2+x^2\sin^2\varphi]^{1/2}[1+2\delta_L(\varphi)]}\right\}. \qquad (3.31)$$

Naturally, this result coincides with the one which follows by differentiation of Kasteleyn's expression[3]) for the partition function of infinite cylindrical strips. Indeed, the latter expression in our notation reads

$$\lim_{M\to\infty} \frac{1}{M} \ln Z_{\Lambda}^{(K)}(x,y) = \sum_{\ell=1}^{L/2} \ln\left\{ y \sin\frac{(2\ell-1)\pi}{L} + \left[x^2 + y^2 \sin^2\frac{(2\ell-1)\pi}{L}\right]^{1/2} \right\} . \tag{3.32}$$

Hence

$$\rho_y^{(K)} = \frac{1}{L} \sum_{\ell=1}^{L/2} y \sin\frac{(2\ell-1)\pi}{L} \left[x^2 + y^2 \sin^2\frac{(2\ell-1)\pi}{L}\right]^{-1/2} = \frac{1}{2}\left\{1 - \frac{1}{\pi}\int_0^{\pi} d\varphi\, \frac{2}{L} \sum_{\ell=1}^{L/2} \left[1 + u^{-2}(\varphi) \sin^2\frac{(2\ell-1)\pi}{L}\right]^{-1} \right\}, \tag{3.33}$$

where $u(\varphi) = (x/y)\sin\varphi$. Now, the coincidence of expressions (3.31) and (3.33) can be easily shown by using the identity [3])

$$\prod_{\ell=1}^{L/2} 2\left[u^2 + \sin^2\frac{(2\ell-1)\pi}{L}\right]^{1/2} = \left[(1+u^2)^{1/2} + |u|\right]^{L/2} + \left[(1+u^2)^{1/2} - |u|\right]^{L/2} \tag{3.34}$$

instead of (3.22).

4. Results and Discussion

Expressions (2.24), (2.24), (3.2) and (3.19) give the required dependence of ρ_ξ , ρ_η and hence of the ordering parameter Δ on the bond activities and the lattice size L . In the limit $L\to\infty$, according to (3.24), the expressions for the average densities of bond occupation ρ_ξ , ρ_η become

$$\rho_\xi = \rho_\eta = \frac{\xi\eta}{2\pi}\int_0^{\pi} d\varphi\, \frac{1 - x\sin\varphi\,(y^2 + x^2\sin^2\varphi)^{-1/2}}{y^2 + \xi\eta + (y^2 - \xi\eta)\, x\sin\varphi\,(y^2 + x^2\sin^2\varphi)^{-1/2}} . \tag{4.1}$$

Hence it follows that $\Delta = 0$ in the thermodynamic limit $M \to \infty$, $L \to \infty$ for all values of x, y, ξ and ζ.

Let us turn now to the finite - size effects. In the leading order $O(L^{-1})$, we obtain from (2.24) and (3.28) the finite--size correction $\rho_{\xi}^{(1)}$ to ρ_{ξ} in the form

$$\rho_{\xi}^{(1)} = \frac{1}{\pi L} \frac{\xi y^2 (y^2 - \zeta^2)}{x (y^2 + \xi\zeta)^2} \int_0^{\infty} dz \left[ch\, z + \frac{y(\xi + \zeta)}{y^2 + \xi\zeta} \right]^{-1}, \quad \left(\frac{x}{y} L \to \infty\right). \tag{4.2}$$

The expression for $\rho_{\zeta}^{(1)}$ follows from (4.2) by exchanging the places of ξ and ζ. Therefore, the leading-order finite-size correction $\Delta^{(1)}$ to the ordering parameter is

$$\Delta^{(1)} = \rho_{\xi}^{(1)} - \rho_{\zeta}^{(1)}. \tag{4.3}$$

At $\xi = \zeta = y$ the finite-size corrections to ρ_{ξ} and ρ_{ζ} according to (3.30) are $O(L^{-2})$, namely

$$\rho_{\xi}^{(2)} = \rho_{\zeta}^{(2)} = \frac{y}{x} \frac{\pi}{12 L^2}, \quad \left(\frac{x}{y} L \to \infty\right). \tag{4.4}$$

The results obtained for Δ indicate that we deal with a specific thermodynamic quantity that originates from a correction addition to the free energy rather than from its bulk or surface components. Indeed, the presence of a modified layer of bonds in the infinite cylindrical lattice leads to the appearance in the free energy density of a surface term and corrections (in the limit of large L):

$$\lim_{M \to \infty} \frac{1}{M} \ln Z_{LM}(x,y,\xi,\zeta) = L f_{bulk}(x,y) + f_{surf}(x,y,\xi,\zeta) + \frac{1}{L} f_{corr}(x,y,\xi,\zeta) \tag{4.5}$$

Our result

$$\lim_{L \to \infty} \rho_{\xi} = \lim_{L \to \infty} \rho_{\zeta}$$

implies that

$$\xi \frac{\partial}{\partial \xi} f_{surf} = \eta \frac{\partial}{\partial \eta} f_{surf} . \tag{4.6}$$

Hence

$$f_{surf}(x, y, \xi, \eta) = \varphi(x, y, \xi\eta) . \tag{4.7}$$

The explicit form of the function φ can be found by integration of the equation

$$z \frac{\partial}{\partial z} \varphi(x, y, z) \Big|_{z=\xi\eta} = \rho_\xi \tag{4.8}$$

with ρ_ξ given by (4.1). Thus we find the surface contribution in the form

$$f_{surf}(x, y, \xi, \eta) = \frac{1}{2\pi} \int_0^{2\pi} d\varphi \ln \left\{ y^2 + \xi\eta + (y^2 - \xi\eta) \frac{x \sin \varphi}{\sqrt{y^2 + x^2 \sin^2 \varphi}} \right\} . \tag{4.9}$$

Evidently, the nonzero value (4.3) of the ordering parameter is ensured exclusively by the correction term $L^{-1} f_{corr}(x, y, \xi, \eta)$ in the large L expansion (4.5). In a finite system with homogeneous boundaries, f_{corr} is supposed to be universal and in some geometries to be simply related to the conformal anomaly number c of the theory [8,9]. Besides the conformal properties, f_{corr} depends, in general, on the nature of the boundary conditions. Differentiation of f_{corr} with respect to boundary parameters gives thermodynamic quantities, an example of which is the parameter Δ in our model of crystallization.

Appendix

For the sake of completeness we write down here in full the solution of the system of linear equations (3.10) at finite values of L and M, both assumed to be even numbers. For convenience of notation the solution is given in the form

$$\begin{pmatrix} \tilde{W}_{11}(0,a_2) \\ \tilde{W}_{21}(0,a_2) \\ \tilde{W}_{11}(L-1,a_2) \\ \tilde{W}_{21}(L-1,a_2) \end{pmatrix} = \frac{2}{tMd_0(a_2)} \begin{pmatrix} d_1(a_2) \\ d_2(a_2) \\ d_3(a_2) \\ d_4(a_2) \end{pmatrix},$$

where

$$d_0(a_2) = d^2(a_2) + \\ + t^{-2}A_{11}^2(0,a_2)\left\{(\xi+y)^2\left[1+(\eta+y)A_{11}(1,a_2)\right]^2 + (\eta+y)^2\left[1+(\xi+y)A_{11}(1,a_2)\right]^2\right\},$$

$$d(a_2) = 1 + \frac{y^2-\xi\eta}{y}A_{11}(1,a_2) + (\xi+y)(\eta+y)\varepsilon_L(a_2),$$

$$d_1(a_2) = 1 + \frac{y^2-\eta^2}{y}A_{11}(1,a_2) + (\eta+y)^2\varepsilon_L(a_2) + \\ + t^{-2}(\eta+y)^2A_{11}^3(0,a_2),$$

$$d_2(a_2) = x\left(e^{-4\pi i a_2/M}-1\right)A_{11}(0,a_2)\left[d(a_2) + t^{-2}(\xi+y)(y-\eta)A_{11}^2(0,a_2)\right],$$

$$d_3(a_2) = \frac{1}{\xi+y}\left\{d^2(a_2) - \left[1+(\eta+y)A_{11}(1,a_2)\right]d(a_2)\right\} + \\ + t^{-2}A_{11}^2(0,a_2)\left[\xi+y - \frac{(\eta+y)(2\xi\eta+y\eta-y^2)}{y}A_{11}(1,a_2) + 2(\xi+y)(\eta+y)^2\varepsilon_L(a_2)\right] + \\ + t^{-4}(\xi+y)(\eta+y)^2A_{11}^4(0,a_2),$$

$$d_4(a_2) = x\left(e^{-4\pi i a_2/M}-1\right)(\xi-\eta)A_{11}^2(0,a_2),$$

Here,

$$\varepsilon_L(a_2) = A_{11}^2(1,a_2) + 4x^2\sin^2\frac{2\pi a_2}{M}A_{11}^2(0,a_2) + \frac{1}{y}A_{11}(1,a_2),$$

$$A_{11}(0,a_2)=\frac{2}{L}\sum_{a_1=1}^{L/2}\left[4y^2\sin^2\frac{2\pi a_1}{L}+4x^2\sin^2\frac{2\pi a_2}{M}+t^{-2}\right]^{-1},$$

$$A_{11}(1,a_2)=-\frac{2}{L}\sum_{a_1=1}^{L/2}2x\sin^2\frac{2\pi a_1}{L}\left[4y^2\sin^2\frac{2\pi a_1}{L}+4x^2\sin^2\frac{2\pi a_2}{M}+t^{-2}\right]^{-1}.$$

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