Equilibrium Crystal Shapes and Correlation Lengths: A General Exact Result in Two Dimensions

Mark Holzer
Department of Physics, Simon Fraser University, Burnaby, British Columbia, Canada V5A 1S6
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We show that the exact equilibrium crystal shape (ECS) for a wide class of two-dimensional Ising models can simply be read off from the analytical expression for the *bulk* free energy: The ECS is given as the locus of purely imaginary zeros of the "momentum"-space lattice-path propagator. From these shapes, one may obtain numerically, to arbitrary accuracy, the high-temperature direction-dependent correlation lengths of the dual system. These exact ECS's and corresponding correlation lengths were previously known only for the rectangular, triangular, and honeycomb lattices.

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Equilibrium crystal shapes (ECS's) have received considerable attention in recent years.[1] In particular, two-dimensional (2D) Ising ECS's are interesting because exact solutions are possible. Moreover, these exact solutions may be experimentally relevant, since they are, under appropriate conditions, good approximations to the facet shapes of *three*-dimensional ECS's.[2] To date, exact solutions for the complete temperature- (T-) dependent ECS exist only for the Ising model on rectangular,[3] triangular, and honeycomb lattices.[4,5] These solutions were obtained from the known high-T correlation lengths of these lattices[6] by exploiting a duality relation[7] which connects the ECS of the direct lattice $\mathcal{L}$ with the high-T ($T > T_{\text{critical}}$) correlation length of the dual system on the dual lattice $\mathcal{L}^*$.

In this paper we take a more direct approach, which combines a grand canonical formulation of the ECS problem[1,8] with a recent generalization[9] of the Feynman-Vdovichenko random-walker method[10] of solving the Onsager[11] problem. Surprisingly, we find that a closed-form, exact equation for the ECS can simply be read off from the analytical expression for the *bulk* free energy for a wide class of Ising models with noncrossing bonds. *The ECS is given as the locus of purely imaginary zeros of the "momentum"-space lattice-path propagator.* More precisely, the central result of this paper may be stated as follows: If the bulk free energy f_b^* of the Ising model on $\mathcal{L}^*$ can be written in terms of the $q \times q$ Feynman-Vdovichenko lattice-walk matrix $\mathbf{\Lambda}$ as

$$\beta f_b^* = -\ln \operatorname*{Tr}_{\text{unit cell}} \prod (\cosh K_{ij}^*) - \text{const} \times \int\int dk_x\, dk_y \ln \mathrm{Det}[1 - \mathbf{\Lambda}(k_x, k_y; \tanh K_{ij}^*)] \tag{1}$$

[where $\mathrm{Det}(1-\mathbf{\Lambda})$ is the propagator for lattice paths, and q is finite and in simple cases equal to the coordination number of the lattice], then the ECS of the dual system on $\mathcal{L}$, represented in Cartesian coordinates as $Y(X)$, is given by

$$\mathrm{Det}\{1 - \mathbf{\Lambda}(k_x = i\beta\lambda Y, k_y = -i\beta\lambda X; \exp(-2K_{ij}))\} = 0, \quad T < T_c, \tag{2}$$

subject to some (weak) conditions to be given below. Throughout this paper starred (*) quantities refer to the dual lattice $\mathcal{L}^*$ and $\tanh K_{ij}^* = \exp(-2K_{ij})$.[12] In Eqs. (1) and (2), Tr denotes trace, Det denotes determinant, $\beta \equiv (k_B T)^{-1}$, where k_B is Boltzman's constant, $K_{ij} \equiv \beta J_{ij}$ is the coupling between sites i and j of $\mathcal{L}$, and λ is a constant which controls the volume of the ECS by setting its overall length scale. To the best of our knowledge all known exact solutions for the bulk free energy of 2D Ising models are, indeed, of the form (1) and do satisfy the conditions alluded to.[13] The ECS (2) can be inverted via a Legendre transform[14] (inverse Wulff construction[15]) to obtain the interfacial free energy per unit length $\gamma(\hat{\mathbf{n}})$ (surface tension) for a macroscopically flat interface of normal $\hat{\mathbf{n}}$. The high-T correlation length $\xi^*(\hat{\mathbf{u}})$ for correlations in the $\hat{\mathbf{u}}$ direction on $\mathcal{L}^*$ are then simply given by $\xi^*(\hat{\mathbf{u}}) = 1/\beta\gamma(\hat{\mathbf{n}})$, $\hat{\mathbf{n}} \cdot \hat{\mathbf{u}} = 0$.[7] While this inversion is not generally possible in closed form, it can easily be carried out numerically with arbitrary accuracy. The correlation lengths of 2D Ising models for arbitrary direction $\hat{\mathbf{u}}$ have until now only been known exactly for the rectangular, triangular, and honeycomb lattices.[6]

The method we shall use to evaluate the sums over microscopic configurations which arise in the derivation of Eq. (2) has a venerable history. The root of this method may be considered to be an unpublished conjecture by Feynman which was proved by Sherman[16] (the Sherman theorem). Feynman reinterpreted the seminal work of Kac and Ward[17] on a combinatorial solution of the Ising model in terms of an identity between lattice-path sums and the graphical expansion of the Ising model. (The content of the Sherman theorem is closely related to the free-fermion point of view of Hurst and Green.[18]) Making implicit use of the Sherman theorem, Vdovichenko[10] gave an elegant, intuitive solution to the Onsager problem, which is now textbook material.[19] The first application of these methods to Ising interfaces was recently reported by Calheiros, Johannesen, and Merlini.[9] We shall utilize this technology to derive Eq. (2).

Consider first the "canonical" formulation of the ECS problem: The thermodynamic quantity to be calculated from the microscopic Hamiltonian is the surface tension $\gamma(\hat{\mathbf{n}})$. Throughout this paper we take the Ising system to be defined on an $(|N|+1)\times R$ rectangular strip of a periodic lattice $\mathcal{L}$, with R tending towards infinity. For $T<T_c$ and zero magnetic field, an interface can be forced into this system by dividing the boundary of $\mathcal{L}$ into two connected (1D) regions and fixing the spins to be "up" (+) on one region and "down" (−) on the other. We shall take this interface to extend from spin $\sigma^*_{(0,0)}$ to spin $\sigma^*_{(N,M)}$ on the boundary of the dual strip $\mathcal{L}^*$ (Fig. 1). With this choice of boundary condition (+ −), denote the partition function of the system by $Z^{+-}_{N,M}$; if all boundary spins are fixed to be up (no interface), denote it by Z^{++}. $\gamma(\hat{\mathbf{n}})$ is then defined by

$$\beta\gamma(\hat{\mathbf{n}})\equiv\lim_{L\to\infty}\frac{1}{L}\ln\left(\frac{Z^{+-}_{N,M}}{Z^{++}}\right) \tag{3}$$

$$=\lim_{L\to\infty}\frac{1}{L}\ln\langle\sigma^*_{(0,0)}\sigma^*_{(N,M)}\rangle=\frac{1}{\xi^*(\hat{\mathbf{u}})}, \tag{4}$$

where $L\equiv(N^2+M^2)^{1/2}$, $\hat{\mathbf{n}}=(-M,N)/L$, and $\hat{\mathbf{u}}=(N,M)/L$. The duality statement (4) has been derived by a number of authors[7] and forms the basis of the known exact solutions: A calculation of the dual-lattice correlations $\langle\sigma^*_{(0,0)}\sigma^*_{(N,M)}\rangle$ in the thermodynamic limit $N,M\to\infty$ with $\hat{\mathbf{n}}$ ($\hat{\mathbf{u}}$) fixed gives $\gamma(\hat{\mathbf{n}})$, from which the ECS is determined via the well-known Wulff construction.[15]

To see what the interface has to do with random walkers, consider the low-T expansions[12] of $Z^{+-}_{N,M}$ and Z^{++},

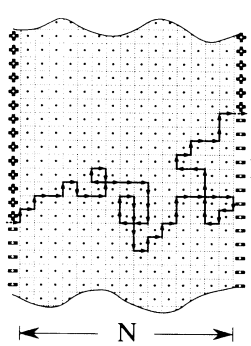

FIG. 1. The boundary conditions considered in this paper illustrated on a rectangular lattice: The strip $\mathcal{L}$ is defined by the heavy dots and the spins on its boundary are forced to be either "up" (+) or "down" (−) as shown. Its dual $\mathcal{L}^*$ is indicated by the grid of dotted lines. The + − boundary conditions force an interface into the system which runs from dual spin $\sigma^*_{(0,0)}$ to dual spin $\sigma^*_{(N,M)}$. The lattice walk shown illustrates a term in the sum of Eq. (5).

expressed in terms of graphs G on the dual lattice $\mathcal{L}^*$. The links of these graphs are the bonds of $\mathcal{L}^*$ dual to the broken bonds of $\mathcal{L}$ (i.e., bonds of $\mathcal{L}$ between spins of opposite sign). Each graph G represents a microscopic interface configuration and has, therefore, weight $W(G)=\prod_{\text{links}}\exp(-2K_{ij})$. The expansion of $Z^{+-}_{N,M}$ contains closed polygons (loops) and open graphs connecting (0,0) to (N,M). The expansion for Z^{++} contains loops only. If (○) denotes the sum of $W(G)$ over all single closed loops, (○∼○) the sum over all pairs of closed loops, (——) the sum over the open graphs, (——∼○) the sum over open graphs in the presence of single closed loops, etc., we can write symbolically

$$Z^{++}=1+(\circ)+(\circ\sim\circ)+\cdots,$$
$$Z^{+-}_{N,M}=(\text{——})+(\text{——}\sim\circ)+(\text{——}\sim\circ\sim\circ)+\cdots.$$

Instead of evaluating the sums over closed loops, it turns out to be easier, following Feynman and Vdovichenko,[10,19] to sum over closed *directed* lattice paths. (The directed links of such lattice walks will be called "steps.") Give weight

$$W(\vec{G})=(-1)^S\prod_{\text{steps}}\exp(-2K_{ij})$$

to each single directed closed path $\vec{G}$, where S is the number of self-intersections of the path and the product is over the steps of the path. The upshot of the Sherman theorem,[16] which holds for any planar embedded lattice with noncrossing bonds, is that $Z^{++}=A\exp(\circlearrowright)$, where ($\circlearrowright$) denotes the sum of $W(\vec{G})$ over all possible $\vec{G}$ and A is just $\mathrm{Tr}(\prod_{\text{links}}\cosh K^*_{ij})$. The critical point is that the n-loop term of the directed paths has uncoupled into $(\circlearrowright)^n/n!$.[20] Hence, if (—>—) denotes the sum over open graphs which are counted using directed paths weighted in the same manner as the closed paths of ($\circlearrowright$), one is led to expect that (—>—) uncouples from the ($\circlearrowright$)'s, so that $Z^{+-}_{N,M}=(\text{—>—})Z^{++}$. Calheiros, Johannesen, and Merlini[9] showed that, indeed, this follows rigorously from the Sherman theorem by considering the closed-loop expansion with an auxiliary bond J^*_a external to $\mathcal{L}^*$ connecting the dual sites (0,0) and (N,M). In the limit as $J^*_a\to 0$, one finds that

$$\frac{Z^{+-}_{N,M}}{Z^{++}}=\sum_{(0,0)\to(N,M)}(-1)^S\prod_{\text{steps}}e^{-2K_{ij}}, \tag{5}$$

where the sum is over all paths or lattice walks from (0,0) to (N,M) (Fig. 1).

Following Refs. 10, 17, and 19, the sums over walks (5) can now easily be evaluated, at least in the thermodynamic limit. Let $\{\mathbf{d}_\mu\}$, with $\mu\in\{1,2,\ldots,q\}$, be the set of vectors which correspond to all possible distinct directed bonds of $\mathcal{L}^*$. If $\mathcal{L}^*$ is a Bravais lattice, q is the coordination number; otherwise, q is the sum of the coordination numbers for each type of site. Denote by $\mathbf{d}_\mu(n)$ the nth step of the walk. We associate with each change of direction a phase factor $\exp(i\phi_{\mu\nu}/2)$, where $\phi_{\mu\nu}$ is the angle ("of turn") from $\mathbf{d}_\nu(n)$ to $\mathbf{d}_\mu(n+1)$, defined such that $|\phi_{\mu\nu}|\le\pi$. This keeps track of the parity of self-intersections because the product of these phase factors over a single closed loop gives $-(-1)^S$, a topological property of planar embedded loops.[17] Let $\Psi_{\mu\kappa}(x,y;n)$ be the sum over all weighted walks (including the phase factors) which step onto the origin with $\mathbf{d}_\kappa(0)$, and n steps later onto site (x,y) with $\mathbf{d}_\mu(n)$. These $\Psi_{\mu\kappa}(x,y;n)$ then obey a recursion equation which, in the limit as the strip width $|N|\to\infty$, can be diagonalized via a Fourier transform to obtain[10,19]

$$\Psi_{\mu\kappa}(k_x,k_y;n+1)=\sum_\nu \Lambda_{\mu\nu}(k_x,k_y)\Psi_{\nu\kappa}(k_x,k_y;n). \quad (6)$$

The $\Lambda_{\mu\nu}$ are the elements of the $q\times q$ matrix $\mathbf{\Lambda}$ and have the form

$$\Lambda_{\mu\nu}(k_x,k_y;e^{-2K_{ij}})=e^{-2K_{ij}}e^{i\phi_{\mu\nu}/2}e^{-i\mathbf{k}\cdot\mathbf{d}_\mu}(1-\delta_{\mathbf{d}_\mu,-\mathbf{d}_\nu}), \quad (7)$$

where $\mathbf{k}=(k_x,k_y)$. The Kronecker δ in (7) ensures that walks cannot immediately backtrack.[10,19] The right-hand side of Eq. (5) can now be written in terms of Λ as

$$\iint_{-\pi}^{\pi}\frac{dk_x\,dk_y}{4\pi^2}e^{i(k_xN+k_yM)}\sum_{m=0}^{\infty}[\mathbf{\Lambda}^{|N|+|M|+1+m}]_{\mu_{\rm out}\nu_{\rm in}}. \quad (8)$$

In principle, the boundaries of the lattice should be chosen such that $\mu_{\rm out}=\nu_{\rm in}$, so that self-intersections are properly accounted for; however, in the thermodynamic limit this is not important, as we can replace

$$[\mathbf{\Lambda}^{|N|+|M|+1+m}]_{\mu_{\rm out}\nu_{\rm in}} \text{ with } \mathrm{Tr}\,\mathbf{\Lambda}^{|N|+|M|+m}.$$

If the 2D ECS is represented in Cartesian coordinates as $Y(X)$, the analytical statement of the Wulff construction[14] takes a form particularly useful in the derivation of Eq. (2):

$$\lambda Y(X)=f(s)+\lambda Xs;\quad \lambda X=-\frac{\partial f}{\partial s},\quad s=\frac{\partial Y}{\partial X}, \quad (9)$$

where $f(s)\equiv\gamma(\hat{\mathbf{n}})(1+s^2)^{1/2}$ and $\hat{\mathbf{n}}=(-s,1)/(1+s^2)^{1/2}$. Equation (9) is a Legendre transform: In going from $f(s)$ to $Y(X)$ we pass from a "canonical" ensemble at fixed macroscopic slope s to a grand "canonical ensemble," in which all s are allowed and the field variable X selects a particular slope s as $\partial Y/\partial X$. We may, therefore, write[1,8]

$$\beta\lambda Y(X)=-\lim_{|N|\to\infty}\frac{1}{N}\ln\left\{\frac{1}{Z^{++}}\{\mathrm{Tr}\}\exp\left[-\beta\left(\mathcal{H}-\lambda X\hat{\mathbf{x}}\cdot\sum\hat{\boldsymbol{n}}\right)\right]\right\} \quad (10a)$$

$$=-\lim_{|N|\to\infty}\frac{1}{N}\ln\sum_M e^{-\beta\lambda XM}\left(\frac{Z^{+-}_{N,M}}{Z^{++}}\right), \quad (10b)$$

where $\{\mathrm{Tr}\}$ denotes the trace over all possible configurations containing an interface extending from (0,0) to (N,M) for *any* M. $\hat{\boldsymbol{n}}$ is the microscopic normal of the bonds dual to broken bonds and points from + to −. The field $X\hat{\mathbf{x}}$ is constant and, therefore, couples only to the normals of *open* paths from (0,0) to (N,M). Because the net field contribution depends only on M, the field term of Eq. (10) can be neatly incorporated into $\mathbf{\Lambda}$ by making the substitution $k_y\to k_y-i\beta\lambda X$. Substituting (8) into (10b) with $\mathbf{\Lambda}=\mathbf{\Lambda}(k_x,k_y-i\beta\lambda X)$ and summing over m, we obtain

$$\beta\lambda Y(X)=-\lim_{|N|\to\infty}\frac{1}{N}\ln\left\{\sum_{M=-\infty}^{+\infty}\iint_{-\pi}^{\pi}dk_x\,dk_y\,e^{i(k_xN+k_yM)}\mathrm{Tr}\frac{\mathbf{\Lambda}^{|N|+|M|}}{\mathbf{1}-\mathbf{\Lambda}}\right\}, \quad (11)$$

where X must be bounded such that $\mathbf{\Lambda}^P\to\mathbf{0}$ as $P\to\infty$. Only the saddle point of the integrand of Eq. (11) contributes to the thermodynamic limit. It is straightforward to show that this saddle point occurs when $\mathrm{Det}(\mathbf{1}-\mathbf{\Lambda})=0$. Thus, in the limit $|N|\to\infty$, we can replace $\mathrm{Tr}[\mathbf{\Lambda}^{|N|+|M|}/(\mathbf{1}-\mathbf{\Lambda})]$ with $1/\mathrm{Det}(\mathbf{1}-\mathbf{\Lambda})$. This substitution allows us immediately to sum over M to obtain a delta function $2\pi\delta(k_y)$. After integrating over k_y and making the change of variable $e^{ik_x}=z$, Eq. (11) becomes

$$\beta\lambda Y(X)=-\lim_{|N|\to\infty}\frac{1}{N}\ln\left\{\oint\frac{dz}{2\pi i}\frac{z^N}{z\,\mathrm{Det}(\mathbf{1}-\mathbf{\Lambda})}\right\}, \quad (12)$$

where $\mathbf{\Lambda}=\mathbf{\Lambda}(k_x,0-i\beta X)$ and the contour of integration is counterclockwise around the unit circle $|z|=1$.

For all Ising models of Ref. 13 for which the exact (bulk) solution is known, (12) can be evaluated very simply: For all these models the propagator $\mathrm{Det}(\mathbf{1}-\mathbf{\Lambda})$ is a polynomial in z and $1/z$ and, for appropriate orientation of the axis, $z\,\mathrm{Det}(\mathbf{1}-\mathbf{\Lambda})$ is of the form $[z-z_1(X)][z-z_2(X)]$. The roots $z_1(X)$ and $z_2(X)$ are real and positive for $X\in[X_{\min},X_{\max}]$ and $T<T_c$. For a range of the field variable $X\in[X_Z,X_B]\subset[X_{\min},X_{\max}]$, $z_1(X)\le 1$ and $z_2(X)\ge 1$. Thus, for $X\in[X_A,X_B]$, Eq. (12) is evaluated as $\beta\lambda Y(X)=-\ln[z_1(X)]$, if $N>0$, and as $-\ln[z_2(X)]$, if $N<0$. Since the outward normal of the interface is $\hat{\mathbf{n}}=(-\langle M\rangle(X),N)/L$, $N>0$ ($N<0$) corresponds to the "upper (lower) half" of the ECS. If $X_A\neq X_{\min}$ and $X_B\neq X_{\max}$, and $X\in[X_{\min},X_A]\cup[X_B,X_{\max}]$, then (by definition) either both or neither of the poles z_1,z_2 lie inside $|z|=1$. In this case we find that $\mathbf{\Lambda}^P(k_x,k_y-i\beta\lambda X)$ no longer converges for all (k_x,k_y) as $P\to\infty$. Hence, for $X\in[X_{\min},X_A]\cup[X_B,X_{\max}]$, the substitution $\mathbf{\Lambda}(k_x,k_y)\to\mathbf{\Lambda}(k_x,k_y-i\beta\lambda X)$, which incorporates the field term of Eq. (10) into the matrix $\mathbf{\Lambda}$, is no longer well founded mathematically. For such X, Eq. (10) would, therefore, in principle have to be calculated by first evaluating the integrals for $Z^{+-}_{N,M}/Z^{++}$ and then performing the sum over M. However, since the ECS of any 2D system with short-range forces is smooth[1-4] for $0 < T < T_c$, it follows from *analytical continuity* that the upper half of the ECS must be given by $-\ln[z_1(X)]$, and the lower half by $-\ln[z_2(X)]$, for the *entire* range of field $X \in [X_{\min}, X_{\max}]$. To summarize, we have for $T < T_c$ and $X_{\min} \le X \le X_{\max}$

$$\beta\lambda Y(X) = \begin{cases} -\ln z_1, & \text{if } N \ge 0, \\ -\ln z_2, & \text{if } N \le 0, \end{cases} \tag{13}$$

which can succinctly be expressed in the form of Eq. (2). Since $\mathrm{Det}(1-\Lambda)$ does not have to be explicitly evaluated, if the bulk free energy for the dual lattice is known in the form of Eq. (1), we arrive at the promised result Eq. (2). For the rectangular, triangular, and honeycomb lattices the ECS's as obtained from Eq. (2) agree with those calculated independently[3-5] via the canonical formulation. A number of new results are obtained immediately by applying Eq. (2) to the known bulk solutions.[13]

The results of this paper generalize to free-fermion models not in the Ising universality class,[21] provided that the ECS problem is well defined. We hope to explore these cases in a future publication.

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