DUALITY TRANSFORMATION FOR DEFECT MELTING

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Received 22 February 1982
Revised manuscript received 6 July 1982

For a simple lattice model of defect melting we calculate the transition temperature in terms of the elastic constants, using the technique of duality transformations. The Lindemann parameter comes out to be $L \approx 100$ for strong steric repulsion g between the dislocation lines and can be increased by weakening this parameter (experimentally $L \sim 120$–200). Thus g must be small. This also ensures the first-order nature of the transition, as recently shown by the author.

Duality transformations permit a direct change from an order to a disorder description of a physical system [1]. In this note we use this technique for a simple lattice model of defect melting and calculate the transition temperature.

Consider an ideal crystal whose linear elasticity is described by an energy

$$F_{\rm el} = \int {\rm d}^3x\ [\tfrac{1}{4}\mu(\partial_i u_j + \partial_j u_i)^2 + \tfrac{1}{2}\lambda(\partial_i u_i)^2] = \int {\rm d}^3x\ \frac{1}{4\mu}\left(\sigma_{ij}^2 - \frac{\nu}{1+\nu}\sigma_{ii}^2\right), \tag{1,2}$$

where μ, λ are Lamé's constants, $\nu = \frac{1}{2}\lambda/(\lambda+\mu)$ is Poisson's ratio, σ_{ij} is the stress and u_i are the displacements of the atoms. We shall assume the perfect crystal at zero temperature to consist of a periodic array of potential wells located at $\boldsymbol{x} = \Sigma_{i=1}^{3} n_i \boldsymbol{a}_i = (n_1, n_2, n_3)a$ each being occupied by one atom. As the temperature is increased, the atoms are allowed to move across the barriers to any other well without being disturbed by the presence of the atom lying there. In nature, there will be repulsion and the atom remains at an interstitial place. This detail will be neglected at first and included heuristically at a later stage.

Thus we shall study the energy

$$F_{\rm el} = a\sum_{\boldsymbol{x}} [\tfrac{1}{4}\mu(\nabla_i u_j + \nabla_j u_i - 2n_{ij}a)^2 + \tfrac{1}{2}\lambda(\nabla_i u_i - n_{ii}a)^2]\ . \tag{3}$$

Here $\nabla_i u_j = u_j(\boldsymbol{x}+\boldsymbol{a}_i) - u_j(\boldsymbol{x})$ are the lattice derivatives, the variables u_i cover the unit cell of the crystal, $|u_i| \leqslant a/2$, and the integers $n_{ij} = 0, \pm1, \pm2, \ldots$ account for the jumps across the barriers. Obviously, for smooth configurations, (3) coincides with (1).

The partition function

$$Z = \prod_{\boldsymbol{x},i} \int_{-a/2}^{a/2} \frac{{\rm d}u_i(\boldsymbol{x})}{\sqrt{\pi T/a\mu}} \sum_{n_{ij}(\boldsymbol{x})} \exp[-F_{\rm el}(u_i, n_{ij})/T] \tag{4}$$

can be transformed via an auxiliary triplet of symmetric tensor fields $\bar{\sigma}_{ij}$ to the form

$$Z = \prod_{\boldsymbol{x},i} \int_{-a/2}^{a/2} \frac{{\rm d}u_i(\boldsymbol{x})}{\sqrt{\pi T/a\mu}} \prod_{i,j} \int_{-\infty}^{\infty} {\rm d}\bar{\sigma}_{ij}(\boldsymbol{x}) \sqrt{\tau/\pi} \sum_{n_{ij}(\boldsymbol{x})} \exp \sum_{\boldsymbol{x}} \left[-\tau\left(\bar{\sigma}_{ij}^2 - \frac{\nu}{1+\nu}\bar{\sigma}_{ii}^2\right) + 2\pi {\rm i}\bar{\sigma}_{ij}\left(\frac{1}{2a}(\nabla_i u_j + \nabla_j u_i) - n_{ij}\right)\right], \tag{5}$$

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where we have abbreviated the dimensionless factor $\pi^2 T/\mu a^3$ by τ. Executing the sum over $n_{ij}(x)$ via Poisson's formula, $\Sigma_n \, e^{i2\pi n\alpha} = \Sigma_l \, \delta(\alpha - l)$, the integral over $d\bar{\sigma}_{ij}$ reduces to a sum over integer values $\bar{\sigma}_{ij} = 0, \pm 1, \pm 2, \ldots$. After this the integral over u_i enforces $\bar{\sigma}_{ij}$ to be divergenceless on the lattice $\overset{*}{\nabla}_i \bar{\sigma}_{ij} = \overset{*}{\nabla}_i \bar{\sigma}_{ji} = 0$. Here we have performed the lattice analogue of partial integration under which $\Sigma_x \, (\nabla_i \psi)\varphi = \Sigma_x \, \psi \overset{*}{\nabla}_i \varphi$ with $\overset{*}{\nabla}_i \varphi(x) = \varphi(x) - \varphi(x - a_i) \equiv \nabla_i \varphi(x - a_i)$. We may introduce a symmetric integer tensor field $\bar{h}_{nl}$ such that

$$\bar{\sigma}_{ij}(x) = \epsilon_{ikl}\epsilon_{jmn} \overset{*}{\nabla}_k \overset{*}{\nabla}_m \bar{h}_{ln}(x - a_l - a_n) \, , \tag{6}$$

i.e., $\bar{\sigma}_{ij}$ is a double lattice curl of h_{nl}. There is a freedom under arbitrary local lattice gauge transformations

$$\bar{h}_{nl} \to \bar{h}_{nl} + \nabla_n \bar{\xi}_l + \nabla_l \bar{\xi}_n \, . \tag{7}$$

In terms of $\bar{h}_{nl}$, Z takes the form [2]

$$Z = \prod_{l,n} \sum_{\bar{h}_{ln}(x)=0,\pm 1,\ldots} \sqrt{\tau/\pi} \, \delta_{\nabla \bar{h}_{ln},0} \exp\left(-\tau \sum_x \bar{h}_{ln} \bar{D}_{ln,l'n'} \bar{h}_{l'n'}\right) , \tag{8}$$

where $\bar{D}_{ln,l'n'}$ is the difference operator

$$\bar{D}_{ln,l'n'} = \overset{*}{\nabla}_i \nabla_i \overset{*}{\nabla}_j \nabla_j \left(P^{(2,2)} + P^{(2,-2)} + \frac{1-\nu}{1+\nu} P^{\mathrm{L}}\right)_{ln,l'n'} \, . \tag{9}$$

The expressions $P^{(s,\lambda)}$ stand for the lattice versions of the spin s helicity λ projection matrices with P^{L} projecting into the mixed state corresponding to $(1/3)^{1/2}|2, 0\rangle - (2/3)^{1/2}|0, 0\rangle$. The form (9) permits an immediate inversion such that the correlation function of $\bar{h}_{ln}$ becomes

$$\overline{\bar{h}_{ln}(x)\bar{h}_{l'n'}(0)} = \frac{1}{2\tau} \sum_k e^{ik\cdot x} a^{-4} \kappa^{-4} \left(P^{(2,2)}(k) + P^{(2,-2)}(k) + \frac{1+\nu}{1-\nu} P^{\mathrm{L}}(k)\right)_{nl,n'l'} \, , \tag{10}$$

where $a^2\kappa^2 \equiv 2 \, \Sigma_{i=1}^{3} \, (1 - \cos k_i a)$ and $P^{(s,\lambda)}(k)$ arise from the familiar rotational forms by replacing $\hat{k}_{l'}$ by $[\exp(ik_{l'}a) - 1]/ia\kappa \equiv \kappa_{l'}/\kappa$ and $\hat{k}_l$ by $[1 - \exp(-ik_l a)]/ia\kappa \equiv \overset{*}{\kappa}_l/\kappa$.

The awkward restriction to integer $\bar{h}_{ln}$ can be lifted by one more use of Poisson's formula by which Z becomes

$$Z = \prod_{x,l,n} \int dh_{ln}(x) \sqrt{\tau/\pi} \, \delta(\nabla_l h_{ln}) \exp\left(-\tau \sum_x h_{ln} \bar{D}_{ln,l'n'} h_{l'n'}\right) \sum_{\bar{\eta}_{ij}(x)} \delta_{\overset{*}{\nabla}_i \bar{\eta}_{ij},0} \exp\left(2\pi i \sum_x \bar{\eta}_{ij} h_{ij}\right) . \tag{11}$$

Here $\bar{\eta}_{ln}$ is a symmetric integer tensor. It is recognized as the lattice version of the incompatibility tensor, well-known in the classical theory of elasticity [3] [‡1]. This may be decomposed into dislocation and disclination densities $\bar{\alpha}_{in}$ and $\bar{\theta}_{ij}$, respectively, via

$$\bar{\eta}_{ij} = \bar{\theta}_{ij} - \tfrac{1}{2} \overset{*}{\nabla}_m (\epsilon_{mjl}\bar{\alpha}_{il} + (i \leftrightarrow j) + \epsilon_{ijl}\bar{\alpha}_{ml})(x) \, , \tag{12}$$

which is symmetric and satisfies $\overset{*}{\nabla}_i \eta_{ij} = 0$, due to the relations $\overset{*}{\nabla}_i \bar{\alpha}_{in} = \epsilon_{nij}\bar{\theta}_{ij}$, $\overset{*}{\nabla}_j \bar{\theta}_{ij} = 0$. From now on we shall

[‡1] Integrating h_{ln} out gives

$$Z = \sum_{\bar{\eta}_{ij}} \delta_{\overset{*}{\nabla}_i \bar{\eta}_{ij},0} \exp(-2\pi^2 \sum_x \bar{\eta}_{ln} \bar{D}^{-1}_{ln,l'n'} \bar{\eta}_{l'n'}) \, ,$$

where $\bar{D}^{-1}$ can be taken as

$$\{\tfrac{1}{2}(\delta_{nn'}\delta_{ll'} + \delta_{nl'}\delta_{n'l}) + [\nu/(1-\nu)]\delta_{nl}\delta_{n'l'}\} \sum_k e^{ik\cdot x} a^{-4}\kappa^{-4} \, ,$$

due to $\overset{*}{\nabla}_i \bar{\eta}_{ij} = 0$. For a defect line along L, $\bar{\theta}_{ij} = b_i \delta_j(L)$, $\alpha_{in} = \delta_i(L)[b_n + \epsilon_{jmn}\Omega_j(x - x^0)_m]$ where $\boldsymbol{b}$, $\boldsymbol{\Omega}$ are Burgers and Frank vectors, respectively, This generalizes Blin's formula to $\boldsymbol{\Omega} \neq 0$.

consider only dislocations because of their lower elastic energy. Then the last factor in (11) becomes

$$\sum_{\bar{\alpha}_{in}} \delta^{*}_{\nabla_i \bar{\alpha}_{in},0} \exp\left(-2\pi i \sum_x \bar{\alpha}_{in} A_{in}\right), \tag{13}$$

where we introduced the auxiliary field $A_{in}(x) \equiv \epsilon_{nmj}\nabla_m h_{ij}(x)$. In terms of this, the elastic exponent is $\exp(-\tau\, \Sigma_x A_{in}\tilde{D}_{ini'n'}A_{i'n'})$ with

$$\tilde{D}_{in,i'n'} = \overset{*}{\nabla}_l \nabla_l \left(P^{(2,2)} + P^{(2,-2)} + \frac{1-\nu}{1+\nu}P^{(1,0)}\right)_{in,i'n'}, \tag{14}$$

such that A_{in} has the correlation function

$$\overbrace{A_{in}(x)A_{i'n'}(0)} = \frac{1}{2\tau}\sum_k e^{ik\cdot x} a^{-2}\kappa^{-2}\left(P^{(2,2)} + P^{(2,-2)} + \frac{1+\nu}{1-\nu}P^{(1,0)}\right)_{in,i'n'}. \tag{15}$$

In order to calculate the partition function we observe that it is equivalent to grand canonical ensemble of closed, random loops $(\bar{\alpha}_i)_n$ coupled to an external field $(A_i)_n$ (with $\overset{*}{\nabla}_n A_{in} = 0, A_{ii} = 0$), one vector for every $n = 1, 2, 3$. Consider a random walk of n steps and let $P(x, y, n)$ be the probability of arriving at x after starting from y. For D dimensions, P satisfies

$$P(x,y,n) = \sum_l P(x+l, y, n-1)/2D \quad \text{or} \quad (\nabla_n - \tfrac{1}{2}D^{-1}\overset{*}{\nabla}_l\nabla_l)P(x,y,n) = 0\,.$$

With the initial condition $P(x, y, 0) = \delta_{x,y}$, this is solved by

$$P(x,y,n) = \frac{1}{N}\sum_k e^{ik\cdot(x-y)-T(k)n}, \quad T(k) \equiv -\log(1 - a^2\kappa^2/2D)\,, \tag{16}$$

where N is the number of sites on the lattice. The total number of different closed loop configurations is therefore $N(2D)^n P(x, x, n)/n$. Allowing for a chemical potential ϵ per link, the one loop partition function is

$$Z = \sum_{n=0}^{\infty}\sum_k \frac{1}{n} e^{-\alpha n} = \sum_{n=0}^{\infty}\sum_k \int_{\alpha}^{\infty} d\xi\, e^{-\xi n} = -\log(e^{\alpha} - 1)\,, \tag{17}$$

where we have abbreviated $\alpha = T(k) + \epsilon/T - \log 2D$. If this is exponentiated we obtain the partition function of a grand canonical ensemble of closed loops. For $T \lesssim T_c = \epsilon/\log 2D$, we use the approximation $Z \sim \exp(-\Sigma_k \log \alpha(a^2K^2))$ which can also be written as a path integral over a fluctuating defect field:

$$Z \approx \int D\varphi D\varphi^{+} \exp\left(-\sum_x \varphi^{+}(x)\alpha(\overset{*}{\nabla}_l\nabla_l)\varphi(x)\right).$$

Here we see that for $T > T_c$, the fluctuations destabilize due to the high configurational entropy of the dislocation lines such that there is a phase transition order→disorder. Actually, when summing up the loop configurations we have committed some counting errors. Random walks which backtrack or pass through a point twice should be omitted. This will be taken into account phenomenologically by adding, in the exponent of (20), a steric repulsion $-g(\varphi^{+}\varphi)^2$. Leaving the size of g adjustable we may simulate the atomic repulsions which forces the defected atoms into interstitial places. Such a quartic term is necessary in order that the system restabilizes, above T_c, at some new value $\varphi_0 \neq 0$. Let us now calculate the temperature at which the transition takes place. For this we must include the elastic forces. This can be done simply via the minimal gauge invariant replacement [2], standard in electrodynamics,

$$\sum_{x,n} \varphi_n^{+}\alpha(\overset{*}{\nabla}_l\nabla_l)\varphi_n \to \sum_{x,n} \varphi_n^{+}\alpha(\overset{*}{D}_l D_l)\varphi_n\,, \quad D_l\varphi(x) \equiv \varphi(x + a_l)\exp[-2\pi i A_l(x + a_l)] - \varphi(x),$$

$$\overset{*}{D}_l\varphi(x) \equiv \varphi(x) - \varphi(x - a_l)\exp[2\pi i A_l(x - a_l)]$$

and we have introduced the index $n = 1, 2, 3$ for the three different dislocation lines. It was shown by us in ref. [2] that this coupling leads to the correct longrange forces between dislocation lines. Consider the induced effective potential for the φ_n fields. Neglecting $\delta\varphi_n$ fluctuations we can use a gauge φ_n = real and integrate out the A_{in} fields. This leads to a fluctuation determinant

$$\text{const.}\exp\left[-\frac{1}{2}\sum_k \text{tr}\log\left(\tilde{D}_{in,i'n'}(k) + \frac{2\pi^2}{3D\tau}\delta_{ii'}\delta_{nn'}\sum_n\left|\varphi_n\right|^2\right)\right].$$

The exponent can be split into $P^{(2,2)}, P^{(2,-2)}, P^{(1,0)}$ parts and becomes

$$\left(\text{const} - \frac{3}{2}\sum_k \log a^2\kappa^2\right) - \frac{\pi^2}{D\tau}\left(1 + \frac{2}{3}\frac{\nu}{1-\nu}\right)v(0)\sum_n\left|\varphi_n\right|^2 - \frac{1}{2}\sum_k\left[2\log'\left(1 + \frac{2\pi^2}{3D\tau}\frac{1}{a^2\kappa^2}\sum_n\left|\varphi_n\right|^2\right)\right.$$

$$\left. + \log'\left(1 + \frac{2\pi^2}{3D\tau}\frac{1}{a^2\kappa}\frac{1+\nu}{1-\nu}\sum_n\left|\varphi_n\right|^2\right)\right]$$

where the prime records the fact that the $\varphi_n^+\varphi_n$ terms have been removed from the Taylor series of the logarithms and $v(0) \equiv \Sigma_k\, a^{-2}\kappa^{-2} \approx 0.253$ denotes the lattice Coulomb potential [4]. The first term gives an entropy of elastic fluctuations, the second a self-energy of the dislocation loops. This remormalizes

$$\frac{\epsilon}{T}\sum_n\left|\varphi_n\right|^2 \to \left[\frac{\epsilon}{T} + \frac{\pi^2}{D\tau}\left(1 + \frac{2}{3}\frac{\nu}{1-\nu}\right)v(0)\right]\sum_n\left|\varphi_n\right|^2.$$

Actually, there was no ϵ in the beginning such that the chemical potential is entirely due to elasticity and this puts us in a position to determine T_c. At the transition we have $\tau_c = \pi^2[1 + \frac{2}{3}\nu/(1-\nu)]v(0)/D\log 2D$. Comparison with experiment is most convenient in terms of the Lindemann parameter L which is defined as [5] $L \equiv 22.8\sqrt{\mu a^3/T_{\text{melt}}} = 22.8 \times \pi/\sqrt{\tau_c} \approx 100$. This value is somewhat smaller than what is found for most materials ($L \sim 120$–200).

Therefore we turn to the third fluctuation terms in (21) neglected so far. Since the integral converges rapidly for small k, we can replace it by the continuum limit $a \to 0$ and find a term $(\Sigma_n\,|\varphi_n|^2)^{3/2}$. Such a cubic term is capable of destabilizing the $\varphi_n \approx 0$ fluctuations for $T_{\text{melt}} < T_c$ thereby lowering the transition temperature and raising L^2. Moreover, the phase transition, which up to now was of second order, becomes first order just as observed expreimentally [2]. The precise position of T_{melt} depends on the size of the steric repulsion $\Sigma_{nn'}\, g_{nn'} \times |\varphi_n|^2|\varphi_{n'}|^2$ between defect lines [2]. The coupling g has to be very small if T_{melt} lies substantially below T_c. The consequence is a large latent heat and the absence of precritical fluctuations which justifies the assumption used in arriving at (21), a posteriori. Under these circumstances, the φ field theory corresponds to a type I superconductor [2,6,7].

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