DEFECT MEDIATED PHASE TRANSITIONS IN SUPERFLUIDS, SOLIDS, AND THEIR RELATION TO LATTICE GAUGE THEORIES

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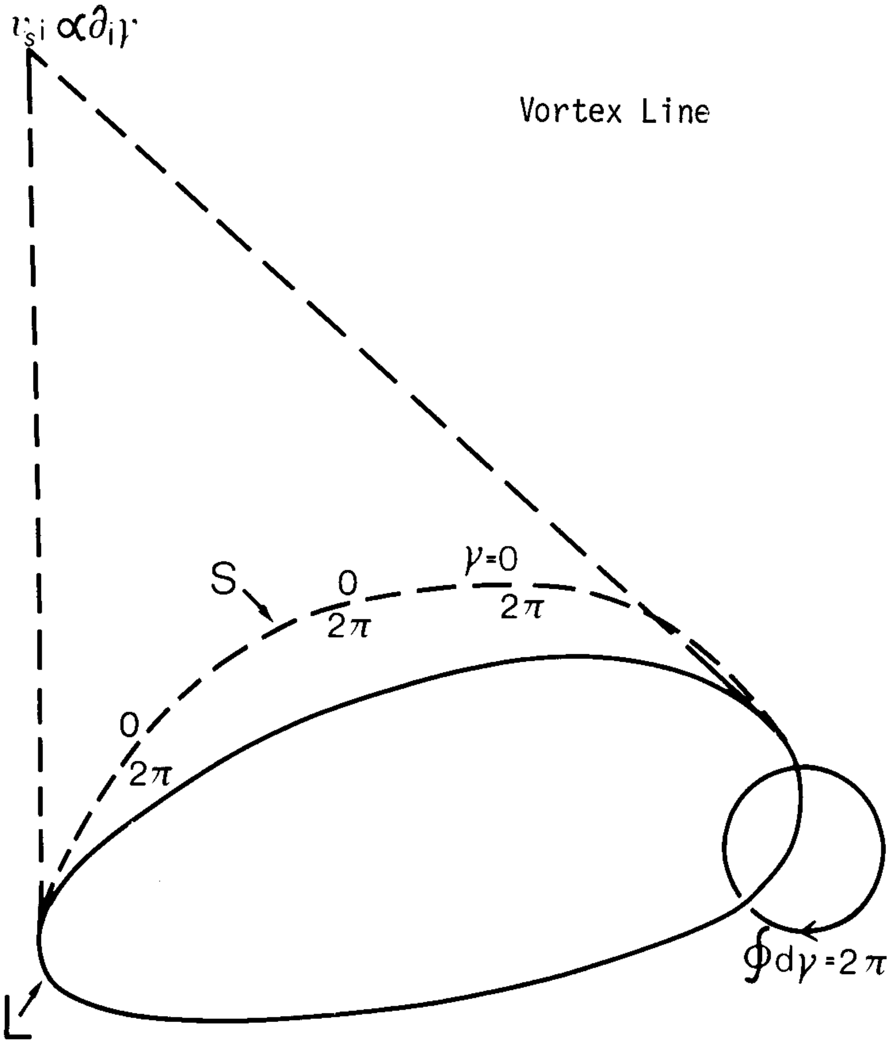
ABSTRACT

We compare the defects in different physical systems, exhibit their relevant properties for phase transitions, and point out the similarity of the lattice field theories by which their ensembles can be studied.

In recent years it has become clear that phase transitions of many non-linear systems are caused by the proliferation of topological excitations.[1-4] These are characterized by the failure of certain fields to satisfy integrability conditions and will therefore be called defects.

For example, in superfluid Helium II, there are vortex lines along which the phase of the order parameter has non-commuting derivatives (see Fig. 1).

$$\varepsilon_{kij}\,\partial_i\partial_j\,\gamma(\underset{\sim}{x}) = \alpha_k(\underset{\sim}{x}) \neq 0 \qquad (1)$$



$$\varepsilon_{\ell ij}\partial_i\partial_j\gamma = 2\pi\delta_\ell(L)$$

$$(\partial_i\partial_j - \partial_j\partial_i)\gamma \neq 0$$

Fig. 1. A vortex line with its non-integrable phase angle which satisfies $\varepsilon_{\ell ij}(\partial_i\partial_j - \partial_j\partial_i)\gamma = 2\pi\delta_\ell(L)$

If

$$\delta_k(L) \equiv \int ds \, \frac{dx_k(s)}{ds} \, \delta^{(3)}(\underset{\sim}{x} - \underset{\sim}{x}(s)) \tag{2}$$

denotes the delta function singular along a vortex line L, parametrized by x(s), the vortex density is

$$\alpha_k(\underset{\sim}{x}) = 2\pi n \, \delta_k(L) \tag{3}$$

In a crystal, the displacement vector $u_i(\underset{\sim}{x})$ may be non-integrable due to dislocation lines (see Fig. 2-4)[5]

$$\varepsilon_{kij} \partial_i \partial_j u_\ell(\underset{\sim}{x}) = \alpha_{\ell k}(\underset{\sim}{x}) \neq 0 \tag{4}$$

where $\alpha_{lk}(\underset{\sim}{x})$ is called the dislocation density. A single line along L is characterized by a Burgers vector b_i (which is a multiple of a lattice vector) and $\alpha_{lk}(\underset{\sim}{x})$ reads

$$\alpha_{\ell k}(\underset{\sim}{x}) = b_\ell \, \delta_k(L) \tag{5}$$

Dislocations may pile up to form disclinations (see Fig. 5) in which case the local rotation field $\omega_i \equiv \frac{1}{2}\varepsilon_{ijk}\partial_j u_k$ may become non-integrable with[6]

$$\varepsilon_{kij} \partial_i \partial_j \omega_\ell(\underset{\sim}{x}) = \Theta_{\ell k}(\underset{\sim}{x}) \neq 0 \tag{6}$$

For a single disclination line one has (see Fig. 6,7,8)

$$\Theta_{\ell k}(\underset{\sim}{x}) = \Omega_\ell \, \delta_k(L) \tag{7}$$

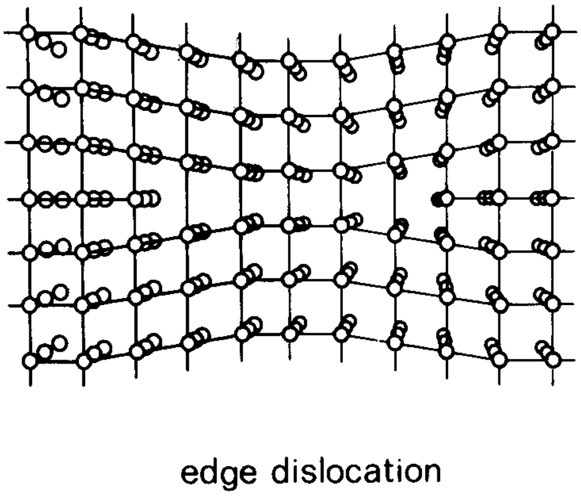


Fig. 2. An edge dislocation as the boundary line of a missing section of a lattice plane.

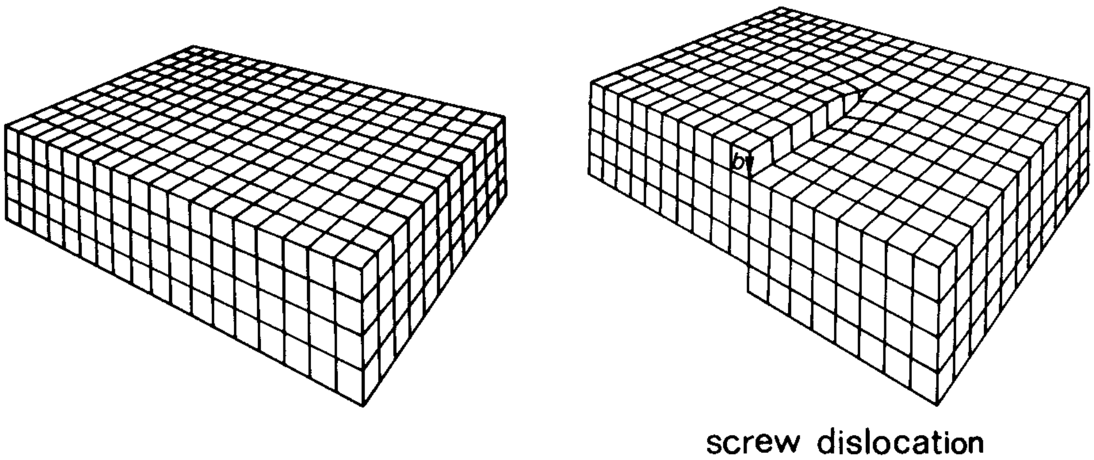


Fig. 3. A screw dislocation as the boundary line of a torn part of the crystal.

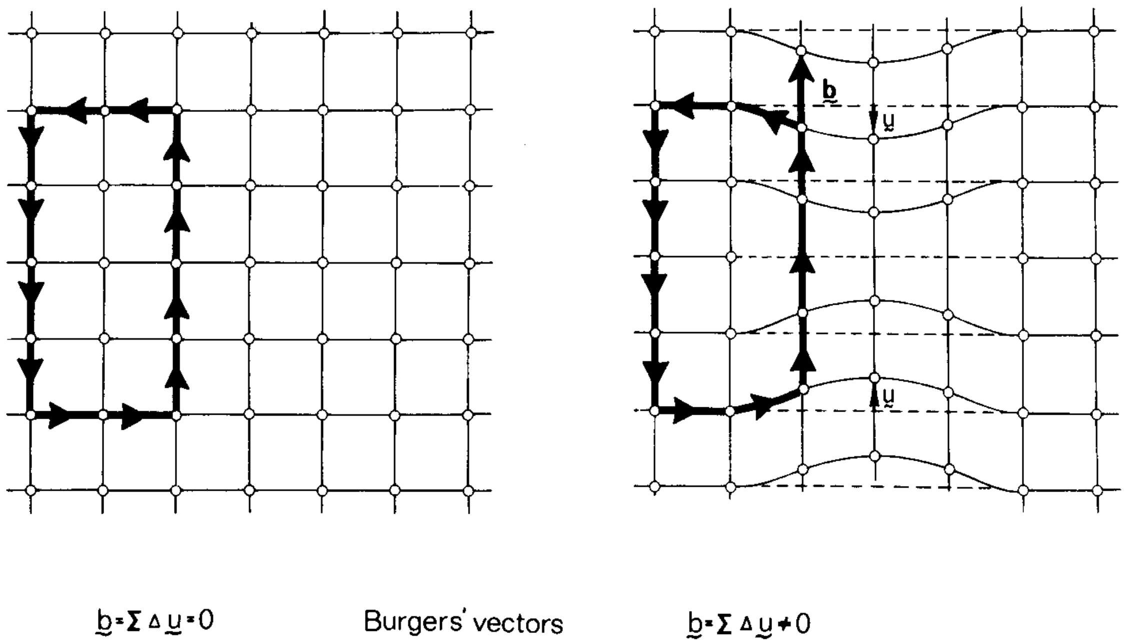


Fig. 4. The non-integrability of the displacement field at a dislocation line.

and Ω_l is called the Frank vector of the line. Instead of a differential characterization, one can state (1),(4),(6) also in the form of circuit integrals around the defect line L

$$\oint d\gamma = 2\pi n \tag{8}$$

$$\oint du_i = b_i \tag{9}$$

$$\oint d\omega_i = \Omega_i \tag{10}$$

These show that γ, u_i, ω_i are not single valued. There is a surface S Spanned by the line L, whose precise position is irrelevant, across which these variables have a jump by $2\pi n, b_i, \Omega_i$ (see Figs. 1,2,3,6,7,8).

Apart from these defects, the fields γ, u_i, ω_i are supposed to be smooth such that the physical quantities formed from its derivatives are integrable. For example, the superfluid velocity is given by $v_{s_k} \propto \partial_k \gamma$ and satisfies

$$(\partial_i \partial_j - \partial_j \partial_i) \partial_k \gamma(\underset{\sim}{x}) = 0 \tag{11}$$

The strain is given by $u_{ln} = \frac{1}{2}(\partial_l u_n + \partial_n u_l)$ and satisfies

$$(\partial_i \partial_j - \partial_j \partial_i) u_{ln}(\underset{\sim}{x}) = 0 \tag{12}$$

Moreover, also the derivative of strain and rotation field are supposed to be integrable

$$(\partial_i \partial_j - \partial_j \partial_i) \partial_k u_{ln}(\underset{\sim}{x}) = 0 \tag{13}$$

$$(\partial_i \partial_j - \partial_j \partial_i) \partial_k \omega_l(\underset{\sim}{x}) = 0 \tag{14}$$

These integrability conditions imply conservation laws.[7] Contracting (11) with ε_{ijk} shows that $\alpha_k(x)$ is divergenceless

$$\partial_k \alpha_k(\underset{\sim}{x}) = 0 \tag{15}$$

such that vortex lines can never end. Similarly, writing the dislocation density (4) as

$$\begin{aligned} \alpha_{\ell k}(\underset{\sim}{x}) &= \varepsilon_{kij}\,\partial_i \partial_j u_\ell = \varepsilon_{kij}\left(\partial_i u_{j\ell} + \varepsilon_{j\ell n}\,\omega_n\right) \\ &= \varepsilon_{kij}\,\partial_i\, u_{j\ell} + \delta_{k\ell}\,\partial_i \omega_i - \partial_\ell \omega_k \end{aligned} \tag{16}$$

and differentiating with respect to ∂_k, equ. (12) leads to

$$\partial_\ell \alpha_{k\ell}(\underset{\sim}{x}) = \varepsilon_{kij}\,\Theta_{ij} \tag{17}$$

which says that dislocations can end only on disclinations. For disclinations themselves, a few manipulations lead from (9),(10) and (11) to the conservation law

$$\partial_\ell \Theta_{k\ell}(\underset{\sim}{x}) = 0 \tag{18}$$

which says that disclination cannot end.

The conservation laws (17) and (18) can be used to construct a defect tensor

$$\eta_{ij} = \Theta_{ij} - \varepsilon_{jnk}\,\partial_k\left(\alpha_{ni} - \tfrac{1}{2}\delta_{ni}\,\alpha_{\ell\ell}\right) \tag{19}$$

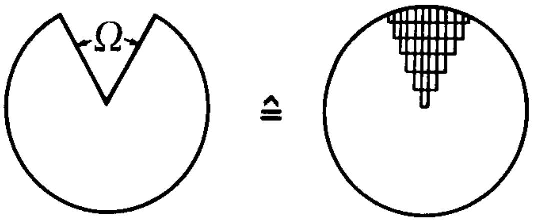


Fig. 5. Dislocation lines can stack up to form a rotational defect, a disclination.

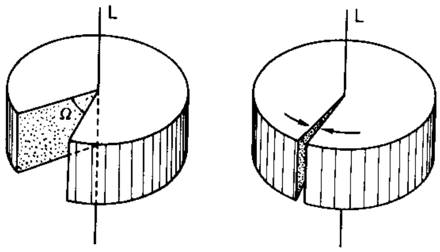


Fig. 6. A wedge disclination with Frank vector parallel to the line.

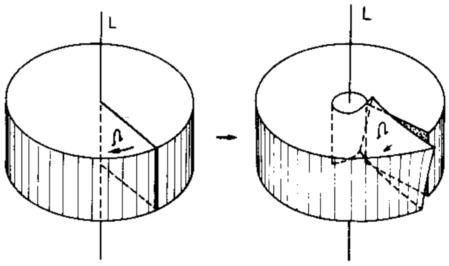


Fig. 7. A twist disclination with Frank vector orthogonal to the line and the cutting interface.

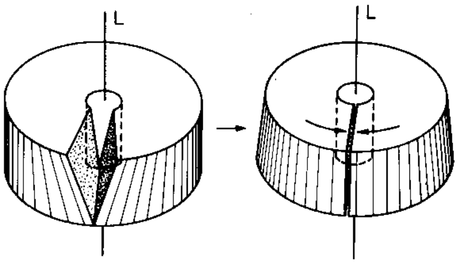


Fig. 8. A splay disclination with Frank vector orthogonal to the line but parallel to the cutting interface.

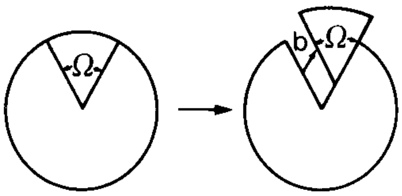


Fig. 9. A disclination and an antidisclination spaced a distance $\underset{\sim}{b}$ apart from a dislocation of Burgers' vector $\underset{\sim}{b}$.

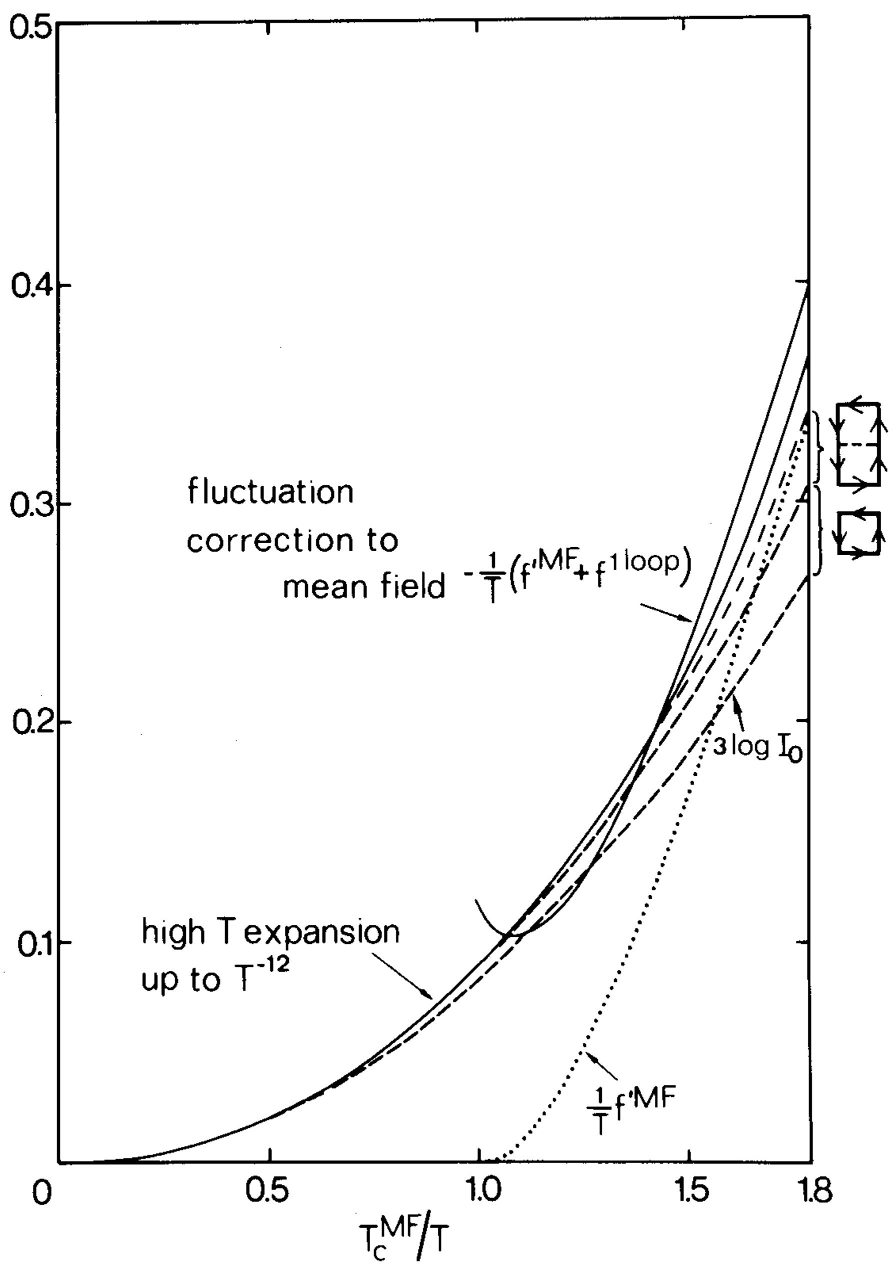


Fig. 10. The mean field potential $-\beta v = -\beta f$ for the XY model plus the one loop correction as compared with the high temperature expansion up to β^{12}. The intercept lies at $\beta_c/\beta_{MF} \sim 1.4$. The exact critical value is 1.36.

which is symmetric, due to (17), and divergenceless, due to (18). Notice that this equals Belinfante's construction of a symmetric energy momentum tensor from a canonical one Θ_{ij} and a spin current density $S_{ij,k} = \varepsilon_{ij\ell}\alpha_{\ell k}$ which reads

$$\eta_{ij} = \Theta_{ij} - \frac{1}{2}\partial_k\left(S_{ij,k} - S_{jk,i} + S_{ki,j}\right) \tag{20}$$

This is no accident since disclination density and dislocation density can be identified with Einstein curvature tensor[8] and torsion tensor of a general affine (metric) space and (17),(18) are the linearized manifestations of the two fundamental identities (in Schouten's[9] convention the so-called second identity for the torsion and the Bianchi identity for the curvature). The expression (20) is a linearized version of the symmetric energy momentum tensor of a gravitational Lagrangian $\int dx\sqrt{g}\,R$. The metric of this space is $g_{ij} = 2u_{ij}$ and the connection $\Gamma_{ijk} = \partial_i\partial_j u_k$. The geometry of this space has a simple operational meaning: Imagine a distorted crystal to be embedded in Euclidean space. Distances are measured by counting atoms in the <u>distorted crystal</u>. Vectors are parallel if they correspond to parallel vectors <u>before</u> the distortion (remaining attached to the crystalline atoms during the distortion).

Inserting the explicit forms (16),(6) into (19) we find

$$\eta_{ij} = \varepsilon_{ik\ell}\varepsilon_{jmn}\,\partial_k\partial_m\,u_{\ell n} \tag{21}$$

This double curl operation is called incompatibility.[5] It plays the same role for symmetric tensors as the single curl does for vectors. If a curl of a vector vanishes everywhere, the vector can be written as a gradient of an integrable scalar field. Similarly, if the double curl vanishes, the strain tensor can be written as $\frac{1}{2}(\partial_i u_j + \partial_j u_i)$ with integrable u_i fields! Hence we can conclude: A crystal is free of defects if $\eta_{ij}=0$.

The phenomenon of quark confinement arises if a gas of magnetic monopoles squeezes electric flux lines into thin tubes. In the usual description of magnetism it is customary to use a vector potential A_i whose curl is the magnetic field

$$B_i = \varepsilon_{ijk}\partial_j A_k \tag{22}$$

A magnetic monopole of charge m is a source of B_i field lines, defined by the condition

$$\partial_i B_i = \varepsilon_{ijk}\partial_i\partial_j A_k = m\,\delta^{(3)}(\underset{\sim}{x}) \tag{23}$$

Thus, in the presence of monopoles, the vector potential fails to satisfy the integrability condition

$$(\partial_i\partial_j - \partial_j\partial_i)A_k(\underset{\sim}{x}) = 0 \tag{24}$$

Monopoles are <u>defects</u> in the vector potential!

Notice that in a scalar description

$$B_i = \partial_i u \tag{25}$$

this would not be the case. The scalar field of a monopole $u(\underset{\sim}{x}) = (\underset{\sim}{\partial}^2)^{-1} m\,\delta(\underset{\sim}{x})$ is singular but integrable. However, in the scalar description, electric currents would cause defects since along them

$$\varepsilon_{ijk}\,\partial_i B_k = \varepsilon_{ijk}\,\partial_j \partial_k u = I\,\delta_i(L) \qquad (26)$$

which is a relation analogous to (1),(3) for vortex lines in superfluid ^{4}He.

Thus, in a system with electric currents and magnetic monopoles there are always defects. With the traditional choice of a vector potential, these are the monopoles.

Lattice formulations of partition functions permit a simple study of ensembles of defects. If these are line-like, there is usually a certain temperature where the entropy overwhelms the energy and causes a proliferation of lines. On a lattice in 3 dimensions, a line involving n links has $(2D)^n$ configurations. If the energy per link is ε , the partition function

$$Z = \sum_n (2D)^n e^{-\frac{\varepsilon}{T} n}$$

indicates a proliferation for[2] $T > T_c = \varepsilon / \log 2D$. Vortex lines destroy the superfluid order[10], dislocation lines the translational order (creating liquid crystals)[11] and disclination lines the rotational order.[12]

The magnetic monopoles in three dimensions behave like a classical Coulomb gas. Since Debye, it has been known that there is screening which changes the propagation of fields for all temperatures, i.e. independent of how dilute the gas is. This Debye screening causes quark confinement, as was first observed by Polyakov.[4]

It is interesting to discover a great similarity between the three models describing such different systems:

Superfluid He is studied by means of an XY model on a simple cubic lattice with sites $\underset{\sim}{x}$.[13]

$$Z_{XY} = \prod_{\underset{\sim}{x}} \int_{-\pi}^{\pi} \frac{d\gamma(\underset{\sim}{x})}{2\pi}\, e^{\beta \sum_{x,i} (\cos \nabla_i \gamma(\underset{\sim}{x}) - 1)} \tag{27}$$

where $\nabla_i \gamma = \gamma(\underset{\sim}{x}+\underset{\sim}{i}) - \gamma(\underset{\sim}{x})$ is the lattice gradient across the links $\underset{\sim}{i}=(1,0,0),(0,1,0),(0,0,1)$ connecting $\underset{\sim}{x}$ and $\underset{\sim}{x}+\underset{\sim}{i}$. The Villain approximation,[14]

$$Z_{XY} \simeq Z_V = R_V^N \sum_{\{n_i(x)\}} \prod_{\underset{\sim}{x}} \int_{-\pi}^{\pi} \frac{d\gamma(x)}{2\pi} \quad e^{-\frac{\beta_V}{2}\sum_{x,i}(\nabla_i\gamma - 2\pi n_i)^2} \tag{28}$$

with $R_V = (I_0(\beta) e^{-\beta} \sqrt{2\pi\beta_V})$ and $\beta_V = -[2\log(I_1(\beta)/I_0(\beta))]^{-1}$ displays the surfaces over which γ jumps ($n_3(o)=1$ means that γ jumps when passing the XY plane for 0 to 1). Instead of integrating from $-\pi$ to π we can integrate over the entire γ axis, if we remove from n_i the gradient of an integer field, i.e.

$$n_i \to n_i - \nabla_i n \tag{29}$$

By choosing $n = \nabla_3^{-1} n_i$, the remaining n_i can be taken to satisfy $n_3=o$. Hence

$$Z_V = R_V^N \sum_{\{n_i(x)\}} \delta_{n_3,0} \prod_{\underset{\sim}{x}} \int_{-\infty}^{\infty} \frac{d\gamma(x)}{2\pi} e^{-\frac{\beta_V}{2}\sum_{x,i}(\nabla_i\gamma - 2\pi n_i)^2} \tag{30}$$

Introducing a conjugate variable B_i, which is the superfluid velocity and plays the same role as a magnetic field for electric currents, in the gradient representation (25), we can rewrite this as

$$Z_V = R_V^N \sum_{\{n_i(\mathbf{x})\}} \delta_{n_3,0} \prod_{\mathbf{x},i} \int_{-\infty}^{\infty} \frac{dB_i}{\sqrt{2\pi\beta}} \prod_{\mathbf{x}} \int_{-\infty}^{\infty} \frac{d\gamma}{2\pi}\, e^{-\frac{1}{2\beta_V}\sum_{\mathbf{x},i} B_i^2 + i\sum_{\mathbf{x},i} B_i(\nabla_i\gamma - 2\pi n_i)} \tag{31}$$

The integrals over γ force B_i to be divergenceless. Hence we can express B_i in terms of a vector potential

$$B_i = \varepsilon_{ijk}\partial_j A_k \tag{32}$$

and write

$$Z_V = R_V^N \sum_{\{n_i(\mathbf{x})\}} \delta_{n_3,0} \int_{-\infty}^{\infty} \frac{dA_i}{\sqrt{2\pi\beta}}\, \delta(\nabla_i A_i)\, e^{-\frac{1}{2\beta_V}\sum_{\mathbf{x}}(\nabla\times\mathbf{A})^2 + 2\pi i\sum_{\mathbf{x},i} A_i l_i} \tag{33}$$

where we have set

$$l_i(\mathbf{x}) = (\nabla\times\mathbf{n})(\mathbf{x}) \tag{34}$$

This is an integer field satisfying $\bar{\nabla}_i l_i = 0$. It can be pictured as superposition of closed integer lines and is the lattice version of the vortex density $\alpha_k(\mathbf{x})$ (recall (3)). Due to (33), the vortex lines interact in the same way as electric currents (Biot-Savart forces). From (34) we see that the l_i form the boundary lines of the surfaces across which the phase γ jumps. Hence l_i are the vortex lines. The smallest is given by a single $n_i(x)$ being equal to one which gives a loop around one plaquette. This can be identified with a roton. In fact, its energy turns out to be about the same as that of a roton. Rotons have dipole forces. These do not change the field propagators as long as they are dilute. Only when they proliferate does screening set in and there is a close relation to the Meissner screening of magnetic field lines in super conductors. There exists a disorder field theory of the Ginzburg-Landau type describing this proliferation of vortices and the Meissner like screening.[10]

In a crystal, we can construct a similar model containing dislocations and disclinations. The linear elastic energy is, in terms of the displacement vector

$$e(\underset{\sim}{x}) = \frac{\mu}{4} (\partial_i u_j + \partial_j u_i)^2 \tag{35}$$

if we neglect the Lamé constant λ, for brevity. Dislocation lines are characterized by jumps of u_i across certain surfaces. Their ensemble can be studied by[15,16]

$$Z_{1\,\text{melt}} = \prod_{\underset{\sim}{x},i} \int_{-\pi}^{\pi} \frac{dA_i(\underset{\sim}{x})}{2\pi}\, e^{\beta\left[\sum_{\underset{\sim}{x},i>j} \left(\cos(\nabla_i A_j + \nabla_j A_i) - 1\right) + 2\sum_{\underset{\sim}{x},i} (\cos \nabla_i A_i - 1)\right]} \tag{36}$$

which has a Villain approximation

$$Z_{1\,\text{melt}} \approx Z_{\text{melt},V} = R_V^{6N} \sum_{\{n_{ij}(\underset{\sim}{x})\}} \prod_{\underset{\sim}{x},i} \int_{-\pi}^{\pi} \frac{dA_i}{2\pi}\, e^{-\frac{\beta_V}{2}\left[\sum_{\underset{\sim}{x},i>j} (\nabla_i A_j + \nabla_j A_i - 2\pi n_{ij})^2 + \frac{1}{2}\sum_{\underset{\sim}{x},i} (\nabla_i A_i - 2\pi n_{ii})^2\right]} \tag{37}$$

We have renormalized u_i to $A_i = \frac{2\pi}{a} \cdot u_i$ such that it is periodic in 2π, and set $\beta \equiv \mu a^3/((2\pi)^2 T)$. We can again extend the A_i integrations over all real values by restricting n_{ij} to

$$n_{3j} = n_{j3} = 0 \tag{38}$$

Just as in (30) it is possible to introduce a conjugate stress variable σ_{ij} and write

$$Z_{met,V} = R_V^{(N} \prod_{\mathbf{x}, i \geq j} \int_{-\infty}^{\infty} \frac{d\sigma_{ij}}{\sqrt{2\pi\beta_V}} e^{\frac{1}{4\beta_V} \sum_{\mathbf{x}, i,j} \sigma_{ij}^2} \tag{39}$$

$$\cdot \sum_{\{n_{ij}(\mathbf{x})\}} \delta_{n_{3i},0}\, e^{\frac{i}{2}\sum_{\mathbf{x}, i>j} \sigma_{ij}(\nabla_i A_j + \nabla_j A_i - 2\pi n_{ij}) + i \sum_{\mathbf{x}, i} \sigma_{ii}(\nabla_i A_i - 2\pi n_{ii})}$$

The integrals over A_i force

$$\bar{\nabla}_i \sigma_{ij} = 0 \tag{40}$$

which is the standard equation for linear elasticity. This can be taken advantage of to express σ_{ij} in terms of a symmetric gauge field

$$\sigma_{ij} = \varepsilon_{ikl}\, \varepsilon_{jmn}\, \bar{\nabla}_k \bar{\nabla}_m \chi_{ln} \tag{41}$$

In this way, (39) becomes

$$Z_{met,V} = R_V^{6N} \prod_{\mathbf{x}, i \geq j} \int_{-\infty}^{\infty} \frac{d\chi_{ij}(\mathbf{x})}{\sqrt{4\pi\beta_V}} \Phi[\chi] \tag{42}$$

$$\sum_{\{n_{ij}(\mathbf{x})\}} \delta_{n_{3j},0}\, e^{-\frac{1}{4\beta_V}\sum_{\mathbf{x}} (\varepsilon\varepsilon\bar{\nabla}\bar{\nabla}\chi)^2 + 2\pi i \sum_{\mathbf{x}, ij} \chi_{ij}\eta_{ij}}$$

where $\Phi[\chi]$ is a gauge fixing factor (for example $\prod_{\mathbf{x}, i} \delta(\chi_{3i}(\mathbf{x}))$) and

$$\eta_{ij} = \varepsilon_{ikl}\, \varepsilon_{jmn}\, \bar{\nabla}_k \bar{\nabla}_m n_{ln} \tag{43}$$

is a symmetric integer tensor satisfying

$$\nabla_i \eta_{ij}(\underset{\sim}{x}) = 0 \tag{44}$$

This is the lattice version of the defect density (21). integrating out the χ fields gives

$$Z_{melt,V} = \beta_V^{6N} \frac{1}{(4\pi\beta_V)^{\frac{3N}{2}}} e^{-\beta_V 4\pi^2 \sum_{\underset{\sim}{x},\underset{\sim}{x}'} \eta_{ln}(\underset{\sim}{x}) v_4(x-x') \eta_{ln}(x')} \tag{45}$$

where

$$v_4(\underset{\sim}{x}) = \int \frac{d^3k}{(2\pi)^3} \left(2D - 2\sum_i \cos k_i\right)^{-2} \tag{46}$$

is the lattice version of the $1/k^4$ potential. It diverges which implies that only such defect configurations $\eta_{ln}(\underset{\sim}{x})$ can contribute which are neutral

$$\sum_{\underset{\sim}{x}} \eta_{ln}(\underset{\sim}{x}) = 0 \tag{47}$$

For these, in turn, we can use the finite subtracted potential

$$v_4'(\underset{\sim}{x}) \equiv v_4(\underset{\sim}{x}) - v_4(\underset{\sim}{0}) \tag{48}$$

Similar to the XY model, the melting model has a critical temperature at which dislocation loops proliferate. These cause a screening of the elastic forces, which can again be viewed as a Meissner effect, by going to a disorder field description.[17] Contrary to the XY model, the transition is now of first order. The reason for this is quite simple: Lattice defects allow for certain collective formations whose energy is much lower than the sum of the individual energies. An example was given before: Many dislocation lines can pile up on top of each other and form a disclination line (see Fig. 5). If two such disclination lines run through the crystal in opposite directions the energy between line elements grows like R. Hence they are permanently confined. In fact, one may consider the disclinations as fundamental defect lines as confined pairs (see Fig. 9). When the dislocation lines proliferate, they screen the elastic forces from R to 1/R.[18] This leads to the deconfinement of its constituents. The proliferation alone would be a second order transition, the ensuing deconfinement opens up an additional reservoir of entropy and this is what causes the discontinuity of the transition.

An ensemble of monopoles in a magnetic field can be studied with the model[4]

$$Z_{\text{gauge}} = \prod_{\mathbf{x},i} \int_{-\pi}^{\pi} \frac{dA_i(\mathbf{x})}{2\pi}\, e^{\beta \sum_{\mathbf{x},i>j} \left(\cos(\nabla_i A_j - \nabla_j A_i) - 1\right)} \tag{49}$$

called lattice QED. Its Villain approximation reads

$$Z_{\text{gauge},V} = R_V^{\,3N} \sum_{\{n_{ij}(\mathbf{x})\}} \prod_{\mathbf{x},i} \int_{-\pi}^{\pi} \frac{dA_i(\mathbf{x})}{2\pi}\, e^{-\frac{\beta_V}{2} \sum_{\mathbf{x},i>j} \left(\nabla_i A_j - \nabla_j A_i - 2\pi n_{ij}\right)^2} \tag{50}$$

Introducing a conjugate magnetic field gives

$$Z_{\text{gauge},V} = R_V^{\,3N} \sum_{\{n_{ij}(\mathbf{x})\}} \prod_{\mathbf{x},i>j} \int_{-\infty}^{\infty} \frac{df_{ij}(\mathbf{x})}{\sqrt{2\pi\beta_V}} \prod_{\mathbf{x},i} \int_{-\pi}^{\pi} \frac{dA_i(\mathbf{x})}{2\pi} \tag{51}$$

$$e^{-\frac{1}{2\beta_V} \sum_{\mathbf{x},i>j} f_{ij}^2 + i \sum_{\mathbf{x},i>j} f_{ij} \left(\nabla_i A_j - \nabla_j A_i - 2\pi n_{ij}\right)}$$

Summing over the n_{ij} forces f_{ij} to be integer whereupon the integrations over A_i give

$$\bar{\nabla}_i f_{ij} = 0 \tag{52}$$

Therefore one can write

$$f_{ij} = \varepsilon_{ijk} \bar{\nabla}_k \varphi \tag{53}$$

with an integer scalar field $\varphi(\underset{\sim}{x})$. This, in turn, can be integrated over all real values if one couples it to an integer field m(x):

$$Z_{gauge,V} = \left(R_V^3 \frac{1}{2\pi\beta_V}\right)^N \sum_{\{m(\underset{\sim}{x})\}} \prod_{\underset{\sim}{x}} \int \frac{d\varphi(\underset{\sim}{x})}{\sqrt{2\pi\beta^V}} \, e^{-\frac{1}{2\beta_V}\sum_{\underset{\sim}{x}}(\bar{\nabla}\varphi)^2 + 2\pi i \sum_{\underset{\sim}{x}} \varphi(\underset{\sim}{x}) m(\underset{\sim}{x})} \tag{54}$$

Integrating out the φ field gives

$$Z_{gauge,V} = \left(R_V^3 \frac{1}{2\pi\beta_V}\right)^N \sum_{\{m(\underset{\sim}{x})\}} e^{-\frac{\beta_V}{2} 4\pi^2 \sum_{\underset{\sim}{x},\underset{\sim}{x}'} m(\underset{\sim}{x}) v_2(\underset{\sim}{x}-\underset{\sim}{x}') m(\underset{\sim}{x}')} \tag{55}$$

where

$$v_2(\underset{\sim}{x}) = \int \frac{d^3k}{(2\pi)^3} \, e^{i\underset{\sim}{k}\underset{\sim}{x}} \left(2D - 2\sum_i \cos k_i\right)^{-1} \tag{56}$$

is the lattice Coulomb potential. The field $m(\underset{\sim}{x})$ parametrizes the ensemble of monopole charges. It is related to the jumps n_{ij} via

$$m(\underset{\sim}{x}) = \varepsilon_{ijk} \nabla_i n_{jk}(\underset{\sim}{x}) \tag{57}$$

under the constraint $n_{3j} = n_{j3} = 0$.

The Debye screening can be seen by separating the self-energy of the monopoles and writing

$$v_2(\underset{\sim}{x}) = v_2(\underset{\sim}{0}) + v_2'(\underset{\sim}{x}) = .2527 + v_2'(\underset{\sim}{x}) \tag{58}$$

which allows bringing (55) to the form

$$Z_{\text{gauge},V} = \left(R_V^3 \frac{1}{2\pi\beta_V}\right)^N \prod_{\underset{\sim}{x}} \int_{-\infty}^{\infty} \frac{d\varphi}{\sqrt{2\pi\beta_V}}\, e^{-\frac{1}{2\beta_V}\sum_{\underset{\sim}{x},\underset{\sim}{x}'} \varphi(\underset{\sim}{x}) \frac{-\nabla_\ell \bar{\nabla}_\ell}{1+v(0)\nabla_\ell\bar{\nabla}_\ell}(\underset{\sim}{x},\underset{\sim}{x}')\varphi(\underset{\sim}{x}')}$$

$$\sum_{\{m(\underset{\sim}{x})\}} e^{-\beta_V \frac{4\pi^2}{2} v_2(\underset{\sim}{0}) \sum_{\underset{\sim}{x}} m^2(x) + 2\pi i \sum_{\underset{\sim}{x}} \varphi(\underset{\sim}{x}) m(\underset{\sim}{x})} \tag{59}$$

For large β, only $m(\underset{\sim}{x}) = 0, \pm 1$ has to be summed and the last factor becomes

$$e^{2 e^{-\beta_V \frac{4\pi^2}{2} v_2(\underset{\sim}{0})} \cdot \sum_{\underset{\sim}{x}} \cos 2\pi\varphi(\underset{\sim}{x})} \tag{60}$$

The curvature of the cosine term induces a mass

$$m^2 = 8\pi^2 e^{-\beta_V \frac{4\pi^2}{2} v_2(\underset{\sim}{0})} \tag{61}$$

and this is responsible for confinement.[4]

Comparing the partition function (27), (36), and (49) we notice the following relation. The latter two cases can be considered as special constraint versions of an extended XY model for <u>three</u> angular variables

$$Z'_{XY} = \prod_{x,i} \int_{-\pi}^{\pi} \frac{d\gamma_i(x)}{2\pi} \, e^{\beta \sum_{x,i,j} \left(\cos \nabla_i \gamma_j - 1\right)} \tag{62}$$

As long as the angles are independent, this partition function is simply the cube of the individual XY models.

$$Z'_{XY} = Z^3_{XY} \tag{63}$$

The melting model counts only the energy of <u>symmetric</u> combinations, the gauge model that of <u>antisymmetric</u> combinations of $\nabla_i \gamma_j$.

The XY model has a <u>second order</u> phase transition and so does (62). The antisymmetric combination has <u>no phase</u> transition (permanent confinement). The symmetric combination, on the other hand, describes melting which is a <u>first order</u> transition. Thus, symmetrization of the tensor $\nabla_i \gamma_j$ in (62) hardens the transition, antisymmetrization softens it.

The simplest way of studying the phase diagram of such theories is via a mean field approximation plus loop corrections.[19,20] This follows from the possibility of rewriting the partition functions in the following way

$$Z_{XY} = e^{-3N\beta} \prod_{\underset{\sim}{x}} \int_{-\pi}^{\pi} \frac{d\gamma(\underset{\sim}{x})}{2\pi} \, e^{\beta \sum_{\underset{\sim}{x},i} U(\underset{\sim}{x})\, U^{\dagger}(\underset{\sim}{x}+\underset{\sim}{i})} \tag{64}$$

$$Z_{melt} = e^{9N\beta} \prod_{\mathbf{x},i} \int_{-\pi}^{\pi} \frac{dA_i}{2\pi}\, e^{\beta\left[\sum_{\mathbf{x},i>j} U_i(\mathbf{x}) U_j^+(\mathbf{x}+\mathbf{i}) U_i^+(\mathbf{x}+\mathbf{j}) U_j(\mathbf{x}) + 2\sum_{\mathbf{x},i} U_i(\mathbf{x}) U_i^+(\mathbf{x}+\mathbf{i})\right]} \tag{65}$$

$$Z_{gauge} = e^{3N\beta} \prod_{\mathbf{x},i} \int_{-\pi}^{\pi} \frac{dA_i}{2\pi}\, e^{\beta \sum_{\mathbf{x},i>j} U_i(\mathbf{x}) U_j(\mathbf{x}+\mathbf{i}) U_i^+(\mathbf{x}+\mathbf{j}) U_j^+(\mathbf{x})} \tag{66}$$

where $U(\mathbf{x}) = e^{i\gamma(\mathbf{x})}$, $U_i(\mathbf{x}) = e^{iA_i(\mathbf{x})}$. Melting and the first term in the gauge theory differ only by the position of a star on the U's which corresponds graphically to exchanging a rotation graph  by a distortion graph  .

The introduction of two auxiliary complex fields via the identity

$$\prod_{\mathbf{x}} \iint_{-i\infty}^{i\infty} \frac{d\alpha(\mathbf{x})\, d\alpha^+(\mathbf{x})}{(2\pi)^2} \iint_{-\infty}^{\infty} du(\mathbf{x})\, du^+(\mathbf{x})\, e^{\frac{i}{2}\sum_{\mathbf{x}} \alpha^+(u-U) + c.c.} \tag{67}$$

permits a reformulation of the partition functions as integrals over the fluctuating energies[19,20]

$$-\beta F_{xy} = \sum_{\mathbf{x}} \left[\beta \sum_i u(\mathbf{x}) u^+(\mathbf{x}+\mathbf{i}) - \tfrac{1}{2}(\alpha^+(\mathbf{x}) u(\mathbf{x}) + c.c.) - \log I_0(|\alpha|)\right] \tag{68}$$

$$-\beta F_{melt} = \sum_{\mathbf{x}} \Big[\beta \sum_{i>j} u_i(\mathbf{x}) u_j^+(\mathbf{x}+\mathbf{i}) u_i^+(\mathbf{x}+\mathbf{j}) u_j(\mathbf{x}) + 2\beta \sum_i u_i(\mathbf{x}) u_i(\mathbf{x}+\mathbf{i}) \tag{69}$$
$$- \tfrac{1}{2}\sum_i (\alpha_i^+(\mathbf{x}) u_i(\mathbf{x}) + c.c.) - \sum_i \log I_0(|\alpha_i|)\Big]$$

$$-\beta F_{gauge} = \sum_{\underline{x}} \Big[\beta \sum_{i>j} u_i(\underline{x}) u_j(\underline{x}+\underline{i}) u_i^{+}(\underline{x}+\underline{j}) u_j^{+}(\underline{x})$$

$$- \frac{1}{2} \sum_i (\alpha_i^{+}(\underline{x}) u_i(\underline{x}) + c.c.) - \sum_i \log I_0(|\alpha_i|) \Big] \tag{70}$$

The mean field equations are

$$|u| = \frac{I_1(|\alpha|)}{I_0(|\alpha|)} \tag{71}$$

in all three cases and

$$\left.\begin{array}{lll} \alpha = 6\beta u & \text{for XY} & (72) \\ |\alpha_i| = 4\beta(|u_i|^3 + |u_i|) & \text{for melting} & (73) \\ |\alpha_i| = 4\beta|u_i| & \text{for gauge} & (74) \end{array}\right\} \text{model}$$

This gives a second order transition for the XY model at $\beta_c^{MF} = 1/3$. For melting[16] and guage models[20] one finds, on the other hand, a first order transition at

$$\beta_c^{MF} = .49 \qquad \text{melting}$$

$$\beta_c^{MF} = 1.52 \qquad \text{gauge}$$

For $\beta < \beta_c^{MF}$, the mean fields are zero, for $\beta > \beta_c^{MF}$ they grow from zero to $u \sim 1$, $\alpha_i \sim 6\beta, 8\beta, 4\beta$. Fluctuation corrections change the energy for low β by adding a power series in β which is known[21] up to β^{12} . Above β_c^{MF} , the loop correction gives the major contributions and shifts $-\beta f$ slightly upwards. For the XY model, this brings β_c up to .47 (see Fig. 11).

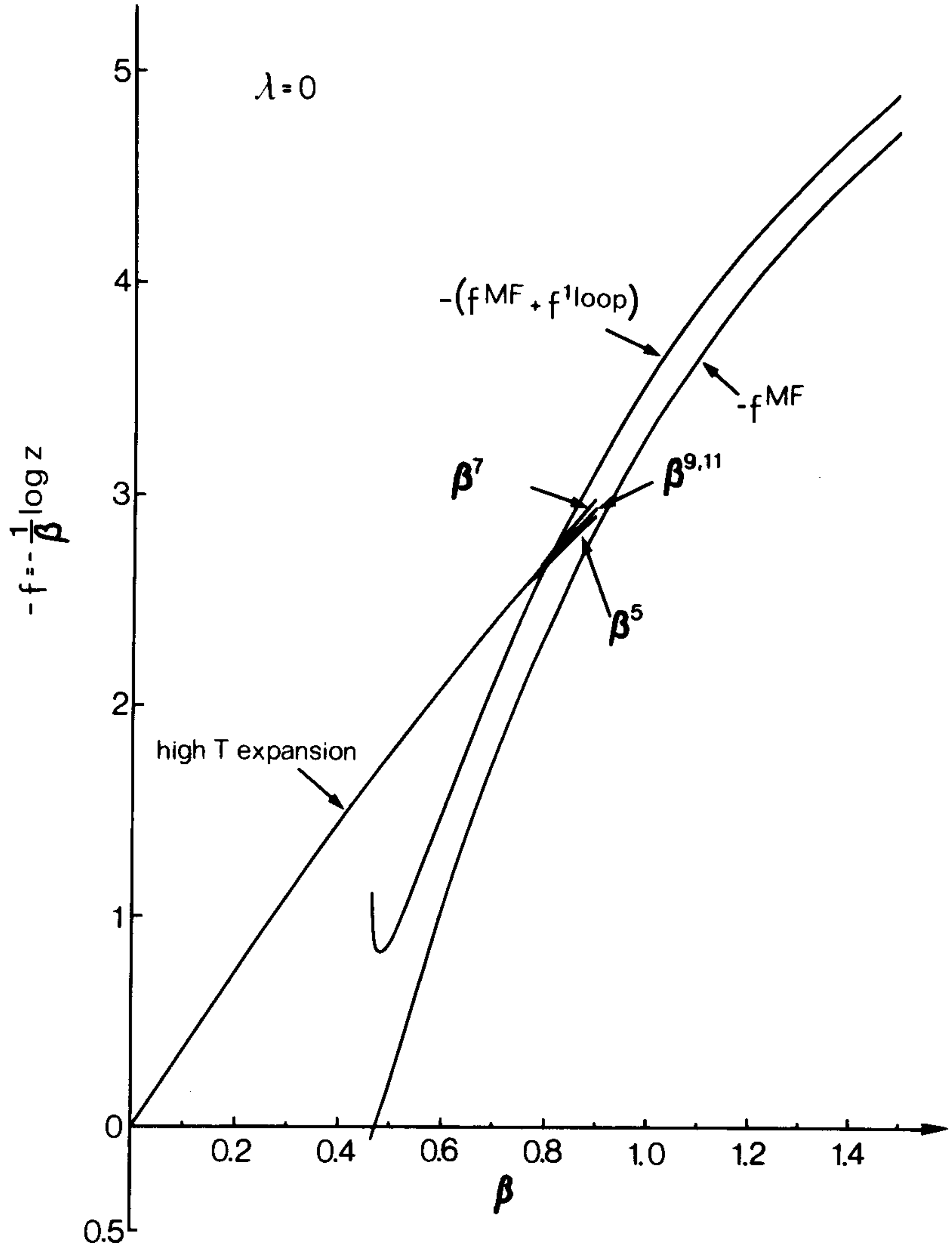


Fig. 11. The same plot as in Fig. 9, but for the melting model.

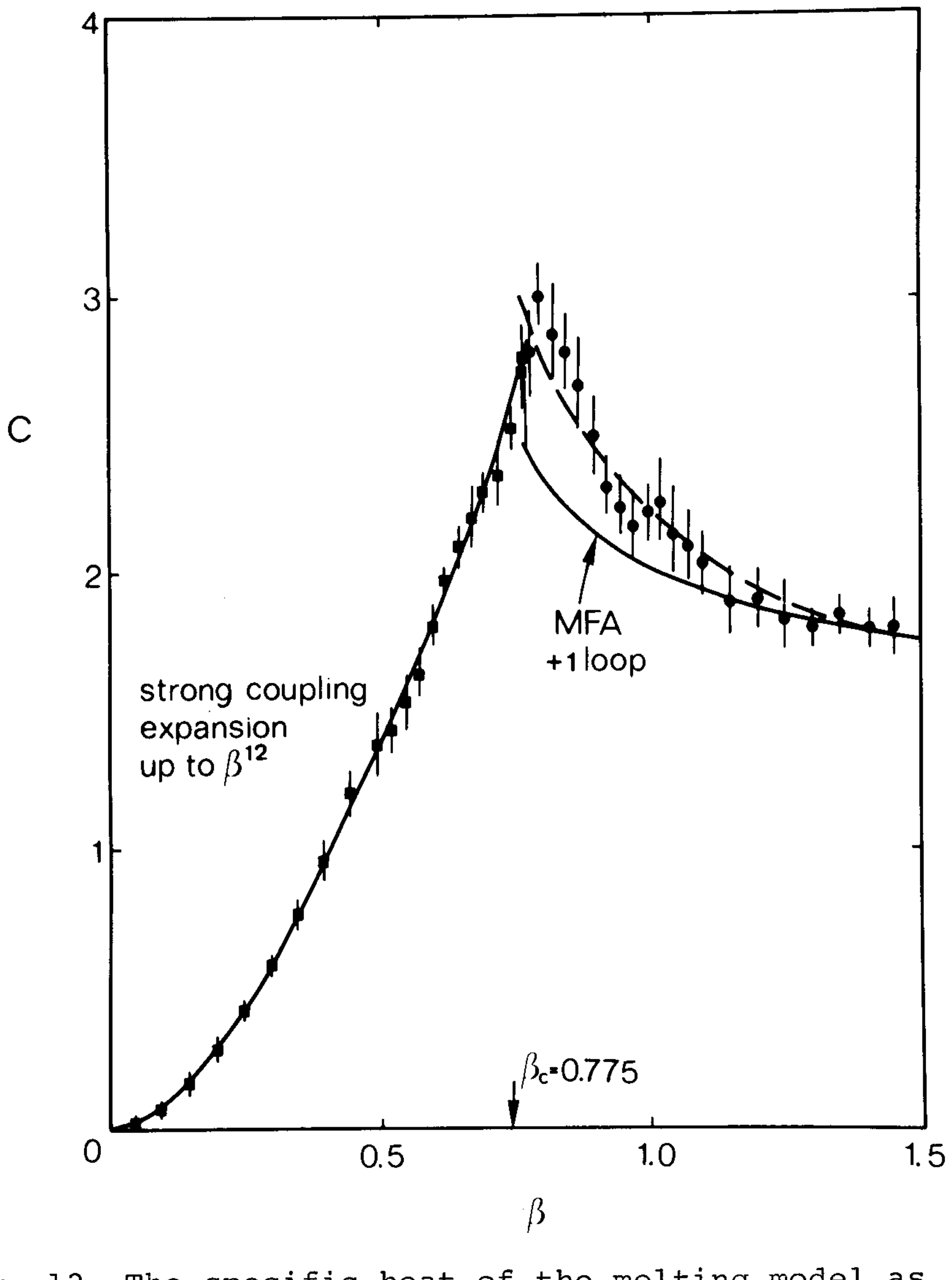


Fig. 12. The specific heat of the melting model as compared with mean field calculation plus one loop correction for $\beta > \beta_c$ and with a low temperature expansion up to β^{12} for $\beta < \beta_c$.

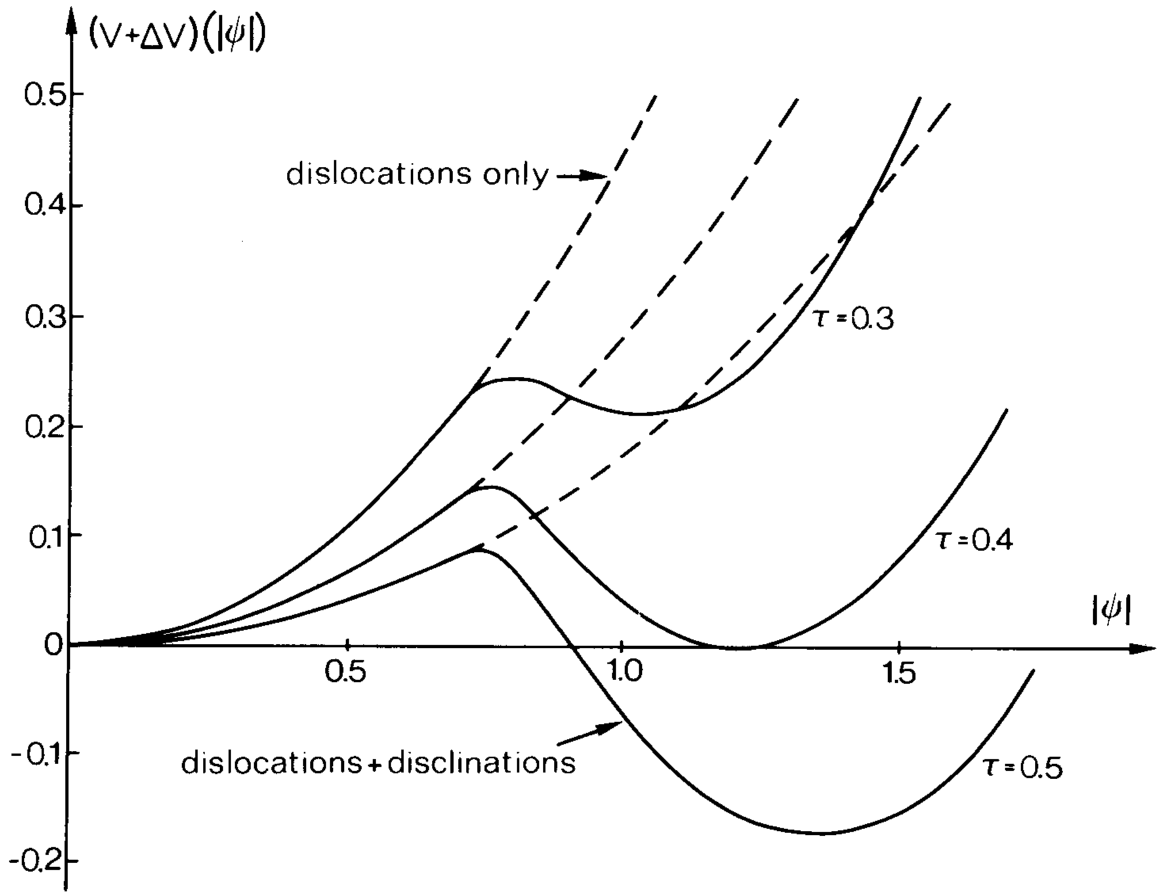


Fig. 13. The potential of the disorder field theory of dislocation plus disclination lines as a function of the dislocation field $|\Psi|$. The curve "dislocations only" corresponds to the pure proliferation (second order transitions). The break-up due to Meissner screening causes the additional lowering of the energy which causes the first order phase transition.

For the gauge theory, the corrections are so important that they wipe out the transition completely. The model always remains on the energy branch obtained by the low β expansion.

The melting theory, on the other hand, retains the first order of the mean field transition. The jump in entropy comes out $S=1.4k_B$ per site, in good agreement with experimental data.[22,23] The shape of the specific heat agrees reasonably with experimental curves (see Fig. 12.)

In conclusion we see that defects form the common basis for the understanding of many phase transitions. Their analysis can give an important clue concerning the order of the transition. Melting and U(1) lattice gauge theory are, in one respect, quite similar, namely by having the same mean field approximations. However, their defects are quite different, and this explains why melting is a first order transition while the gauge theory has confinement at all temperatures.

Closed defect lines have dipole interactions. For this reason, few of them cannot cause screening. Their proliferation is necessary to achieve this. Point defects, with Coulomb forces, on the other hand, screen for all temperatures in three dimensions, as is known from Debye's classical work. If closed defect lines can break up after screening the coupled transition "proliferation plus break up" is of first order (see Fig. 13.)

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