LETTERE AL NUOVO CIMENTO VOL. 37, N. 12 23 Luglio 1983

Relation between U_1 Lattice Gauge Theory and Defect Melting.

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(ricevuto il 14 Aprile 1983)

PACS. 11.10. – Field theory.
PACS. 61.70. – Defects in crystals.

Summary. – We point out that the U_1 lattice gauge theory and the recently developed theory of defect melting are closely related. They differ mainly by the positions of the « daggers » in the plaquette energy, *i.e.* $U_1(\boldsymbol{x})\,U_j(\boldsymbol{x}+\boldsymbol{i})\,U_i^\dagger(\boldsymbol{x}+\boldsymbol{j})\,U_j^\dagger(\boldsymbol{x})$ is replaced by $U_i(\boldsymbol{x})\,U_j^\dagger(\boldsymbol{x}+\boldsymbol{i})\,U_i^\dagger(\boldsymbol{x}+\boldsymbol{j})\,U_j(\boldsymbol{x})$. As a consequence, both theories have essentially the same mean-field approximation with a first-order transition at that level. In the gauge theory, this result is wrong and modified completely by fluctuations. Melting, on the other hand, is a first-order transition such that the mean-field result is in qualitative agreement with experiment.

The Abelian U_1 lattice gauge theory has a partition function [1]

$$(1)\qquad Z=\prod_{\boldsymbol{x},i}\int_{-\pi}^{\pi}\frac{\mathrm{d}A_j(\boldsymbol{x})}{2\pi}\exp\left[\frac{1}{2}\beta\sum_{\boldsymbol{x},i,j}\left(\cos\left(\nabla_i A_j-\nabla_j A_i\right)-1\right)\right]=$$

$$=\prod_{\boldsymbol{x},i}\int\mathrm{d}U_i(\boldsymbol{x})\exp\left[\frac{1}{2}\beta\sum_{\boldsymbol{x},i,j}\mathrm{Re}\,(U_{ij}-1)\right],$$

where

$$(2)\qquad U_{ij}=U_i(\boldsymbol{x})\,U_j(\boldsymbol{x}+\boldsymbol{i})\,U_i^\dagger(\boldsymbol{x}+\boldsymbol{j})\,U_j^\dagger(\boldsymbol{x})$$

(*) Supported in part by the National Science Foundation, grant No. PHY77-27084.
(1) K. WILSON: *Phys. Rev. D*, **10**, 2445 (1974).

is a product of four U_1 transformations $U_i(\boldsymbol{x}) = \exp[iA_j(\boldsymbol{x})]$ encircling each plaquette as  .

Recently it was shown that defect melting can be studied by means of a partition function [2]

$$(3)\qquad Z = \sum_{\{n_{ij}(\boldsymbol{x})\}} \prod_{\boldsymbol{x},i} \int_{-\pi}^{\pi} \frac{\mathrm{d}A_i(\boldsymbol{x})}{2\pi} \cdot \exp\left[-\frac{\beta}{4}\left[\sum_{\boldsymbol{x},i,j} (\nabla_i A_j + \nabla_j A_i - 2\pi n_{ij})^2 + \frac{2\lambda}{\mu}\left(\sum_{\boldsymbol{x}} (\nabla_i A_i - \pi n_{ii})\right)^2\right]\right],$$

where μ, λ are the elastic constants $\left(\nu = \lambda/(2(\mu+\lambda)) = \text{Poisson ratio}\right)$ and $\beta = \mu a^3/((2\pi)^2 T)$, with T being the temperature. The sum over symmetric integer numbers n_{ij} $(i \neq j)$ and even numbers n_{ii} produces precisely the dislocation lines existing in crystal lattices, including the proper elastic forces between them [3]. This partition function, however, is simply the Villain approximation [4] to

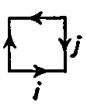
$$(4)\qquad Z = \prod_{\boldsymbol{x},i} \int_{-\pi}^{\pi} \frac{\mathrm{d}A_i(\boldsymbol{x})}{2\pi} \exp\left[\beta\left\{\sum_{\boldsymbol{x},i>j} (\cos(\nabla_i A_j + \nabla_j A_i) - 1) + 2\sum_{\boldsymbol{x},i} (\cos(\nabla_i A_i) - 1) + \frac{\mu}{\lambda}\sum_{\boldsymbol{x}}\left(\cos\left(\sum_i \nabla_i A_i\right) - 1\right)\right\}\right],$$

which, in turn, can be written as

$$(5)\qquad Z = \prod_{\boldsymbol{x},i} \int \mathrm{d}U_i(\boldsymbol{x}) \exp\left[\beta\left\{\sum_{\boldsymbol{x},i>j} \mathrm{Re}\,(V_{ij} - 1) + 2\sum_{\boldsymbol{x},i} \mathrm{Re}\,(V_i - 1) + \frac{\lambda}{\mu}\sum_{\boldsymbol{x}} \mathrm{Re}\,(V - 1)\right\}\right],$$

where V_{ij} is the *distortion* analogue of U_{ij}, namely

$$(6)\qquad V_{ij} \equiv U_i(\boldsymbol{x})\, U_j^{\dagger}(\boldsymbol{x} + \boldsymbol{i})\, U_i^{\dagger}(\boldsymbol{x} + \boldsymbol{j})\, U_j(\boldsymbol{x})$$

in which the U_i lines in the plaquettesm ay be pictured as  . Further

$$V_i \equiv V_{ii}^{\frac{1}{2}} = U_i(\boldsymbol{x})\, U_i^{\dagger}(\boldsymbol{x} + \boldsymbol{i}),$$

and

$$V \equiv V_1 V_2 V_3 .$$

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(2) H. KLEINERT: *Phys. Lett. A*, **91**, 295 (1982).
(3) H. KLEINERT: *Phys. Lett. A*, **89**, 294 (1982); *Lett. Nuovo Cimento*, **34**, 464 (1982).
(4) J. VILLAIN: *J. Phys. (Paris)*, **30**, 581 (1975).
(5) J. GREENSITE and B. LAUTRUP: *Phys. Lett. B*, **104**, 41 (1981).

The mean-field approximation for both partition functions (1) and (5) are obtained by inserting the factor ([5,6])

$$\prod_{x,i} \int \mathrm{d}u_i \int_{-i\infty}^{i\infty} \mathrm{d}\alpha_i \exp\left[\sum_{x,i} (U_i - u_i)\alpha_i\right] = \prod_{x,i} \int \mathrm{d}u_i\, \delta(U_i - u_i) = 1\,, \tag{7}$$

after which one can replace U_i by u_i in Z and integrate out the single remaining U_i variable in front of α_i. For smooth fields $u_i \sim u$ and $\alpha_i \sim \alpha$ this gives

$$Z \sim \exp\left[\sum_x (\beta E - 3\alpha u + 3 \log I_0(\alpha))\right], \tag{8}$$

where in the gauge theory

$$E = E^{\mathrm{g}} \equiv 3(u^4 - 1) \tag{9}$$

and in the melting theory

$$E = E^{\mathrm{melt}} \equiv 3(u^4 - 1) + 6(u^2 - 1) + \frac{\lambda}{\mu}(u^6 - 1)\,. \tag{10}$$

The exponent is extremal at

$$u = I_1(\alpha)/I_0(\alpha) \tag{11}$$

and

$$\begin{cases} \alpha = 4\beta u^3\,, & \text{for the gauge theory} \\ \alpha = 4\beta(u^3 + u^2 + (\lambda/2\mu)u^5)\,, & \text{for the melting theory.} \end{cases} \tag{12}$$

There is a first-order transition at $\beta^{\mathrm{g}} \sim 1.92$, $\beta^{\mathrm{melt}} \sim 0.47$, 0.43 and 0.42 for $\lambda/2\mu = v/(1-2v) \sim 0.6$, 0.75, and 1.05 in Be, Fe and Al, respectively. This amounts to a Lindemann parameter ([7]), $L \sim 22.8 \cdot 2\pi\sqrt{\beta^{\mathrm{melt}}} \sim 98$, 94, 93. Experimentally, L varies between 100 and 200 in most materials ([8]) and is 150, 121 and 138 in Be, Fe and Al. The discrepancy should be explained by fluctuation corrections which certainly tend to increase β^{melt}, as we know from gauge models ([9]).

At β^{melt}, $W = (\partial/\partial\beta)\log Z$ jumps from zero to 4, 5.2 and 5.7 after which it approaches smoothly $(9 + \lambda/\mu)$. The jump in entropy is $\Delta S \simeq -\beta\Delta W \sim -1.9$, -2.2 and -2.4. Fluctuation corrections, however, will lower this number considerably. In fact, the high-T expansion gives, to lowest oder in β (*), $\log Z \sim (15/4 + (\lambda/2\mu)^2)\beta^2$, such that ΔS is brought down to ~ 1.1, -1.5 and -1.34 close to the experimental values 1.1, 1.3 and 1.4 in Be, Fe and Al, respectively.

When comparing the model with real crystals it should be kept in mind that the stress energy is actually anisotropic and reads

$$f = \tfrac{1}{2} C_{ijkl} u_{ij} u_{kl}\,,$$

([6]) E. BREZIN and J.-M. DROUFFE: *Nucl. Phys. B*, **200**, 93 (1982).
([7]) H. KLEINERT: *Lett. Nuovo Cimento*, **34**, 471 (1982).
([8]) A. R. UBBELOHDE: *The Molten State of Matter* (New York, N.Y.), p. 63.
([9]) H. FLYVBJERG, B. LAUTRUP and J. B. ZUBER: *Phys. Lett. B*, **110**, 279 (1982).
(*) We omit the trivial contribution $-9\beta - (\lambda/\mu)\beta$ in the esponent (4).

where $u_{ij} = (\nabla_i u_j + \nabla_j u_i)/2a$ is the strain tensor. For cubic systems this simplifies to

$$\tfrac{1}{2} C_{1111}(u_{11}^2 + u_{33}^2 + u_{33}^2) + C_{1122}(u_{11}u_{22} + u_{22}u_{33} + u_{33}u_{11}) + 2C_{1212}(u_{12}^2 + u_{23}^2 + u_{31}^2) .$$

Defining

$$\mu \equiv C_{1212} , \qquad \lambda \equiv C_{1122} , \qquad r \equiv \frac{(C_{1111} - C_{1122})}{2C_{1212}}$$

and introducing defects via the substitutions $(4\pi u_{ij})^2 \to 2(1 - \cos 4\pi u_{ij})$ for $i \neq j$, $(2\pi u_{ii})^2 \to 2(1 - \cos 2\pi u_{ii})$, $\big(2\pi \sum u_{ii}\big)^2 \to 2\big(1 - \cos 2\pi \sum_i u_{ii}\big)$, $u_i \to (a/2\pi)A_i$, the energy in (4) changes merely by a factor r in front of the second term. Experimentally, $r \sim 0.2 \div 0.7$ in many materials. From eq. (10) we see that r multiplies the u^2 term such that $r < 1$ increases the transition entropy.

Let us mention that the model can easily be modified to incorporate additional point defects like interstitial atoms. All we have to do is allow the variables n_{ij} to take, with some probability, half-integer values. In the energy (4) this amounts to admitting cosine terms with twice the argument. Since these appear with twice the power of u in (10), this hardens the transition. Monte Carlo calculations are necessary for a detailed study of this interesting class of models.

From the present discussion it appears that the existing mean-field methods are really the ideal tool for studying melting rather than gauge theories, for which they were originally developed ([5]). The three-dimensional U_1 gauge theory has no phase transition at all ([10]) such that the first-order transition at the mean-field level is qualitatively wrong and smoothed out completely by fluctuations ([9]). The value β^g merely indicates the temperature region where the magnetic monopoles, the defects of that theory, decrease strongly in number, albeit in a continuous fashion. To make things worse, the approximation violates the important fundamental gauge symmetry of the system.

Both diseases are absent in the present application. There is no gauge symmetry to be destroyed and the transition to be explained is of first order, in qualitative agreement with the mean-field result.

Notice that both gauge and melting theory can be considered as two orthogonal generalizations of the XY model from one to three angular variables. The XY model has a second-order transition at the mean-field level as well as after fluctuation corrections and describes the λ-transition of superfluid ^{4}He. The Abelian lattice gauge theory is the antisymmetric generalization and has no transition at all. The present model of defect melting is the symmetric generalization and the transition is of first order at the mean-field level. If this mean-field result survives more detailed fluctuation studies it would explain an old puzzle as to how defect melting differs from the λ-transition when described as an ensemble of vortex lines (the defects in the XY model) ([11]). It was recently shown that the λ-transition can be made first order by artificially lowering the core energy of the vortex lines below the purely elastic self-energy ([12]). This was achieved by coupling an extra short-range vector field to the XY model. It will be interesting to see, whether the simple partition function (4) has the correct first-order transition as it stands or whether some modification will be necessary in order to fit experimental data.

([10]) A. M. POLYAKOV: *Nucl. Phys. B*, **120**, 429 (1977).
([11]) H. KLEINERT: *Phys. Lett. A*, **93**, 86 (1982).
([12]) H. KLEINERT: *Lett. Nuovo Cimento*, **35**, 405 (1982).

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The author thanks S. AMI, T. HOFSÄSS and R. HORSLEY for discussions.

Note added in proofs.

The simple partition function does have a first-order transition with $\Delta S = 1.4$ as shown meanwhile by L. JACOBS and H. KLEINERT: Santa Barbara preprint (to be published). See also the very accurate low-β expansion (up to β^{12}) as well as the one-loop correction to the mean field theory by S. AMI, T. HFSÄSS and R. HORSLEY, Berlin preprint, July 1973. The crucial role of disclinations in producing a first-order transition is discussed in H. KLEINERT: *Phys. Lett. A*, **95**, 381, 493 (1983).