DEFECT MELTING AS AN SO(3) LATTICE GAUGE THEORY

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We show that defect melting is closely related to SO(3) lattice gauge theory. The phase transition of this system corresponds to a Lindemann melting parameter $L \sim 50\gamma$ where $\gamma \sim 2$ is a parameter characterizing the unharmonic content in the elastic forces. This is in rough agreement with experiment. The equivalence may help in visualizing the crucial role of defects in quark confinement.

On the basis of a recently developed field theory of line-like defects interacting via linear elasticity [1] it has become possible to give a simple description of the melting transition. The theory has the same form as the Ginzburg–Landau theory of superconductivity, i.e. it consists of a scalar field coupled to a gauge field (scalar QED). Melting proceeds via the usual Meissner–Higgs effect, only that the scalar field represents disorder rather than order such that φ becomes unstable above some critical temperature, $T > T_c$, rather than below.

The explicit representation of fluctuating defect lines in terms of a disorder field is a powerful tool in isolating the essential non-linear characteristics of the system and treating them separately. The residual interaction between defects can then be linearized without changing the phenomena. Certainly, in the actual crystal, the defect lines are caused by the non-linearities of the forces and appear in the thermal partition function due to their high configurational entropy while being almost extremal in the energy.

In fact, this understanding has led to the suggestion [2] that other non-linear theories such as QCD could be understood in more simple terms by finding their relevant line-like defects, and parametrizing their fluctuations in terms of a Higgs-like disorder field. Moreover, the Higgs fields employed presently in the description of the spontaneous symmetry breakdown between weak and electromagnetic interactions could be disorder fields of just this type and therefore of a pure gauge field nature.

In order to further support this suggestion we would like to show that the melting problem is related to the standard SO(3) lattice gauge theory, thus showing our first Higgs-like theory of defects with linear elastic interactions [1] to carry information on this non-abelian gauge theory. As a useful physical side result we use the transition temperature of this theory to calculate a melting temperature with Lindemann parameter $L \sim 100$ in agreement with the experimental values for many materials.

A crystal lattice consists of mass points in a periodic, say simple cubic, array of potential wells of spacing l. There is an elastic next-neighbor coupling such that small and smooth distortions $u_i(x)$ lead to an elastic energy

$$f = \tfrac{1}{2}\mu(\partial_i u_j)^2 + \tfrac{1}{2}(\lambda + \mu)(\partial_i u_i)^2$$

or, in terms of stresses

$$\sigma_{ij} \equiv \mu(\partial_i u_j + \partial_j u_i) + \lambda\delta_{ij}\partial_k u_k \,,$$

$$f_{\rm el} = (1/4\mu)\{\sigma_{ij}^2 - [\nu/(1+\nu)]\,\sigma_{ii}^2\} \,, \qquad (1)$$

where $\nu \equiv \lambda/2(\mu + \lambda)$ is the Poisson ratio of the elastic constants μ, λ. In order that the material properly fits to its neighborhood, in spite of the distortion, the incompatibility [3]

$$\eta_{ij}(x) = \epsilon_{ikl}\epsilon_{jmn}\partial_k\partial_m\partial_l u_n(x) \qquad (2)$$

has to vanish. Due to the non-linearity of elastic forces not described in (1), however, defects will form. They

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can be incorporated phenomenologically at the linear level by allowing for discontinuities in u_i which show up in a non-vanishing $\eta_{ij}(x)$. Most important are defect lines for which [4]

$$\eta_{ij}(x) = [\epsilon_{jmn}\partial_m \alpha_{ni} + \theta_{ij} + (i \leftrightarrow j)]/2 ,$$

with

$$\alpha_{ni} = b_n \delta_i(L) \equiv b_n \int \mathrm{d}\tau\, \dot{\bar{x}}_i\, \delta^{(3)}(x - \bar{x}(\tau)) ,$$

$$\theta_{ij} = \Omega_i \delta_j(L) ,$$

where b, Ω are the Burgers and Frank vectors, respectively. In our field theory of defects, their grand-canonical ensemble was studied by using the fact that $\partial_i \sigma_{ij} = \partial_j \sigma_{ij} = 0$ such that we could introduce a stress potential h_{ln} via the double curl $\sigma_{ij} = \mu l^2 \epsilon_{ikl}\epsilon_{jmn}\partial_k \partial_m h_{ln}$ which is invariant under local gauge transformations $h_{ln} \to h_{ln} + \partial_l \xi_n(x) + \partial_n \xi_l(x)$. The field h_{ln} is coupled minimally to a scalar field describing fluctuating defect lines. The correct conserved current turns out to be the Belinfante momentum tensor ${}^{\mathrm{B}}\theta_{ij}$ of the defect field just as though h_{ln} were linearized gravitational fields [2].

As a matter of fact, (1) may be seen as the linear approximation to a certain non-linear theory in which $\gamma\sigma_{ij}/\mu l^2$ is replaced by the Einstein tensor G_{ij} of a riemannian space such that one arrives at a coordinate-independent elastic energy

$$F_{\mathrm{el}} = \int \mathrm{d}^3x\, \sqrt{g}(\mu l^4/4\gamma)\{G_i{}^j G_j^i - [\nu/(1+\nu)]\, G_i^{i\,2}\} , \tag{3}$$

with the metric $g^{ij} = \delta^{ij} + \gamma h^{ij}$ describing the stresses. The parameter γ characterizes the non-linearities in the elastic forces. The defects can be shown to move in this space just as spinning particles in a gravitational field [2].

In three dimensions, the Einstein tensor is related to the curvature by $G_{ij} = \frac{1}{4}\epsilon_{ikl}\epsilon_{jmn}R^{klmn}$ such that $G_i^{j\,2} = \frac{1}{4}R^2_{klmn}{}^2$ and $G_i^{i\,2} = \frac{1}{4}(R_{kl}{}^{kl})^2$. In the following we shall neglect ν since it is usually small ($\lesssim 0.4$). The phase transition of melting should not suffer much from this. Thus we are led to studying

$$F_{\mathrm{el}} = \int \mathrm{d}^3x\, \sqrt{g}(1/16\mu)\, R_{klmn}R^{klmn} . \tag{4}$$

For this theory, however, there exists a simple lattice version. In order to see this let us introduce dreibein vectors $e^a{}_i(x)$, and their reciprocals $e^{ai}(x)$, such that the metric is $g_{ij}(x) = e^a{}_i e^a{}_j(x)$. This decomposition leaves room for arbitrary local rotations $e^a{}_i(x) \to O(x)^a{}_b\, e^b{}_i(x)$. Under these, the connection

$$\Gamma_i^{ab}(x) \equiv e^{aj}\partial_i e^b{}_j \equiv e^{aj} e^b{}_k\, \Gamma_{ij}{}^k \tag{5}$$

transforms like an SO(3) gauge field

$$\Gamma_i^{ab}(x) \to O\Gamma_i O^{-1} + O\partial_i O^{-1} . \tag{6}$$

The curvature tensor is defined as

$$R_{ijk}{}^l = e^{al}(\partial_i\partial_j - \partial_j\partial_i)\, e^a{}_k , \tag{7}$$

and becomes

$$R_{ijk}{}^l = e^{al} F_{ij}{}^{ab}\, e^b{}_k , \tag{8}$$

where

$$F_{ij}{}^{ab} \equiv \partial_i \Gamma_j^{ab} - \partial_j \Gamma_i{}^{ab} + [\Gamma_i, \Gamma_j]^{ab}$$

is the covariant curl of the gauge field. Thus we find

$$R_{ijkl}R^{ijkl} = F_{ij}{}^{ab}F^{ijab} . \tag{9}$$

But with this expression, (3) may just as well be considered as the weak and smooth field limit of an SO(3) lattice theory [5]

$$F_{\mathrm{el}}^{\mathrm{latt}} = -\tfrac{1}{6}\beta \sum_{x,i,j} \mathrm{tr}(O^{\square}{}_{ij} - 1) , \tag{10}$$

where x denotes the sites and a, b the ordered links. The rotation $O^{\square}{}_{ij}$ is defined for each square plaquette as the product of four arbitrary rotations $O_j(x) = \exp[\mathrm{i}l\Gamma_j(x)]$

$$O^{\square}{}_{ij} = O_i(x)\, O_j(x+i)\, O_i^{\mathrm{T}}(x+j)\, O_j^{\mathrm{T}}(x) . \tag{11}$$

Expanding the exponential we find

$$F_{\mathrm{el}}^{\mathrm{latt}} \to \frac{\beta T l^4}{12} \int \mathrm{d}^3x \sum_{i,j} (F_{ij}{}^{ab})^2 ,$$

such that we can identify

$$(\mu l^3/T)^{1/2} = \gamma \cdot 2(\beta/3)^{1/2} . \tag{12}$$

The partition function of (10) has a marked change of phase at $\beta_{\mathrm{c}} \sim 3.92$ [5] [‡1]. This leads to the melting temperature T_{melt} satisfying $(\mu l^3/T_{\mathrm{melt}})^{1/2} \sim 2.3\gamma$. Experimentally, the most accessible number is the

‡1 The author is grateful to R. Horsley and E. Kröner for useful discussions on lattice gauge theories and defects, respectively, as well as to B. Lautrup for running the SO(3) theory through his improved mean-field calculation and determining $\beta_{\mathrm{c}} \sim 3.92$.

Lindemann parameter $L \equiv 22.8(\mu l^3/T_{\text{melt}})^{1/2}$ which ranges around $L \sim 120$ [6]. The parameter of non-linearity γ may be estimated by Grüneisen's constant γ which is defined in a different way but characterizes the same physical property of crystal forces. For most materials $\gamma \sim 2$ as a reflection of the rather hard repulsion cores between atoms. With this value, the Lindemann number agrees reasonably well with experiment.

Let us interpret the result physically. Thermal excitations can move a lattice constituent from one well to an interstitial place. If this happens for an entire section of a lattice plane in $\hat{x}, \hat{y}$, or the $\hat{z}$ direction, then the circumference appears as a dislocation line of Burgers vector $l\hat{x}$, $l\hat{y}$, or $l\hat{z}$. Disclination lines can be built as superpositions of dislocation lines [4,7]. In the SO(3) gauge theory, this is simulated in a rather indirect way. Stress is built up if entire SO(3) rotations, around each of the three spatial axes, becomes thermally excited. This stress can be associated with a crystal defect density η_{ij} via the relation

$$\epsilon_{ikl}\epsilon_{jmn}\partial_k\partial_m\sigma_{ln} - [\nu/(1+\nu)](\delta_{ij}\partial^2 - \partial_i\partial_j)\,\sigma_{\text{el}} = 2\mu\eta_{ij}\,.$$

At a certain temperature, the stress energy is relaxed by a transition to disorder which is equivalent to an avalanche-like proliferation of crystal defects.

As was discussed previously [1], the order of the transition depends sensitively on the size of the steric repulsion between defect lines. When extrapolating the linear elasticity theory into the non-linear regime, which certainly is a non-unique procedure, this corresponds to a certain choice of steric repulsion which may not be the same as that chosen by the crystal. In fact, this does seem to be the case here since in the SO(3) lattice theory the phase changes continuously, while melting always happens in first order. It is weak steric repulsion [1] which makes a transition first order and it was shown [1] that this draws the transition to lower temperature corresponding to an increase in Lindemann's parameter L, just as required by the data.

A final remark is necessary as to the neglect of the ν term in (3). In the SO(3) gauge theory this amounts to coupling spin and orbital indices, a situation which has not been treated there since SO(3) was always considered to be an internal "color" group not capable of hybridizing with the SO(3) of space. Here, this occurs in the form $\Sigma_{x,i,j,ab}\delta_{ia}\delta_{jb}(O_{\square ij} - 1)^{ab}$ and for estimating the effect of ν upon melting, it would be interesting to see this term included in SO(3) lattice calculations.

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