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GAUGE THEORY OF DEFECT MELTING-STATUS 1984

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We show that the grand-canonical ensemble of line-like defects in crystals can be described by a gauge theory of the Ginzburg-Landau type which normally governs the magnetic phenomena in superconductors. We use this theory to study the melting transition. It leads to a close structural correspondence between superconductive and crystalline properties: The vector potential of magnetism and the order parameter correspond to the potential of stress and the disorder parameter, respectively. The Meissner effect which prevents magnetism from invading the ordered state of a superconductor corresponds to the screening of stress in the disordered molten state.

There is, however, an important difference which causes melting to be a first order transition: It is the presence of two types of disorder fields, one for dislocations and one for disclinations with different long-range interactions. The melting process is the result of a combined proliferation of both types of defects. We exhibit the important backfeeding mechanism which is responsible for the first order of the transition.

The theoretical ideas are exemplified by a simple statistical model, similar to the *XY* model of magnetism, which is dually equivalent to an ensemble of crystalline defects including their long-range stress interactions. Since it is a local model with next-neighbour coupling it can be simulated on a computer and shows a proper first order melting transition.

1. Introduction

I would like to report on progress made during the last couple of years* in describing the solid–liquid phase transition as a proliferation of line-like crystalline defects. The usefulness of such an approach was emphasized by Shockley [1] as early as 1952, but it was not until recently [2, 3, 4] that this idea was translated into a proper theory. With such a theory being available we can now calculate thermodynamic properties and correlation functions of a defect system.

For some time, theoretical efforts were limited to two dimensions where a prototype study of the vortex driven phase transition of superfluid ^{4}He has been successful [5]. It helped pointing out the importance of defects in driving a number of other phase transitions.

In trying to understand crystal melting, however, a simple copy of the vortex description with the replacement vortices $\rightarrow$ dislocations is not sufficient and leads to unphysical results [6]. It overlooks the larger variety of topological defects in a crystal [7]. While a superfluid has only the periodicity $u(x) \rightarrow u(\boldsymbol{x}) + 2\pi$ of a phase variable, a crystal has translational periodicity

$$u_i(\boldsymbol{x}) \rightarrow u_i(\boldsymbol{x}) + b_i \tag{1}$$

by lattice vectors b_i, as well as rotational invariance

$$u_i(\boldsymbol{x}) \rightarrow u_i(\boldsymbol{x}) + \Omega_k \varepsilon_{kij} x_j . \tag{2}$$

In the topological classification of defects, these two symmetry groups are associated with dislocations and disclinations, respectively, with b_i being the Burgers vector and Ω_k the Frank vector [8].

In statistical considerations, disclinations have always been thought to play only a minor role [8], because of their large formation energy. Due to the coupling of stress to dislocations, however, disclinations represent a considerable reservoir of entropy which, in fact, is responsible for driving the melting transition to first order.

In addition, the joint proliferation of both types of defects is necessary to destroy both translational and rotational order and produce a proper isotropic liquid.

I have focused attention from the beginning on

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three-dimensional systems [2–4]. I did this not only since they are closer to physical reality. There are several reasons:

1) In three dimensions, ensembles of defects under stress posses two types of beautiful gauge structures [9] which are fun investigating. In two dimensions, one half of these is lost (the stress half) and the beauty is greatly reduced.

2) The defects form oriented closed lines. Ensembles of such lines can be described efficiently by a complex scalar field theory [10]. It is well known that field theories can be evaluated perturbatively by expanding the partition function in terms of Feynman graphs. Usually, these graphs are considered to be an auxiliary device for counting the different algebraical contributions. A close look, however, teaches us that the diagrams, which have the form of closed loops, are the direct pictures of the closed particle orbits. By replacing 'particle orbits' by defect lines we realize immediately the usefulness of field theory for summing defect lines.

3) The stress forces between defect lines can be obtained from a minimal coupling to the stress gauge field [2]. Such minimal couplings are familiar from other branches of field theory. The most prominent and best understood example is the Ginzburg–Landau theory of superconductivity which the field theorists call scalar QED or Abelian–Higgs model. Let us briefly recall the features which are relevant for our discussion.

2. Reminder of Ginzburg–Landau theory

The partition function is

$$Z=\int \mathscr{D}\mathbf{A}\Phi[\mathbf{A}]\int \mathscr{D}\varphi\mathscr{D}\varphi^{+}\times\exp\left\{-\frac{1}{2e^2}\int \mathrm{d}^3x(\partial\times\mathbf{A})^2-\int \mathrm{d}^3x\tfrac{1}{2}|(\partial_l-\mathrm{i}A_l)\varphi|^2+\frac{m^2}{2}|\varphi|^2+\frac{g}{4}|\varphi|^4+\cdots\right\}, \tag{1}$$

where $\varphi(\boldsymbol{x})$ is called the order field and describes the Cooper pairs of the system with a charge e. The m^2 term becomes negative when lowering the temperature below a critical value T_c. The gauge field A_l describes magnetism, $\boldsymbol{B}=\partial\times\mathbf{A}$ being the closed magnetic field lines. The functional $\Phi[\mathbf{A}]$ fixes the gauge (for example $\Phi=\delta[\boldsymbol{\partial}\mathbf{A}]$).

For $T<T_c$, the lowest energy lies at $|\varphi|=\sqrt{-m^2/g}$. This implies that the magnetic field acquires a mass term $\mu=e\,|\varphi|$ which amounts to a finite inverse penetration depth $\lambda=\mu^{-1}$. This is the Meissner effect. The ordered state does not support a magnetic field. The ratio $K=\lambda/\xi\equiv\lambda/\sqrt{-m^2}=\sqrt{g/e^2}\gtrless 1/\sqrt{2}$ differentiates type II or type I superconductors, depending on whether they like or dislike to be penetrated by magnetic flux lines. In the type II regime, the Ginzburg–Landau theory has a second order phase transition [11].

The coupling to the gauge field appears only in the co-variant derivatives (= minimal coupling)

$$D_l=\partial_l-iA_l \tag{2}$$

This ensures the covariance of (1) under local gauge transformations

$$\begin{aligned}&A_l(\boldsymbol{x})\rightarrow A_l(\boldsymbol{x})+\partial_l\Lambda(\boldsymbol{x}),\\&\varphi(\boldsymbol{x})\rightarrow \mathrm{e}^{\mathrm{i}e\Lambda(\boldsymbol{x})}\varphi(\boldsymbol{x}).\end{aligned} \tag{3}$$

The minimal coupling is the field theoretic version of the local coupling to particle orbits

$$\mathrm{e}^{\mathrm{i}e\int_L \mathrm{d}x_lA_l(x)}. \tag{4}$$

The duality between many particle systems and fluctuating fields teaches us that the field theory (1) is equivalent to the partition function

$$Z=\int \mathscr{D}\mathbf{A}\Phi[\mathbf{A}]\exp\left\{-\frac{1}{2e^2}\int \mathrm{d}^3x(\boldsymbol{\partial}\times\mathbf{A})^2\right\}\times\sum_{\{L\}}\exp\left\{\mathrm{i}e\oint_L \mathrm{d}x_lA_l(x)\right\}, \tag{5}$$

where $\sum_{\{L\}}$ denotes the sum over all closed particle orbits of the system [12]. The integration over the $\mathbf{A}$ field produces a partition function

$$Z=\sum_{\{L\}}\exp\left\{-e^2\oint_L \mathrm{d}\boldsymbol{x}\oint_{L'}\mathrm{d}\boldsymbol{x}1/4\pi R\right\}, \tag{6}$$

with a $1/R$ type Biot–Savart interaction energy.

It was observed by Feynman [13] in 1955 that the partition function of vortices in superfluid ^{4}He has exactly the same form and he suggested that a study of Z should show the superfluid phase transition. It would take place at a temperature where the entropy s per line element becomes larger than the energy ε per line element divided by temperature, i.e. when $T>\varepsilon/s$. Instigated by his idea we have taken the partition function (6) and developed it backwards using simple functional techniques, until we arrived at a field theory with a Ginzburg–Landau form (1) [11]. In it, the field φ describes the vortex lines, the magnetic field, the current density of superflow.

In the Ginzburg–Landau form, the superfluid transition was obvious. The mass [2] turns out to be proportional to $\varepsilon/T-s$ where $\varepsilon \propto e^2$ and $s \approx \log 6$ (6 = coordination number). This agrees with Feynman's qualitative considerations. The mass term becomes negative for T larger than a critical temperature ε/s and $|\varphi|$ takes a non-zero expectation value in the hot, disordered, phase. This is the signal of the proliferation of vortex lines. The field φ is called a *disorder field* [2, 3]. For $|\varphi| \neq 0$, there is a disorder version of the Meissner effect. Just as magnetic fields avoids the ordered state, super-flow avoids the disordered state.

3. Gauge theory of defect lines

For dislocation lines in a crystal the partition function corresponding to (6) is

$$Z=\sum_{\{L,\boldsymbol{b}\}} \exp -\frac{\mu}{2} \oint_L \oint_{L'} \Big\{ [\boldsymbol{b}\cdot \mathrm{d}\boldsymbol{x}\; \boldsymbol{b}'\cdot \mathrm{d}\boldsymbol{x}' - 2(\boldsymbol{b}\times\boldsymbol{b}')\cdot(\mathrm{d}\boldsymbol{x}\times \mathrm{d}\boldsymbol{x}')]/4\pi R - \frac{2}{1-\nu}(\boldsymbol{b}\times \mathrm{d}\boldsymbol{x})_i \times (\boldsymbol{b}'\times \mathrm{d}\boldsymbol{x}')_j \partial_i\partial_j R/8\pi \Big\}, \tag{7}$$

where $\boldsymbol{b}$ and $\boldsymbol{b}'$ are the Burgers vectors of the dislocation lines L, L'. The energy in the exponent was first derived by Blin. Also for this Z we found an equivalent field theory of the type (1).

First of all, there is no problem in going backwards from (7) to the form (5). The answer is simply [2]

$$Z=\int \mathscr{D}A_{il}\Phi[A_{ie}] \times \exp\left\{-\frac{1}{4\mu\beta}\int \mathrm{d}^3x\left(\sigma_{ij}^2-\frac{\nu}{1+\nu}\sigma_{ll}^2\right)\right\} \times \sum_{\{L,\boldsymbol{b}\}} \exp\left\{ib_i\oint_L \mathrm{d}x_l A_{il}(\boldsymbol{x})\right\}, \tag{8}$$

where A_{il} is the gauge field of the stress tensor σ_{ij} defined by

$$\sigma_{ij}=\varepsilon_{jkl}\partial_k A_{il} \tag{9}$$

and $\Phi[A_{il}]$ is a gauge fixing factor, for example $\Phi=\delta[\partial_l A_{il}]$. In order that σ_{ij} be symmetric, A_{il} has to satisfy the constraint

$$\partial_i A_{il}=\partial_l A_{il}. \tag{10}$$

The constants μ and $\nu=\lambda/2(\mu+\lambda)$ are the shear modulus and the Poisson number, respectively. It can easily be shown that, integrating out the field A_{il} in (8), gives (7). Having eq. (8) it is simple to transform the sum over the lines L into a disorder field theory and obtain the Ginzburg–Landau-like expression [2]

$$Z=\int \mathscr{D}A_{il}\Phi[A_{il}]\int \mathscr{D}\varphi_b\mathscr{D}\varphi_b^+ \times \exp\left\{-\frac{1}{4\mu\beta}\int \mathrm{d}^3x\left(\sigma_{ij}^2-\frac{\nu}{1+\nu}\sigma_{ll}^2\right) - \int \mathrm{d}^3x\left\{\sum_b\left[\tfrac{1}{2}|(\partial_l - \mathrm{i}b_i A_{il})\varphi_b|^2 + \frac{m_b^2}{2}|\varphi_b|^2\right] + \sum_{b,b'}\frac{g_{bb'}}{4}|\varphi_b|^2|\varphi_{b'}|^2+\cdots\right\}\right\}. \tag{11}$$

As in superfluids, m^2 behaves like $\varepsilon_b/T-s_b$ where $\varepsilon_b \propto \mu$ and $s_b \sim \log 6$. For $T>T_b=\varepsilon_b/s_b$ there is a disorder phase transition and the gauge field of stress is screened by a disorder version of the Meissner effect which reflects the fact that stress does not invade into the molten state.

When comparing this transition with melting there are, however, two serious discrepancies:

1) The transition in (11) is of second order.

2) The crystal, in which only the defects of translational order have proliferated, is not a liquid.

Now, from naive symmetry arguments, it is clear what is necessary to produce a liquid: Also, the rotational order has to be destroyed and this requires disclinations. When the field theory (11) is extended such as to include these it turned out that this also repairs the discrepancy [1].

The interaction energy between disclination lines and between dislocation and disclination lines is of the type $-R/8\pi$ and $1/4\pi R$, respectively. There exists a representation of the form (7) which includes both types of lines. In order to proceed with our program, Z has to be brought to the form (8). For this purpose, A_{il} turns out to be no longer adequate. Instead, one has to write σ_{ij} as a double curl

$$\sigma_{ij} = \varepsilon_{imn}\varepsilon_{jkl}\partial_m\partial_k\chi_{nl} \tag{12}$$

(i.e. the old A_{il} is once more curl $\varepsilon_{imn}\partial_m\chi_{nl}$). Then the coupling to dislocation lines L and disclination lines L' with Burgers vector $\boldsymbol{b}$ and Frank vector $\boldsymbol{\Omega}$ is simply

$$\sum_{\{L,\boldsymbol{b}\}\{L',\boldsymbol{\Omega}\}} \exp\left\{\mathrm{i}\left(b_i\oint_L \mathrm{d}x_l\varepsilon_{imn}\partial_m\chi_{nl} + \Omega_i\int_{L'}\mathrm{d}x_l\chi_{il}\right)\right\}. \tag{13}$$

Using this coupling, and expressing σ_{ij} in terms of χ_{nl} via (12), the partition function has the same form as in (8). It is therefore straightforward to introduce disorder fields φ_Ω also for the disclinations. The field energy has the same form (11) as for disclination field φ_b except that the minimal coupling contains the χ_{ln} field, rather than A_{il}, such that the total partition function reads

$$\begin{aligned} Z = &\int \mathcal{D}\chi_{nl}\Phi[\chi_{nl}]\int \mathcal{D}\varphi_b\mathcal{D}\varphi_b^+\int\mathcal{D}\varphi_\Omega\mathcal{D}\varphi_\Omega^+ \\ &\times\exp\left[-\frac{1}{\varphi\mu\beta}\int \mathrm{d}^3x\left(\sigma_{ij}^2+\frac{\nu}{1+\nu}\sigma_{ll}^2\right)\right] \\ &\times\exp\left[-\int\mathrm{d}^3x\left\{\sum_{\boldsymbol{b}}\left[\tfrac{1}{2}|(\partial_l - \mathrm{i}b_i\varepsilon_{imn}\partial_m\chi_{nl})\varphi_b|^2\right.\right.\right. \\ &\left.+\frac{m_b^2}{2}|\varphi_b|^2\right] + \sum_{bb'}\frac{g_{bb'}}{4}|\varphi_b|^2|\varphi_{b'}|^2+\cdots \\ &-\int\mathrm{d}^3x\left\{\sum_{\boldsymbol{\Omega}}\left[\tfrac{1}{2}|(\partial_l-\mathrm{i}\Omega_i\chi_{il})\varphi_\Omega|^2+\frac{m_\Omega^2}{2}|\varphi_\Omega|^2\right]\right. \\ &\left.\left.+\sum_{\Omega,\Omega'}\frac{g_{\Omega\Omega'}}{4}|\varphi_\Omega|^2|\varphi_{\Omega'}|^2+\cdots\right\}\right], \end{aligned} \tag{14}$$

where $m_\Omega^2 \propto \varepsilon_\Omega/T - s_\Omega$ and $\varepsilon_\Omega \propto \mu$. This is the disorder field theory of all line-like defects in crystals which has led to an understanding of the melting transition from the defect point of view [12].

4. The melting transition

Consider, for a moment, the temperature regime above T_b where mass of the dislocation field is negative such that φ_b has a non-zero expectation. Due to the minimal coupling $|(\partial_l - ib_i\varepsilon_{imn}\partial_m\chi_{nl})\varphi_b|^2$ the χ field acquires a mass term of the form $\frac{1}{2}b^2|\varphi_b|^2\boldsymbol{k}^2|\chi|^2$. This changes the energy of the stress gauge field from $(1/\mu\beta)\boldsymbol{k}^4|\chi|^2$ to $(\boldsymbol{k}^4/\mu\beta + \frac{1}{2}b^2|\varphi_b|^2\boldsymbol{k}^2)|\chi|^2$ as a dislocation version of the Meissner effect. At long distances, we can neglect the first purely elastic term and keep only the second. With this screened stress energy the disclinations have an effective partition function of the type

$$\begin{aligned} Z_\Omega^{\mathrm{eff}} = &\int\mathcal{D}\chi\Phi[\chi]\int\mathcal{D}\varphi_\Omega\mathcal{D}\varphi_\Omega^+ \\ &\times\exp\left[-\frac{b^2|\varphi_b|^2}{2}\int\mathrm{d}^3x\,|\boldsymbol{\partial}\chi|^2\right. \\ &-\int\mathrm{d}^3x\left\{\sum_\Omega\left[\tfrac{1}{2}|(\partial_l-\mathrm{i}\Omega_i\chi_{il})\varphi_\Omega|^2\right.\right. \\ &\left.\left.+\frac{m\Omega^2}{2}|\varphi_\Omega|^2\right]+\sum_{\Omega,\Omega'}\frac{g_{\Omega\Omega'}}{4}|\varphi_\Omega|^2|\varphi_{\Omega'}|^2\right\} \end{aligned} \tag{15}$$

When taking this to the orbit form (6), it reads

$$Z_\Omega^{\mathrm{eff}} = \sum_{\{L,\Omega\}}\exp\left\{-\tfrac{1}{2}\frac{\Omega^2}{b^2|\varphi_b|^2}\oint_L\mathrm{d}\boldsymbol{x}\oint_{L'}\mathrm{d}\boldsymbol{x}'\frac{1}{4\pi R}\right\}. \tag{16}$$

This looks just like (5), i.e. the disclinations in a bath of dislocations behave like vortex lines in ^{4}He except with the role of temperature being taken by the expectation value $|\varphi_b|^2$. An increase in $|\varphi_b|^2$ is felt by the disclinations like an increase in temperature. We have seen before that there exists a T_c, i.e. here a $|\varphi_b|^2_c$, above which the vortex lines proliferate, here the disclinations. This leads to a reduction in energy as a function of $|\varphi_b|^2$.

The important point is now that this reduction becomes active even before T_b is reached. This can be seen most easily by considering some *fixed* $T \leqslant T_b$ and increasing virtually the dislocation field $|\varphi_b|$. The φ_b energy alone is positive definite and monotonously increasing. From a point $|\varphi_b|_c$ on, however, the potential bends downwards due to the proliferation of disclinations. It is obvious that the combined curve can in principle touch the φ_b axis before T reaches T_b and this would mean that there is a first order transition in which both dislocations and disclinations proliferate [4, 7].

5. Defect gauge theory

That this really happens was shown by a Monte Carlo simulation of crystal defects with their proper long-range forces. For such a simulation, neither the disorder field theory (14) nor the line representation (7), plus disclinations, is useful. A better form of the partition function is based on the second type of gauge fields, namely those of defects. For vortex lines the corresponding partition function is given by

$$Z = \int_{-\infty}^{\infty} \mathscr{D}u(\boldsymbol{k}) \int \mathscr{D}n_i(\boldsymbol{x}) \Phi[n_i] \times \exp\left\{-\frac{\beta}{2}\int d^3x(\partial_i u(\boldsymbol{x}) - 2\pi n_i(\boldsymbol{x}))^2\right\}, \tag{17}$$

where $\beta = e^2/4\pi^2$. Here $n_i(x)$ are the gauge fields of vortices and $\Phi[n]$ is a gauge fixing factor. The exponential is invariant under the local gauge transformations

$$n_i(\boldsymbol{x}) \to n_i(\boldsymbol{x}) + \partial_i N(\boldsymbol{x}),$$
$$u(\boldsymbol{x}) \to u(\boldsymbol{x}) + 2\pi N(\boldsymbol{x}). \tag{18}$$

These have a simple physical interpretation: The numbers $n_i(\boldsymbol{x})$ denote jumps by 2π of $u(\boldsymbol{x})$ across surfaces S whose boundaries L are given by

$$\boldsymbol{\alpha}(\boldsymbol{x}) = \boldsymbol{\partial} \times n(\boldsymbol{x}). \tag{19}$$

These are the vortex lines. If $n_i(x) = \delta_i(S)$, then $\alpha_i(x) = \delta_i(L)$. This is the Volterra construction of vortex lines. The position of S is irrelevant, only the boundary L is physical. The defect gauge transformation changes S without changing L.

When integrating out the u field one finds

$$Z = \int \mathscr{D}n_i \Phi[b_i] \exp\left\{-\frac{\beta}{2} 4\pi^2 \int d^3x n_i^2\right\}. \tag{20}$$

In the gauge $\partial_i n_i = 0$, this is equal to $\int d^3x \alpha(\boldsymbol{x})(1/-\boldsymbol{\partial}^2)\alpha(\boldsymbol{x})$ which for lines $\alpha_i = \delta_i(L)$ is equal to (6).

6. Computer simulation

The model (17) can be simulated on the computer in the lattice approximation

$$Z = \prod_{\boldsymbol{x}} \int_{-\infty}^{\infty} \frac{du(\boldsymbol{x})}{2\pi} \sum_{\{n_i(x)\}} \Phi[n_i] \times \exp\left\{-\frac{\beta}{2}\sum_{\boldsymbol{x}} (\nabla_i u(\boldsymbol{x}) - 2\pi n_i(\boldsymbol{x}))^2\right\}$$
$$\sim \prod_{\boldsymbol{x}} \int_{-\pi}^{\pi} \frac{du(x)}{2\pi} \exp\left\{\beta \sum_{x} \cos \nabla_i u(\boldsymbol{x})\right\}. \tag{21}$$

This is known as the classical planar Heisenberg model. It shows beautifully the λ-transition of the superfluid.

For crystal defects, we can construct a similar model

$$Z = \int_{-\infty}^{\infty} \mathscr{D}u_i(x) \int \mathscr{D}n_{ij}(x) \Phi[n_{ij}] \exp -\frac{\beta}{4} \int d^3x \times [\mu(\partial_i u_j + \partial_j u_i - 4\pi n_{ij})^2 + 2\lambda(\partial_i u_i - 2\pi n_{ij})^2]. \tag{22}$$

This model is equivalent to (14), i.e., it contains dislocations and disclinations and their proper long-range interactions.

It can be simulated [15, 16] and calculated analytically [17, 18] in the approximate lattice form

$$
\begin{aligned}
Z = & \prod_{\boldsymbol{x},i} \int_{-\infty}^{\infty} \frac{\mathrm{d}u_i(\boldsymbol{x})}{2\pi} \sum_{\{n_{ij}(\boldsymbol{x})\}} \Phi[n_{ij}] \\
& \times \exp -\frac{\beta}{4} \sum_{\boldsymbol{x}} [\mu(\nabla_i u_j + \nabla_j u_i - 4\pi n_{ij})^2 \\
& + 2\lambda(\nabla_i u_i + 2\pi n_{ij})^2] \\
& \approx \prod_{\boldsymbol{x},i} \int_{-\pi}^{\pi} \frac{\mathrm{d}u_i(\boldsymbol{x})}{2\pi} \exp\left[\beta\left\{\sum_{\boldsymbol{x},i>j} \cos(\nabla_i u_j + \nabla_j u_i)\right.\right. \\
& \left.\left. + 2\sum_{\boldsymbol{x},j} \cos(\nabla_i u_i) + \frac{\lambda}{\mu} \sum_{\boldsymbol{x}} \cos\left(\sum_i \nabla_i u_i\right)\right\}\right]. \qquad (23)
\end{aligned}
$$

which the lines are described by complex fields and the stress forces by a stress gauge field. This representation clarifies the nature of the phase transition, in particular the backfeeding mechanism between the two types of defect lines.

The other is the defect gauge field representation, which has the advantage of being easy to simulate on a computer.

The methods presented here are very general and can easily be extended to a variety of other defect mediated phase transitions, in particular in liquid crystals [19].

Let us finally mention that the models of the type (23) (involving the defect gauge field) permit a straight-forward introduction of random quenched disorder by which they become models of glass [20] (just as spin models with random quenched disorder become models of spin glass).

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