Parameters for Systems Exhibiting Local Lattice Distortions, Charge and Spin Ordering

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Abstract

Keeping in mind the experimental results that indicate local lattice distortions, charge and spin orderings, we have developed a phenomenological approach which allows us to describe the electronic phase diagram of cuprates and related systems in terms of few parameters. In the present work we consider a third-order parameter theory which characterize charge, spin and superconductivity orderings. We are thus led to a theory of three scalar fields. By coupling these scalars to gauge fields we are naturally led to string-like solutions, which we interpret as stripes. This ties nicely with our quantum group conjecture that 1d systems play an important role in the physics of cuprates and related materials. We show that this simple approach can give rough values for two-order parameters which can be naively be interpreted as charge and spin orderings. We also report our attempt to understand how local lattice distortions are involved and what role they play in terms of these two order parameters.
I. INTRODUCTION

In a previous work one of us [1] has advanced the conjecture that one should attempt to model the phenomena of antiferromagnetism and superconductivity by using quantum symmetry group. Following this conjecture to model the phenomena of antiferromagnetism and superconductivity by quantum symmetry groups, three toy models were proposed [2], namely, one based on $\text{SO}_q(3)$ the other two constructed with the $\text{SO}_q(4)$ and $\text{SO}_q(5)$ quantum groups. Possible motivations and rationale for these choices were outlined [2]. In [3] a model to describe quantum liquids in transition from 1d to 2d dimensional crossover using quantum groups was outlined. In [4] the classical group $\text{SO}(7)$ was proposed as a toy model to understand the connections between the competing phases and the phenomenon of pseudo-gap in High Temperature Superconducting Materials [HTSC]. Then we proposed in [5] an idea to construct a theory based on patching critical points so as to simulate the behavior of systems such as cuprates. To illustrate our idea we considered an example discussed by Frahm et al., [4]. The model deals with antiferromagnetic spin-1 chain doped with spin-1/2 carriers. In [6] the connection between Quantum Groups and 1-dimensional [1-d] structures such as stripes was outlined. The main point of [7] is to emphasize that 1-d structures play an important role in determining the physical behaviour [such as the phases and types of phases these materials are capable of exhibiting] of cuprates and related materials.

In this note we examine a phenomenological and classical model to understand the phenomenon of “ordering” in HTSC and related materials.

II. SYMMETRY BREAKING

It is well-known that the Higgs-model in particle physics has its origins in condensed matter physics [CMP] and that Higgs-model is a model of spontaneous symmetry breaking [SSB]. A well-known example of SSB in CMP is ferromagnetism near the Curie temperature. When the temperature is greater than Curie temperature all dipoles are randomly oriented and the ground-state is rotationally invariant, whereas when the temperature is below the Curie temperature all the dipoles are aligned along an arbitrary direction giving rise to spontaneous magnetization and rotational symmetry is hidden. In other words we can say that we have SSB when the symmetry of Hamiltonian or Lagrangian is not explicitly shared by the ground-state or the vacuum. Thus the symmetry breaking condition is the non-invariance of the vacuum (ground-state)

$$U|0> \neq |0>,$$

where $U$ is an element of the symmetry group.

Ginzburg-Landau theory [GL] is a phenomenological model for mainly second-order phase transitions. The main-point of GL can be easily understood by resorting to ferromagnetism as an example. The essential point is that for temperatures near the Curie
temperature, the magnetization \( \mathbf{M} \) is assumed to be small and one can Taylor expand the free energy density as

\[
f(\mathbf{M}) = (\partial_i \mathbf{M})^2 + V(\mathbf{M}),
\]

\[
V(\mathbf{M}) = \alpha_1(T)(\mathbf{M} \cdot \mathbf{M}) + \alpha_2(T)(\mathbf{M} \cdot \mathbf{M})^2,
\]

assuming slowly varying field. By construction in (2) the energy densities \( f \) and \( V \) are clearly rotationally invariant (symmetric). Higher powers of \( \mathbf{M} \) are neglected, the term \( \alpha_2(T)(\mathbf{M} \cdot \mathbf{M})^2 \) is kept since at Curie temperature \( \alpha_1 = \alpha(T - T_C) \), \( \alpha > 0 \) vanishes. The kinetic energy term \( (\partial_i \mathbf{M})^2 \) is non-negative as usual, thus to obtain ground-state magnetization we must extremize \( V(\mathbf{M}) \). This yields for \( T < T_C \) the magnitude of magnetization

\[
|M| = \left( -\frac{\alpha_1}{2\alpha_2} \right)^{1/2},
\]

which is the order parameter.

III. ORDER-PARAMETERS

Following the discussion of the previous section we can easily set-up a GL type of model for cuprates. The GL type of phenomenological approach is not uncommon and has been adopted by many authors, for example see [8]. The basic physical components of HTSC materials are

- Charge density.
- Magnetization.
- Superconductivity.

Thus generically we may write the free energy density of such a system in terms of three order parameters, namely, \( \rho \) [charge density], \( \phi \) [complex superconducting order parameter] and \( \sigma \) [order parameter for magnetization]. The free energy density is the sum of the contributions from each of these order parameters [each with functional form as in (2)] plus an interaction term.

*The main differences between reference [8] and our model is that unlike them we don’t assume that the scalar field corresponding to charge is real and that we deal with couplings of scalar fields with gauge fields.
\[ f = f_\phi + f_\rho + f_\sigma + f_{\text{int}}, \]
\[ f_\phi = (\partial_i \phi)^2 + \alpha_1^2 \phi^* \phi - \alpha_2^2 (\phi^* \phi)^2, \]
\[ f_\sigma = (\partial_i \sigma)^2 + \alpha_1^2 \sigma^* \sigma - \alpha_2^2 (\sigma^* \sigma)^2, \]
\[ f_\rho = (\partial_i \rho)^2 + \alpha_1^2 \rho^* \rho - \alpha_2^2 (\rho^* \rho)^2, \]
\[ f_{\text{int}} = f_{\phi\sigma} + f_{\phi\rho} + f_{\rho\sigma}. \] (4)

The simplest choice of the crossed interaction terms if higher powers than fourth are neglected are of the form \( \alpha_2^2 (\phi^* \phi)(\sigma^* \sigma) \) for the \( \phi-\sigma \) term and similarly for the rest.

What we have is essentially three scalar fields, which represent the order parameters. One way to proceed is to consider the interaction of scalar fields with gauge fields and subject this to some symmetry group. As it is known from particle physics such considerations lead to some interesting non-perturbative solutions such as t’Hooft-monopole, Nielsen-Olsen vortices, instantons and several others. Clearly we have many choices for gauge group, but we consider the most basic ones which can cover the essential physics. We have to broad choices abelian and non-abelian groups. The abelian group of direct relevance is \( U(1) \) or \( O(2) \) and the one of the simplest non-abelian choice is \( SU(2) \) or \( SO(3) \). We may also consider higher groups such as \( SU(N) \), \( SO(N) \), \( CP^{n-1} \) and others.

The Lagrangian \[ \mathcal{L} \] of gauge-field \( A_\mu \) interacting with a scalar field \( \phi \) may be written as for abelian case
\[ \mathcal{L} = \frac{1}{2} (D_\mu \phi)^\dagger (D^\mu \phi) + \mu^2 \phi^\dagger \phi - \lambda (\phi^\dagger \phi)^2 - \frac{1}{4} F_{\mu\nu} F^{\mu\nu}, \]
\[ D_\mu \phi = \partial_\mu \phi - ig A_\mu \phi, \]
\[ F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu, \] (5)
and
\[ \mathcal{L} = \frac{1}{2} (D_\mu^{ij} \phi_j)^\dagger (D^\mu_{ij} \phi^j) + \mu^2 \phi^\dagger_i \phi^i - \lambda (\phi^\dagger_i \phi^i)^2 - \frac{1}{4} F_{\mu\nu}^{ij} F^{\mu\nu}_{ij}, \]
\[ D_\mu^{ij} \phi_j = \partial_\mu \phi^{ij} - ig F^{ijk} A_\mu^j \phi_k, \]
\[ F_{\mu\nu}^{ij} = \partial_\mu A_{\nu}^{ij} - \partial_\nu A_{\mu}^{ij} + g F^{ijk} A_\mu^j A_\nu^k, \] (6)
for the non-abelian case. The group indices are denoted by \( i, j, k, \ldots \), whereas \( \mu, \nu, \ldots \) are the space-time indices.

Let us consider SSB in the abelian case. If the scalar potential is extremized and the scalar field acquires a vacuum expectation value [VEV]
\[ |<0|\phi|0> = v/\sqrt{2}, \]
\[ |\phi| = v/\sqrt{2}, \]
\[ v = (\mu^2/\lambda)^{1/2} \] (7)
the symmetry is spontaneously broken. To see this we first write the \( \phi \) field in terms of two real fields \( \phi_1 \) and \( \phi_2 \), and choose an arbitrary direction to achieve SSB, as discussed above, viz
\[
\phi = \frac{1}{\sqrt{2}} (\phi_1 + i \phi_2),
\]
\[
| < 0 | \phi_1 | 0 > | = v,
\]
\[
| < 0 | \phi_2 | 0 > | = 0,
\]

(8)

After shifting the fields \(\phi_1\) and \(\phi_2\) about their respective vacuum expectation values we will end up with the gauge-boson \(A_\mu\) having acquired a mass \(M = gv\), and a scalar field with mass \(m = \sqrt{2} \mu\). The degrees of freedom [DOF] must correctly add up. We started with massless gauge boson [2 DOF] and complex \(\phi\) field [2 DOF] and ended up with a massive gauge-boson [3 DOF] and one real scalar field [1 DOF] and so the DOF correctly add up. The same procedure easily carries over to the non-abelian case. For example if we consider the group \(SU(2)\), we would start with three massless gauge fields [6 DOF]. Choosing \(\phi\) to be a complex doublet [4 DOF] and assuming SSB we will arrive at 3 massive gauge bosons [9 DOF] and one real scalar field [i.e. Higgs field] [1 DOF] as one should.

The Lagrangian in Eq. (8) is called the Abelian-gauge model [AGM]. The connection between the static solution of AGM and GL model was elegantly pointed out by Nielsen and Olsen [11]. Using the vortex solution of AGM the connection with the dual model of strings [Nambu action] was also pointed out in this work. Thus by looking at particular solution of a field theory one arrives at a string model. It is rather unfortunate that although lot of people in CMT use vortices in context of GL, reference to [11] is almost never made, to our knowledge.

In the above scenario of SSB there is a physical Higgs, however we may consider other scenarios where there is no physical Higgs and symmetry breaking is non-linearly realized [10] [and references therein]. This approach is same as non-linear sigma model, which is discussed in [5]. For our purposes we can think of non-linear sigma model as a type of scalar field theory, whose structure is different from \(\phi^4\) theory discussed above and which gives an alternative description of SSB.

### IV. RESULTS

Our phenomenological model given in Eq. (8) consists of three scalar fields. Even without including gauge fields it is non-trivial to solve this model. We thus break it into simpler logical parts which we have discussed above. For example we can choose to introduce a single Abelian gauge field which interacts with charged complex field, clearly there are several interesting choices one can make. We now outline our results for some of our choices.

- Consider the choice that an Abelian gauge field interacts with a complex scalar. In the usual manner we can obtain the string-like vortex solution. We interpret the string-like solution as charged stripes. We note that so far the treatment is classical. The interaction of the other two scalar fields [which represent superconductivity and magnetism] with these charged strings can be studied. In a simple sense we can take the charged scalar field to represent the holons. The string-like solution [11] can be
obtained by assuming that the scalar field approaches a constant value at large distance. It is straightforward to see that the minimum of potential is at

$$|\phi| = \phi_0 = (\alpha_1/(2\alpha_2)^{1/2}. \quad (9)$$

If we expand about this VEV, and denote fluctuations by $\phi'$, it can be shown that the fluctuations are defined by a characteristic length $\xi$,

$$\phi' = e^{-r/\xi}, \quad \xi = 1/\sqrt{(2\alpha_1)}. \quad (10)$$

$\xi$ measures the distance before $|\phi|$ reaches its asymptotic value, it is the measure of the transverse extension of the string. Another relevant parameter is directly related to the ratio $[r]$ of the strength of the self-coupling of scalar field to the interaction strength of scalar field ($\alpha_2$) with the gauge field ($e$)

$$r = (2\alpha_2/(e^2 \alpha_1)^{1/2}. \quad (11)$$

$r$ is a measure over which the electromagnetic field is appreciably different from zero. A well-defined string results if $\xi$ and $r$ have roughly the same magnitude. Thus the deviation from an exact string structure or deformed string may be got by choosing suitable values for these parameters. Such a parameterization is useful for modeling realistic stripes. Although the string-like solution of the AGM is well-known, our interpretation is new, namely to interpret the string-like solution as charge stripe. We note that Nielsen and Olsen [11] found the solution by realizing that AGM is the relativistic generalization of GL Lagrangian which has a vortex solution as for example found by Abrikosov. Yet another new feature is to use the deviation of the parameters $\xi$ and $r$ from each other for modelling realistic stripes.

- If we choose a non-abelian group such as $SU(2)$, $SU(3)$ or $SO(3)$ we can still obtain a string-like solution provided we have at least two scalar fields [which are “vectors” under the symmetry groups]. The same arguments go through as discussed for the abelian case. We may use these solutions to models spin stripes or regions of spins or spinons. By considering the interactions of charge and spin stripes we can hope to obtain a phenomenological model for cuprates and related materials.

- It is also known [see [11]] that in 2+1 dimensions the simplest non-trivial string-model [or vortex] arises from the sine-Gordon theory, with Lagrangian, equation of motion and static solution [with string lying along the x-axis],

$$L = \frac{1}{2} (\partial_\mu \phi)^2 + c \cos(d\phi),$$

$$\Box \phi + cd \sin(d\phi) = 0,$$

$$\phi = \frac{1}{4} \arctan e^{\sqrt{cd} \ y}, \quad (12)$$
where \( \Box \equiv \partial_{\mu} \partial^{\mu} \equiv (1/v^2) \frac{\partial^2}{\partial t^2} - \nabla^2 \) is the familiar wave operator.

We may thus interpret this solution as giving rise to charge stripes. The above are classical field theory results. On the other hand it is known in CMP according to Luttinger liquid theory of 1d metals that at large wavelengths the relevant degrees of freedom are \textit{collective charge and spin oscillations} which are governed by the quantum sine-Gordon field theories. Our results are supported by the work of Zaanen et al. [12], who have used sine-Gordon theory for separation of spin, charge and string fluctuation.

\section*{V. CONCLUSIONS}

By considering a set of scalar fields without \textit{[global theory]} or with \textit{[local theory]} which we take to define order-parameters of cuprates we are led naturally led to a phenomenological model of strings. These strings and their interactions with the relevant degrees of freedom of systems constitute an interesting direction to pursue. This approach nicely ties with and supports our quantum group conjecture [2], namely that 1d structures are relevant to the understanding of the physics of the cuprates and related materials. It must be pointed out that almost all works have used the argument that since quantum groups were restricted to 1d, it was a problem to use them. On the contrary we have argued that it is precisely the opposite, namely 1d systems or collective excitations are the ones relevant [2] to the physics of the cuprates and related materials.

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