On the possibility of mixed phases in disordered quantum paraelectrics

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We present a theory of phase transition in quantum critical paraelectrics in the presence of a quenched random-Tc disorder using replica trick. The effects of locally ordered regions and their slow dynamics are included by breaking the replica symmetry at a vector level. The occurrence of a mixed phase at any finite value of disorder strength is argued and a a broad power law distribution of quantum critical points is predicted. Results are interesting in the context of a certain class of disordered materials near quantum phase transitions.

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I. INTRODUCTION

Following the recent progress in the understanding of quantum phase transitions in ferroelectrics and the strongly correlated systems with disorder, we make an attempt to explain certain features of disordered quantum paraelectrics. In general, a dilute amount of quenched impurity and associated disorder, can create locally ordered regions even above the transition point of the corresponding pure system. Near a phase transition, large size droplets become more probable and their slow dynamics becomes an important factor to determine the nature of quantum phase transition in the disordered system. Some dielectric materials, like SrTiO3, KTaO3 do not show any ferroelectric transition even at zero temperature in their pure form. These rather end up with a very high, temperature independent, static dielectric susceptibility at low temperatures. The absence of a transition and the saturation at a high dielectric susceptibility in these materials correspond to the smallness of the zero temperature gap in an optical branch and are believed to be near a ferroelectric quantum critical point. These materials have been studied in the past several years and the role of quantum fluctuations in the suppression of ferroelectric transitions and the effects of pressure and impurity were emphasized in earlier literature. A relevant question in this line would be the effects of impurity and disorder in these systems. Most of the disordered quantum paraelectrics show relaxor behavior which is often described as a classical glassy behavior of a dipolar system. In this work we focus on the effects of disorder in quantum critical behavior of certain ferroelectrics. Such issues were addressed in case of classical critical behavior earlier and some attempts to make a quantum generalization of it in the context of itinerant magnets have been proposed in the recent past. We use some of the earlier results and develop a new mean field description of the possible low temperature behavior of a disordered quantum critical paraelectric.

II. THEORY

Polarization fluctuations in these materials are well described by a zone center transverse optic mode. In a Heisenberg spin(dipole) model with dipolar interactions, the longitudinal modes are gapped out and transverse fluctuations are able to become soft. For simplicity, we restrict ourselves to one transverse branch. Assuming that the system is soft in one transverse direction, we start with a one component Landau-Ginzburg-Wilson quadratic action, suitable for near quantum critical paraelectrics.

\[ A_{\text{pure}} = \frac{1}{2\beta} \sum_{n,q} (\omega_n^2 + q^2 + r)|\phi(\omega_n, q)|^2 \]

\[ + \frac{u}{4!} \int dx \int_0^\beta d\tau \phi^4(x, \tau). \]

Here \( \beta = 1/k_B T \) where \( k_B \) is the Boltzmann constant and \( T \) is the temperature. Here \( \omega_n = 2\pi n T \) with integer \( n \), is the Bosonic Matsubara frequency. The parameter \( r \) determines the gap in polarization fluctuations and \( r = 0 \) is the mean field quantum critical point of the pure system. Disorder is introduced into the problem as a random variation of \( r \) in real space and the disorder contribution to the above mentioned quantum action is given by,

\[ A_{\text{dis}} = -\frac{1}{2} \int dx \int_0^\beta d\tau \delta r(x) \phi^2(x, \tau), \]

where \( \delta r(x) \) is assumed to follow a Gaussian probability distribution with variance \( g \), viz.,

\[ P(\delta r(x)) \propto \exp\left\{ -\frac{1}{4g} \int dx \delta r^2(x) \right\}. \]
so that $\delta_r(x) = 0$ and $\delta_r(x)\delta_r(y) = g\delta^d(x-y)$. To calculate the disorder averaged free energy, we introduce replicas of the order parameter $\phi_q$ with replica index $a=1, \ldots, n$ and write $F = -\frac{1}{\beta} \langle \mathcal{Z}^n - 1 \rangle/n$, taking $n \to 0$ at the end of the calculation. Disorder averaging generates interactions between fields with different replica indices and the resulting action becomes,

$$
\mathcal{A} = \frac{1}{2\beta} \sum_{m,q,a,b} (\omega_m^2 + q^2 + r)|\phi_a(\omega_m, q)|^2 \delta_{ab} + \frac{u}{4!} \int dx \int_0^\beta d\tau \phi_a^4(x,\tau) \delta_{ab} - \frac{g}{4} \int dx \int_0^\beta d\tau \int_0^\beta d\tau' \phi_a^2(x,\tau) \phi_b^2(x,\tau').
$$

(4)

Here $a, b$ are the replica indices which take positive integer values up to some integer $n$.

To begin with, first we consider a replica symmetric case. We define replica symmetric solution as replica independent field configurations, i.e.

$$
\phi_a(x, \tau) = \phi(x, \tau) \quad \text{for all } a
$$

(5)

and their replica diagonal two point correlation functions, i.e.

$$
\chi_{ab} = \chi_{aa} \delta_{ab} = \chi_0 \delta_{ab} \quad \text{for all } a, b.
$$

(6)

We consider a paraelectric phase i.e. $<\phi> = 0$ and make a self-consistent quasi-harmonic approximation to decouple the quartic term. In this scheme a quartic term such as $\int dx \int d\tau \phi^4(x,\tau)$ is decomposed as $\lambda_0 \int dx \int d\tau \phi^2(x,\tau)$. Where $\lambda_0 = \int dx \int d\tau \phi^2(x,\tau)$. Thus susceptibility of the disordered paraelectric can be written as,

$$
\chi_0(\omega_m, q) = \frac{1}{(\omega_m^2 + q^2 + r + \lambda_0)}.
$$

(7)

In the above equation $\lambda_0$ describes the fluctuation corrections to ferroelectric gap and is defined by the following self-consistent equation

$$
\lambda_0 = \sum_{m,q} \frac{u \chi_0(\omega_m, q) - g \chi_0(0, q)}{\omega_m^2 + q^2 + r + \lambda_0} = \frac{u}{\beta} \int d^3q \frac{1}{\Omega_q} \coth \beta \Omega_q - \frac{g}{\beta} \int d^3q \frac{1}{\Omega_q^2}.
$$

(8)

where the fluctuation corrected natural frequency $\Omega_q$ is defined as,

$$
\Omega_q^2 = q^2 + r + \lambda_0.
$$

(9)

It is to be noted that the second term in equation (9) is a zero frequency contribution. The reason is that we consider quenched disorder which has no dynamics and thus strongly correlated in time. However the above two equations can be obtained by integrating $\delta_r(x)$ without introducing replica trick and need to be solved self-consistently. It is clear from the expression for $\lambda_0$ that the second integral in the equation (8) gives a shift in gap and depending on its strength controls quantum fluctuations. In this scheme the solution of the equation $r - g \int d^3q \Omega_q^{-2} = 0$ for $r$ gives the quantum critical point. Right at that point various physical quantities follow power law dependencies in temperature, e.g. static dielectric susceptibility $\sim T^{-2}$. The effects of disorder considered here are identical to the effects of hydrostatic pressure as discussed in our previous work.

To include the effects of spatial inhomogeneity created by disorder we need to break the replica symmetry at the vector level. In this approximation field configurations are assumed as

$$
\phi_a(x, \tau) = \phi_k(x, \tau) + \psi(x, \tau) \quad \text{for } a = 1, \ldots, k
$$

(10)

and the correlation functions to be block-diagonal

$$
\chi_{ab}(x, \tau) = \chi_{1}(x, \tau) + \chi_{2}(x, \tau) \delta_{ab} \quad \text{for } a, b = 1, \ldots, k
$$

(11)

Here $k \geq 1$ is an integer that determines the degree of the symmetry breaking process. In classical treatment for $g k > u$, $\phi_k$ corresponds to localized solution given as,

$$
\phi(x) = \sqrt{\frac{r}{\beta (g k - u)}} \psi(\sqrt{T} x).
$$

(12)

So that $\psi(z)$ obeys a scale independent equation

$$
- \nabla_z^2 \psi(z) + \psi(z) - \psi^3(z) = 0.
$$

(13)

The proper boundary conditions are $\psi(0) = \text{constant}$ and $\psi(\pm\infty) = 0$. Equation (13) has exponential decaying solutions for $x \gg \sqrt{T}$ and is smooth for $x < \sqrt{T}$. The size of the droplet $R$ is determined by the dipolar correlation length and $R \sim \sqrt{T}$. At very low temperature the dynamics of the droplets become important. In a simplest approximation spatial and the time dependent parts of the polarization field can be decoupled completely.

$$
\phi(x, \tau) = \phi_k(x) T(\tau).
$$

(14)

Within this approximation the dynamics of the localized solution can be cast in a problem of an undamped Bosonic particle in a double well potential
with frequency $\omega_0 = 2$ in some dimensionless unit. Authors of reference\cite{12} derived a tunnel splitting of ground state energy

$$r_L \approx 2e^{-r_0/r}$$

(15)

with $r_0 \sim E_1/E_2$ a constant, where $E_N = \int dz \phi(z)^{2N}$. Integrating out the fluctuations due to droplets in a Gaussian approximation, an effective action for the paraelectric fluctuations $\psi(x, \tau)$ can be written as,

$$S[\psi] = \frac{1}{2\beta^3} \sum_{m, q, a, b} ((\omega_m^2 + q^2)\delta_{ab} + M_{ab})\psi_a\psi_b. \quad (16)$$

The presence of droplets introduces a “gap-matrix” \{M_{ab}\} which contains $k \times k$ block with elements,

$$M_{ab} = r(1 - \frac{gk - 3u}{gk - u} \lambda_L)\delta_{ab} - \frac{2gk\lambda}{gk - u} \lambda_L \quad (17)$$

and diagonal elements for the remaining $n - k$ replicas

$$M_{ab} = r(1 - \frac{gk}{gk - u} \lambda_L)\delta_{ab}. \quad (18)$$

Here $\lambda_L$ encodes the contributions from the localized solutions along with their dynamics and is given as

$$\lambda_L = \sum_{\omega} \int dz <\psi(z)\mathcal{T}^{(\omega)}\psi(z)\mathcal{T}^{(\omega)} >$$

$$= \int dz \psi^2(z) \sum_{\omega} <\mathcal{T}^{(\omega)}\mathcal{T}^{(\omega)} >$$

$$\sim \frac{1}{\omega - \omega_L} \quad \text{at} \quad \omega = \omega_L \quad (19)$$

Here $\omega_L = 2 \pm r_L$. It is to be noted that the vector breaking of replica symmetry not only introduces inhomogeneous solutions but also glassy effects through off-diagonal elements in the gap-matrix. Putting $\lambda_L = 0$ identically, we get back the behavior of a pure system. However in this scheme replica correlators for disordered paraelectric is given by

$$\lambda_{ab}^{\pm 1}(\omega, q) = ((\omega_m^2 + q^2)\delta_{ab} + M_{ab}). \quad (20)$$

We look for replica diagonal correlations in equations (17) and (18). Diagonalization of the gap-matrix are given as,

$$\hat{M}_{aa} = \begin{cases} r(1 - \frac{gk - 3u}{gk - u} \lambda_L), & a = 1, \ldots, k - 1, \\ r(1 - \frac{3gk - 3u}{gk - u} \lambda_L), & a = k, \\ r(1 - \frac{gk - 3u}{gk - u} \lambda_L), & a = k + 1, \ldots, n \end{cases} \quad (21)$$

Using equation (21) and (19) we find the values of $r$ at which zero temperature diagonal susceptibility ($\sim \frac{1}{\mathcal{M}_{aa}}$) diverges. The instability point depends on the disorder strength and the value of $k$ and is given as,

$$r_c = \begin{cases} -r_0/\log(1 - A \frac{(gk - 3u)}{(gk - u)}), & a = 1, \ldots, k \\ -r_0/\log(1 - A \frac{(gk - 3u)}{(gk - u)}), & a = k \\ -r_0/\log(1 - A \frac{(gk - 3u)}{(gk - u)}), & a = k + 1, \ldots, n \end{cases} \quad (22)$$

and is $k$ dependent. Here $A$ is a system dependent parameter. For a simple minded analysis, let us consider the $a = k + 1, \ldots, n$ elements only. For $\frac{A_{gk}}{(gk - u)} << 1$, $r_c$ can be written in the following form

$$r_c(k) = \frac{r_0}{g} \left( \frac{gk - u}{gk} \right) \quad (23)$$

Since the choice of $k$ is random, depending on its distribution at the limit $n \to 0$, we can estimate a distribution, hence width of $r_c$. In a replicated action with $n$ replicas, $k$ can be chosen in $C_n^k$ ways. Thus we can define a normalized distribution of $\mathcal{P}(k)$ as follows

$$\mathcal{P}(k) = \frac{C_n^k}{\sum_{k=1}^{n} C_n^k} = \frac{1}{2^n - 1} \frac{\Gamma(n)}{\Gamma(n - k)}. \quad (24)$$

Since the gamma function with negative argument is infinity, the limit of $k$ can be extended to infinity. In the limit $n \to 0$, using the asymptotic form of gamma functions, $\mathcal{P}(k)$ can be approximated as \cite{10, 11}

$$\mathcal{P}(k) \approx \frac{1}{\log 2} \frac{(-1)^{k-1}}{k} \approx \frac{1}{\log 2} \frac{\cos \pi \cos \pi k}{k}. \quad (25)$$
Negative values of $P(k)$ for some values of $k$ may turn out to be counter intuitive to the usual notion of a distribution function. But such distributions are allowed in replica scheme. There are several possible broken replica symmetric cases, each characterized by the number $k$ which follows a distribution $P(k)$. For a fixed disorder strength $g$, each $k$ results a different instability point $r_c$. Instead of $k$, if we characterize various possible broken replica symmetric cases by $r_c$, a distribution of $r_c$ can be estimated as

$$P(r_c) = P(k)|\frac{\Delta k}{\Delta r_c}| \sim \frac{1}{B - r_c} \times \cos(\pi k). \quad (26)$$

This is a broad power-law distribution of $r_c$ around a system dependent parameter $B$ with a cosine factor. The probability distribution can be assumed to be smooth around $k = 0$ and any positive integer, excluding zero. The expansion around $k = 0$ is excluded as it corresponds to small $u/g$ limit where the action becomes unstable even in a replica symmetric ansatz. In that limit the system will undergo a first order transition in a replica symmetric analysis, the stability of the system needs a $\phi^6$ term in the action which will lead to more complicated localized solutions in a broken replica symmetry picture. However we focus on those $u/g$ values where the above possibilities are not present and the distribution function is smooth. It is to be noted that the power law nature of $P(r_c)$ arises because of the dynamics of the locally ordered regimes and also depends on the distribution of $k$ used. Neglecting cosine factor within some range of $r_c$ say $(B+R, B-R)$, average susceptibility of the disordered quantum paraelectric can be estimated as,

$$\overline{\chi(r, T)} \sim \int_{B-R}^{B+R} dr_c \frac{1}{B - r_c} \times \frac{1}{r - r_c + T^2} = \frac{1}{r - B + T^2} \log \frac{r - B + R + T^2}{r - B + R - T^2}. \quad (27)$$

It is evident that inclusion of fluctuations due to locally ordered regime introduce a parameter $R \sim O(u/g)$ and changes the usual quantum critical behavior of a paraelectric. In the limit $r \to B$ the temperature dependence of a disordered quantum paraelectric can be predicted as,

$$\overline{\chi(r, T)} \sim \begin{cases} \text{constant, } T < R & \text{1/T^4, } T > R. \end{cases} \quad (28)$$

This is a deviation from the standard quantum critical behavior which predicts $\chi(T) \sim T^{-2}$ in a mean field theory.

### III. DISCUSSIONS

In this work, the low temperature dielectric behavior of a quantum paraelectric in presence of quenched disorder is addressed. A suitable action for these materials, with random $T_c$ type disorder have been studied using a replica trick. The effects of disorder induced locally ordered regimes and their tunnelling in the low temperature are captured in this formalism. We derive an expression for the distribution of instability points for a fixed value of disorder strength and demonstrate the possibility of a mixed phase at non-zero disorder strength. This analysis shows that the instability points follows a broad power law distribution around a system dependent parameter with a cosine correction. By using such distribution we are able to show analytically how the temperature dependence of static dielectric susceptibility of a disordered quantum critical paraelectric deviates from its pure counterpart. Our analysis is a completely new attempt in the context of the effects of disorder in ferroelectrics near a quantum critical point. In a qualitative manner it predicts certain new features such as occurrence of a phase with mixture of critical and non-critical regimes with a distributions of transition points which are missing in earlier works in similar issues in context of itinerant magnets. Moreover the whole analysis is interesting in context of the use of replica trick to incorporate disorder induced inhomogeneities or locally ordered regime in the studies of quantum phase transition and may turn out to be useful in explaining certain experimental results on disordered ferroelectrics near a quantum critical point.

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