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LETTER TO THE EDITOR

Self-consistent treatment of impurity influence in quantum systems at $T = 0$

G Busiello, L De Cesare and I Rabuffo

Dipartimento di Fisica Teorica e SMSA, Università di Salerno, 84100-Salerno, Italy and Gruppo Nazionale di Struttura della Materia, 84100-Salerno, Italy

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Abstract. The zero-temperature properties of quantum systems in the presence of quenched impurities which couple quadratically to the order parameter are investigated by means of a self-consistent treatment. A physical interpretation of the renormalisation group fixed point instability recently discovered is suggested and a comparison with some experiments on doped quantum incipient ferroelectrics is also made.

The influence on quantum critical behaviour of quenched impurities which couple quadratically to the order parameter has been the subject of recent renormalisation group (RG) investigations (Busiello *et al* 1984a, b, Korutcheva and Uzunov 1984). At temperature $T \neq 0$, when quantum fluctuations are irrelevant, the well known results for classical systems both for short-range (Ma 1976, Grinstein *et al* 1977) and long-range (Weinrib and Halperin 1983) correlated impurities are reproduced. At $T = 0$, it turns out that, for dimensionalities such that pure quantum systems show a critical point, the randomness does not create, surprisingly, stable fixed points as it should be whenever a second-order phase transition is present.

An analogous unusual impurity effect occurs at arbitrary temperature also in quantum systems which show tricriticality in the absence of disorder (Busiello *et al* 1984c).

Since the RG results do not allow us to give a clear picture of this strange effect which arises from the competition between quantum and random fluctuations, in our opinion further theoretical and, possibly, experimental investigations need to be done in order to clarify the physical meaning of the above fixed point instability.

In this letter we deal with the problem by using a self-consistent approach, which is exact in the large-n limit (n is the number of order parameter components) but gives a correct qualitative picture of the physics for real systems which show a ($T = 0$) critical point when the disorder is absent. As the above peculiar effect of quenched impurities is independent of the particular quantum model, we refer, for explicit calculations, to bosonised models (Busiello and De Cesare 1980, Busiello *et al* 1983) and a continuous field model for structural phase transitions (Opperman and Thomas 1975, Morf *et al* 1977, Millev and Uzunov 1983). This choice assumes some relevance since these models represent the prototypes of quantum systems without and with dimensional crossover for $T \to 0$, respectively, when the randomness is lacking (Busiello *et al* 1983). Here we limit ourselves to the zero temperature regime which, in our opinion, deserves particular interest from theoretical and experimental (or simulational) point of view.

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In this way we hope to stimulate new deeper investigations in order to obtain a definitive insight into the physical nature of the mentioned impurity effect which occurs in quantum systems when thermal fluctuations vanish.

A complete discussion for arbitrary temperature, also including an analysis of quantum crossover phenomenon which occurs for $T \to 0$, will be given in a future work.

Our starting point is the 'generalised quantum functional' (Busiello *et al* 1984b):

$$\begin{aligned}\mathcal{H}\{\psi,\varphi\} = & \sum_{j=1}^{n/2} \sum_{\substack{q \\ 0<|k|<1}} (r_0 + k^\sigma + f(q))|\psi^j(q)|^2 \\ & + \frac{1}{V^{1/2}} \sum_{j=1}^{n/2} \sum_{\substack{k_1,k_2,\omega_l \\ 0<|k_i|<1}} \varphi(k_1 - k_2)\psi^{j*}(k_1,\omega_l)\psi^j(k_2,\omega_l) \\ & + \frac{u_0 T}{4V} \sum_{i,j=1}^{n/2} \sum_{\substack{\{q_\nu\} \\ 0<|k_\nu|<1}} \delta_{q_1+q_2;q_3+q_4} \psi^{i*}(q_1)\psi^{j*}(q_2)\psi^i(q_3)\psi^j(q_4)\end{aligned} \tag{1}$$

where $q \equiv (k, \omega_l)$, $\omega_l = 2\pi l T$ $(l = 0, \pm 1, \pm 2, \ldots)$, $0 < \sigma \leqslant 2$, $\psi(q) \equiv \{\psi^j(q);\ j = 1, 2, \ldots, n/2\}$ is a complex $n/2$ - component field, V is the volume of the system and $f(q)$ is a function depending on the particular model under study. For instance, one has $f(q) = -\mathrm{i}\omega_l$ for bosonised models and $f(q) = \omega_l^2$ for structural phase transitions. The explicit definition of the coupling parameters r_0 and u_0 for different models is not necessary in the present investigation.

In (1) $\varphi(k)$ is the Fourier transform of the random variable $\varphi(x)$ which describes the quenched impurities with Gaussian averages:

$$[\varphi(k)]_{\mathrm{av}} = 0, \qquad [\varphi(k)\varphi(k')]_{\mathrm{av}} = \delta_{k,-k'} g(k) \tag{2}$$

where for small k (Weinrib and Halperin 1983):

$$g(k) \simeq \Delta_{01} + \Delta_{02} k^{-(d-a)}, \qquad a > 0. \tag{3}$$

With (3) we refer to the general case of quenched impurities which are correlated as $|x-y|^{-a}$ for large distances, a being a positive parameter of the model.

Making use of the replica trick (Edwards and Anderson 1975, Emery 1975), the original random problem without translational invariance can be reduced to a pure one characterised by an effective action

$$\begin{aligned}\mathcal{H}_{\mathrm{eff}}(\{\psi_\alpha\}) = & \sum_{\alpha=1}^{m} \sum_{j=1}^{n/2} \sum_{\substack{q \\ 0<|k|<1}} (r_0 + k^\sigma + f(q))|\psi^j_\alpha(q)|^2 \\ & + \frac{u_0 T}{4V} \sum_{\alpha=1}^{m} \sum_{i,j=1}^{n/2} \sum_{\substack{\{q_\nu\} \\ 0<|k_\nu|<1}} \delta_{q_1+q_2;q_3+q_4} \psi^{i*}_\alpha(q_1)\psi^{j*}_\alpha(q_2)\psi^i_\alpha(q_3)\psi^j_\alpha(q_4) \\ & - \frac{1}{2V} \sum_{\alpha,\beta=1}^{m} \sum_{i,j=1}^{n/2} \sum_{\substack{\{q_\nu\} \\ 0<|k_\nu|<1}} g(k_1 - k_3)\delta_{k_1+k_2;k_3+k_4}\delta_{\omega_{l_1},\omega_{l_3}}\delta_{\omega_{l_2},\omega_{l_4}} \\ & \times \psi^{i*}_\alpha(q_1)\psi^{j*}_\beta(q_2)\psi^i_\alpha(q_3)\psi^j_\beta(q_4)\end{aligned} \tag{4}$$

which is a functional of m replications $\{\psi_\alpha;\ \alpha = 1, \ldots, m\}$ of the original field ψ.

Now, our aim is to calculate the physical susceptibility χ of the random system because the divergence of this quantity constitutes a test of criticality. It is defined as

$$\chi = \lim_{\substack{k\to 0\\ \omega\to 0}} \mathscr{G}_{\mathrm{R}}(\boldsymbol{k}, \omega) \tag{5}$$

where the retarded response function is obtained as the analytical continuation to the real frequency axis of the temperature propagator $\mathscr{G}(q) = [\langle|\psi^i(q)|^2\rangle]_{\mathrm{av}}$. Since this is expressed in terms of the replica fields as

$$\mathscr{G}(q) = \lim_{m\to 0} \frac{1}{m} \sum_{\alpha=1}^{m} \langle|\psi^i_\alpha(q)|^2\rangle_{\mathscr{H}_{\mathrm{eff}}}, \tag{6}$$

the calculation of χ reduces to an evaluation of the replica propagator $G(q) = \langle|\psi^i_\alpha(q)|^2\rangle_{\mathscr{H}_{\mathrm{eff}}}$. With this in mind, let us regard the term:

$$\mathscr{H}^{(0)}_{\mathrm{eff}}(\{\psi_\alpha\}) = \sum_{\alpha=1}^{m} \sum_{j=1}^{n/2} \sum_{\substack{q\\ 0<|\boldsymbol{k}|<1}} (r + k^\sigma + f(q))|\psi^j_\alpha(q)|^2 \tag{7}$$

with $r = \chi^{-1}$, as the 'free part' of the effective action. Of course, this procedure will involve a counterterm in the 'interaction part' of $\mathscr{H}_{\mathrm{eff}}$ given by

$$\mathscr{H}^{(c)}_{\mathrm{eff}}(\{\psi_\alpha\}) = (r_0 - r) \sum_{\alpha=1}^{m} \sum_{j=1}^{n/2} \sum_{\substack{q\\ 0<|\boldsymbol{k}|<1}} |\psi^j_\alpha(q)|^2. \tag{8}$$

Within this scheme the replica propagator will be determined by the Dyson equation

$$G^{-1}(q) = r + k^\sigma + f(q) + \Sigma(q, r) \tag{9}$$

where $\Sigma(q, r)$ is the usual self-energy part (Ma 1976). By valuing this term to the lower order in the coupling parameters u_0, Δ_{01}, Δ_{02} and by inserting the corresponding expression for $G(q)$ in the limit process (6), from (5) we obtain, in the thermodynamic limit, the following self-consistent equation for $r = \chi^{-1}$:

$$r = r_0 + (n+2)\frac{u_0}{4} K_d \int_0^1 \mathrm{d}k\, k^{d-1} \left(T \sum_{\omega_l} \frac{1}{r + k^\sigma + f(q)} \right) - K_d \int_0^1 \mathrm{d}k\, k^{d-1} \frac{\Delta_{01} + \Delta_{02} k^{-(d-a)}}{r + k^\sigma} \tag{10}$$

where $K_d = 2^{1-d}\pi^{-d/2}/\Gamma(d/2)$.

Now, we study (10) at $T = 0$ separately for bosonised models and structural phase transitions.

Bosonised models. In this case, at $T = 0$, the self-consistent equation (10) reduces to:

$$r = r_0 - K_d \sigma^{-1}(\Delta_{01} G_{d/\sigma}(r) + \Delta_{02} G_{a/\sigma}(r)) \tag{11}$$

where

$$G_\mu(r) = \int_0^1 \mathrm{d}x \frac{x^{\mu-1}}{r + x}, \qquad \mu = d/\sigma, a/\sigma. \tag{12}$$

The critical expression $r_{0c} = r_{0c}(\Delta_{01}, \Delta_{02})$ of the parameter r_0 is obtained, as usual, setting $r = 0$ in (11):

$$r_{0c} = K_d \sigma^{-1}(\Delta_{01} G_{d/\sigma}(0) + \Delta_{02} G_{a/\sigma}(0)) \tag{13}$$

where $G_\mu(0)$ ($\mu = d/\sigma$, a/σ) are finite quantities only for $\mu > 1$. This means that for short-range impurity correlations ($\{\Delta_{01} \neq 0, \Delta_{02} = 0\}$ or $\{\Delta_{0i} \neq 0$ $(i = 1, 2)$ with $a \geqslant d\}$) a ($T = 0$) critical point may exist only for $d/\sigma > 1$, while, for long-range ones, it may occur only for $a/\sigma > 1$ and arbitrary $d > 0$, if $\Delta_{01} = 0$, or for $d/\sigma > a/\sigma > 1$ if $\Delta_{0i} \neq 0$ $(i = 1, 2)$.

Remember that for pure bosonised models a ($T = 0$) Gaussian critical point exists for any $d > 0$ (Busiello and De Cesare 1980, Uzunov 1981, De Cesare 1982, Kopec and Kozlowski 1983, Chubukov 1985).

In order to study the behaviour of the random model in terms of the deviation of the parameter r_0 from its ($T = 0$) critical value when a second-order phase transition exists, it is convenient to introduce the variable $g = r_0 - r_{0c}$. Then (11) can be rewritten as:

$$r = g - K_d \sigma^{-1}(\Delta_{01} \tilde{G}_{d/\sigma}(r) + \Delta_{02} \tilde{G}_{a/\sigma}(r)) \tag{14}$$

with $\tilde{G}_\mu(r) = G_\mu(r) - G_\mu(0)$. Of course, we are interested to find solutions of self-consistent (14) for $r \to 0^+$ From a straightforward analysis of (14) in the limit $g \to 0^+$, it emerges that:

(i) When quenched impurities are short-range correlated ($\Delta_{02} = 0$ or $a \geqslant d$), one has a mean field (MF) critical behaviour for $d/\sigma > 2$, but no thermodynamically stable diverging solution for susceptibility is found for $1 < d/\sigma \leqslant 2$. Physically, this may be interpreted as a thermodynamic instability of the ($T = 0$) pure critical behaviour induced by the impurity fluctuations. Thus, for such dimensionalities, the point ($T = 0$, r_{0c}) is inaccessible and no long-range order is possible.

(ii) When long-range correlated disorder is present with $\Delta_{0i} \neq 0$ $(i = 1, 2)$, a MF regime occurs for $d/\sigma > a/\sigma > 2$. For different values of d/σ, $a/\sigma > 1$, no physical solution of (14) approaching the critical point is found and this indicates, as in (i), instability of pure Gaussian critical behaviour towards impurity perturbations.

(iii) Finally, for $\Delta_{01} = 0$, $a/\sigma > 2$ and arbitrary $d > 0$, the randomness is irrelevant and the ($T = 0$) critical behaviour of pure system is reproduced. For $1 < a/\sigma \leqslant 2$ the impurity fluctuations prevent the critical point from being approached along stable thermodynamic paths as in (i) and (ii).

Structural phase transitions. In the quantum regime, (10) for inverse susceptibility becomes:

$$r = r_0 + (n+2) u_0 A(d, \sigma) F_{d/\sigma}(r) - K_d \sigma^{-1}(\Delta_{01} G_{d/\sigma}(r) + \Delta_{02} G_{a/\sigma}(r)) \tag{15}$$

where $A(d, \sigma) = K_d/8\sigma$ and

$$F_{d/\sigma}(r) = \int_0^1 \mathrm{d}x \frac{x^{d/\sigma - 1}}{(r+x)^{1/2}}. \tag{16}$$

The ($T = 0$) critical value of r_0 is therefore given by:

$$r_{0c} = K_d \sigma^{-1}(\Delta_{01} G_{d/\sigma}(0) + \Delta_{02} G_{a/\sigma}(0)) - (n+2) u_0 A(d, \sigma) F_{d/\sigma}(0) \tag{17}$$

where $F_{d/\sigma}(0)$ is finite for $d/\sigma > \frac{1}{2}$. Then, in terms of the variable g, (15) assumes the form:

$$r = g + (n+2) u_0 A(d, \sigma) \tilde{F}_{d/\sigma}(r) - K_d \sigma^{-1}(\Delta_{01} \tilde{G}_{d/\sigma}(r) + \Delta_{02} \tilde{G}_{a/\sigma}(r)) \tag{18}$$

with $\tilde{F}_{d/\sigma}(r) = F_{d/\sigma}(r) - F_{d/\sigma}(0)$.

An analysis of this equation for $r \to 0^+$ yields a physical picture very similar to that for bosonised models. In particular cases (i)-(ii) remain unchanged but in the long-range case for $\Delta_{01} = 0$ some quantitative differences are found as a different manifestation of quantum fluctuations. From (16) it follows in fact that

$$r \propto g^{\gamma} \qquad \text{with } \gamma = \begin{cases} \dfrac{1}{d/\sigma - 1/2}, & \text{for } \{\tfrac{1}{2} < d/\sigma < \tfrac{3}{2},\ a/\sigma \geqslant d/\sigma + \tfrac{1}{2}\} \\ 1, & \text{for } \{d/\sigma > \tfrac{3}{2},\ a/\sigma > 2\} \end{cases} \tag{19}$$

and, in the borderline region $\{d/\sigma = \frac{3}{2},\ a/\sigma \geqslant 2\}$, logarithmic corrections to MF behaviour are present. This is exactly the critical behaviour which appears in the pure system at quantum displacive (Oppermann and Thomas 1975, Morf *et al* 1977) also involving long-range interactions. Thus, for long-range correlated quenched impurities with $\Delta_{01} = 0$ and the parameter a satisfying the conditions above specified, the disorder effects on pure quantum critical behaviour appear to be irrelevant. For different values of $a/\sigma > 1$, the impurity fluctuations are sufficiently strong to prevent the occurrence of criticality.

The previous results show, in particular, that, for short-range interactions ($\sigma = 2$), a ($T = 0$) second-order phase transition is possible in real quantum systems ($d = 3$) with impurities of the type here considered, only if $\Delta_{01} = 0$, $\Delta_{02} \neq 0$ and $a \geqslant 4$ for structural phase transitions and $a > 4$ for bosonised systems. In other cases, for dimensionalities of physical interest, thermodynamic instabilities towards impurity perturbations may occur which inhibit long-range order.

The above picture agrees with the RG predictions (Busiello *et al* 1984a, b) in the sense that we do not find a positive vanishing inverse susceptibility in regions of the (d/σ, a/σ) plane where the RG analysis does not predict stable fixed points. This suggests that the RG fixed point instability, induced by impurity fluctuations in quantum systems at $T = 0$, may be interpreted as corresponding to the physical impossibility of a continuous transition to an ordered phase. By varying the impurity concentrations, $r_{0c} = r_{0c}(\Delta_{01}, \Delta_{02})$ is a line of thermodynamic instability ($\chi \to -\infty$) in the phase diagram of the system. In particular, when short-range disorder is present, we find $\chi \propto -g^{-(d/\sigma-1)}$ for $1 < d/\sigma < 2$ and $\chi \propto -g^{-1} ln^{-1} g^{-1}$ for $d/\sigma = 2$. Notice that from thermodynamic point of view, similar circumstances occur also in other systems of physical interest (Rice 1954, Larkin and Pikin 1969) and are usually considered as indications of the existence of a first-order phase transition.

Of course, new insight into this problem can arise from experiments. Unfortunately no clear experimental results about quenched impurity effects on ($T = 0$) quantum critical behaviour are available at the present. This is mainly due to the difficulty of identifying the relevant type of defects involved in the laboratory samples (Aksenov and Didyk 1984). However, some recent experiments on quantum incipient ferroelectrics in the presence of impurities (Höchli and Boatner 1977, 1979, Höchli *et al* 1977, 1978, Rytz *et al* 1980, Prater *et al* 1981), may give indirect indications on the validity of our previous physical scheme. The term 'incipient ferroelectric' has been employed to describe materials, such as $KTaO_3$ and $SrTiO_3$, which exhibit a rapidly increasing dielectric constant with decreasing temperature consistently with an ultimate ferroelectric transition at $T = 0$. Nevertheless in such pure materials, ferroelectricity can be induced by pressure (Uwe and Sakudo 1975, 1976).

While Li quenched impurities, which are expected to couple linearly to the order parameter in $KTaO_3$ (Höchli *et al* 1978), destroy the ferroelectric order in the host system at $T=0$, a spontaneous polarisation has been found in $KTaO_3$:Nb for a Nb concentration of $x_c=0.008$ (Höchli *et al* 1977, Prater *et al* 1981). Experiments suggest that, in $KTaO_3$, Nb shows no evidence of being a symmetry-breaking defect (Prater *et al* 1981) and it is assumed that it couples quadratically to the order parameter in contrast to Li impurities. Furthermore, there are also indications (Höchli and Boatner 1979) that Nb impurities must be long-range correlated and the involved effective interactions are short-ranged ($\sigma=2$). Finally, a MF behaviour with logarithmic corrections is found at $T=0$ in terms of $r_0-r_{0c}\propto x-x_c$ (Höchli *et al* 1977, Höchli and Boatner 1979, Rytz *et al* 1980) as for pure structural phase transitions at the quantum displacive limit. Analogous properties are also true for $KTaO_3$: Na. All these experimental results can be simply interpreted within our theoretical scheme which may give also information about the structure of the random correlation function. Indeed, the previous theoretical provisions for structural phase transitions impose $g(\boldsymbol{k})\approx\Delta_{02}k^{-(d-a)}$ and, for $d=3$ and $\sigma=2$, long-range order survives only if $a\geqslant 4$; this implies the MF result $\gamma=1$ with logarithmic corrections for susceptibility. As a consequence, for $KTaO_3$: Nb near criticality, we should have $g(\boldsymbol{k})\sim k^{\alpha}$ for $k\to 0$ with $\alpha=a-3\geqslant 1$.

In conclusion, we think that structural phase transitions at the quantum displacive limit will constitute a good framework for clarifying theoretical, experimental and simulational investigations of the strange effect induced by impurities in quantum systems at $T=0$.

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