Comment on “Quantum critical paraelectrics and the Casimir effect in time”

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Abstract

At variance with the authors’ statement [L. Pálová, P. Chandra and P. Coleman, Phys. Rev. B 79, 075101 (2009)], we show that the behavior of the universal scaling amplitude of the gap function in the phonon dispersion relation as a function of the dimensionality $d$, obtained within a self–consistent one–loop approach, is consistent with some previous analytical results obtained in the framework of the $\varepsilon$–expansion in conjunction with the field theoretic renormalization group method [S. Sachdev, Phys. Rev. B 55, 142 (1997)] and the exact calculations corresponding to the spherical limit i.e. infinite number $N$ of the components of the order parameter [H. Chamati. and N. S. Tonchev, J. Phys. A: Math. Gen. 33, 873 (2000)]. Furthermore we determine numerically the behavior of the “temporal” Casimir amplitude as a function of the dimensionality $d$ between the lower and upper critical dimension and found a maximum at $d = 2.9144$. This is confirmed via an expansion near the upper dimension $d = 3$.

PACS numbers: 64.60.an Finite-size systems, 64.60.F- Critical points, 64.70.tg Quantum phase transitions
In a recent paper Pálová, Chandra and Coleman (PCC) studied the quantum paraelectric-ferroelectric phase transition in the framework of the self-consistent one-loop approximation applied to the familiar quantum $\varphi^4$ model that plays an important role in the investigations of the properties of many quantum systems near their quantum critical points. After a suitable normalization of the parameters of the model this approach is formally equivalent to considering an $N$-component model in the spherical limit i.e. when the number $N$ of the components of the order parameter is sent to infinity.

In their equation (33) for the gap function PCC explore the role of the temperature as a boundary effect in the “imaginary time”. Interpreting the inverse temperature as a finite size in this direction, it is possible to map the theory of quantum critical phenomena at low temperatures on the finite size scaling theory which shaped our current understanding of the modern theory of critical phenomena. In this context it is shown in Ref. 1 that at a temperature $T$ above the quantum critical point, the gap function $\Delta(T)$ in the phonon dispersion relation scales as

$$\frac{\Delta(T)}{T} = \alpha_d.$$ 

The corresponding equation for the scaling amplitude $\alpha_d$ was solved numerically for arbitrary dimensions in the range $1 < d < 3$. The bounds on $d$ are imposed by the fact that for $d \leq 1$ no phase transition can survive, while for $d \geq 3$ one obtains a mean field critical behavior. Close to the upper critical dimension, the presented on FIG. 5 dependence of $\alpha_d(T \to 0)$ on dimensionality $d$ exhibits a discrepancy (it is finite) with previous analytical considerations (where it goes to zero) as $\varepsilon \to 0^+$ and/or $N \to \infty^2$, as well as numerical ones for the quantum spherical model.$^8$ Comparing $\varepsilon$-results$^6$ and their numerical prediction PCC suggest that this discrepancy may be attributed to the order in which the limits $\varepsilon \to 0^+$ and $N \to \infty$ are evaluated. In this comment we demonstrate that at variance with PCC’s claims there is no contradiction between previous analytical$^6$ and numerical$^8$ considerations, and the analysis based on self-consistent one-loop approximation presented in Ref. 1.

Our aim is to show that the numerical treatment of Eq. (42) of Ref. 1 is not adequate closely beneath the upper critical dimension $d = 3$. For the sake of completeness, we will outline the main steps of our computations. According to Eq. (33) of PCC one has:

$$\Delta^2 = \Omega_0^2 + 3\gamma_c \Gamma_d \int_0^\Lambda dqq^{d-1} \frac{n_B(\omega_q)}{(2\pi)^d \omega_q} + \frac{3}{2} \gamma_c \Gamma_d \int_0^\Lambda dqq^{d-1} \left( \frac{1}{\omega_q} - \frac{1}{q} \right),$$

where $n_B(\omega) = \left( e^{\omega/k_BT} - 1 \right)^{-1}$, $\Gamma_d^{-1} = \frac{1}{2} \pi^{-d/2} \Gamma(d/2)$, $r$ and $\gamma_c$ are model constants, and $\omega_q = \sqrt{q^2 + \Delta^2}$. The parameter $\Omega_0^2 = r - r_c$ measures the distance of the quantum parameter driving the transition from its critical value $r_c$. In the remainder we use $k_B = 1$. Notice that we clearly separate the thermal ($T > 0$) and quantum ($T = 0$) fluctuations and introduce the cutoff $\Lambda$.

Further, via the substitution $\Delta = \alpha T$ and $q = uT$ we may write

$$\frac{(2\pi)^d}{3\gamma_c \Gamma_d} T^{3-d} \left( \alpha^2 - \frac{\Omega_0^2}{T^2} \right) = \int_0^\Lambda du \frac{ud-1}{\sqrt{\alpha^2 + u^2} \left[\exp \left( \sqrt{\alpha^2 + u^2} \right) - 1 \right]}$$

$$+ \frac{1}{2} \int_0^\Lambda du \frac{ud-1}{\sqrt{\alpha^2 + u^2} - \frac{1}{u}}.$$ 

(2)

In the low temperature region $\frac{\Lambda}{T} \gg 1$, the cutoff in the first integral can be entirely removed neglecting exponentially small corrections. The last integral is convergent in the ultraviolet in
dimensions $1 < d < 3$. It may be computed extending the integration over $u$ up to infinity to get

\[
(4\pi)^{(d+1)/2} \left( \frac{\alpha^2 T^{3-d}}{3\gamma_c} - \varkappa \right) = \Gamma \left( \frac{1 - d}{2} \right) \alpha^{d-1} + 2^d \Gamma \left( \frac{d - 1}{2} \right) h_{d-1}(\alpha^2),
\]

(3)

where we have introduced the scaling variable

\[
\varkappa = \frac{\Omega_0^2}{3\gamma_c} T^{-1/\nu z}
\]

with $\nu = (d - 1)^{-1}$ the critical exponent measuring the divergence of the correlation length, $\xi$, while approaching the quantum critical point and $z = 1$ the dynamical critical exponent. The function $h_\mu(z)$ is defined via

\[
h_\mu(z) = \frac{1}{\Gamma(\mu)} \int_0^\infty \frac{u^\mu du}{\sqrt{z + u^2} \left[ \exp \left( \sqrt{z + u^2} \right) - 1 \right]}.
\]

(4)

In particular one has

\[
h_\mu(0) = \zeta(z),
\]

(5)

where $\zeta(x)$ is the Riemann zeta function.

In the vicinity of the quantum critical point, defined by $\Omega_0 = 0$ and $T = 0$, the term containing $\alpha^2$ in the left hand side may be neglected as it gives only corrections to the leading order of $\alpha$. Then the solution to Eq. (3) has the finite temperature scaling form

\[
\alpha_d = f_d(\varkappa),
\]

(6)

with $f_d(\varkappa)$ an universal scaling function.

For the scaling form (6) to be valid one has to require

\[
T^{3-d} \ll \frac{A(d)}{(\alpha_d)^{3-d}}, \quad A(d) := \frac{3\gamma_c}{(4\pi)^{d/2}} \left| \Gamma \left( \frac{1 - d}{2} \right) \right|.
\]

(7)

This inequality is an estimation of the low temperature region and the magnitude of $\gamma_c$ where the scaling form (6) takes place.

The behavior of the scaling variable $\alpha_d$ above the quantum critical point, obtained numerically by equating the right hand side of (3) to zero, is presented in FIG. 1. To validate our numerical results we choose to perform analytic calculations of $\alpha_d$ by considering some particular cases: namely $d = 2$, and in a close vicinity of $d = 3$ and $d = 1$. This leads us to the results (see e.g. Ref. 7)

\[
\alpha_d = \begin{cases} 
\pi (d - 1), & d - 1 \ll 1, \\
2 \ln \frac{1 + \sqrt{d}}{2}, & d = 2, \\
\sqrt{\frac{2\pi^2}{3}} \sqrt{3 - d}, & 3 - d \ll 1.
\end{cases}
\]

(8)

One sees that the behavior of $\alpha_d$ for the cases $d \to 1$ and $d = 2$ seems to be correctly presented in FIG. 5 of Ref. 1. However both numerical (FIG. 1) and analytical computations (8) show that $\alpha_d$ vanishes as $d \to 3$. This result disagrees with the conclusions drawn by PCC based on the behavior presented on their FIG. 5.
FIG. 1: Dependence of $\alpha_d = f_d(0)$ on dimensionality $d$ at the quantum critical point i.e. $\Omega_0 = 0$ and $T \to 0^+$. 

In the remainder of this comment we will briefly touch on some aspects of the so called temporal Casimir effect or Casimir effect in time considered also some years ago in Ref. 9 in the framework of the quantum spherical model.

The self-consistent one-loop approximation is exact in the spherical limit, i.e. for the theory with $N$ component order parameter in the limit $N \to \infty$. In this case the free energy can be computed using a variational approach based on the Hubbard–Stratonovich decoupling technique of the $P^4$ term ($P$ being $N$–component field) in the model of Ref. 1. Following Ref. 7 we end up with an expression for the free energy per particle and per component

$$F_d(T) = \min_{\Delta} \left\{ -\frac{1}{4\gamma_c} (\Delta^2 - r)^2 + T \int \frac{d^d q}{(2\pi)^d} \ln \left[ \frac{2}{\sinh \left( \frac{1}{2T} \omega_q \right)} \right] \right\}. \tag{9}$$

The equation minimizing the free energy (9) is identical to the self consistency equation (11) up to the substitution $\gamma_c \to 3\gamma_c$. Notice that expression (9) for the free energy can be split into a “pure quantum” free energy and a “finite temperature” contribution as:

$$F_d(T) = \min_{\Delta} \left\{ -\frac{1}{4\gamma_c} (\Delta^2 - r)^2 + \frac{1}{2} \int \frac{d^d q}{(2\pi)^d} \omega_q + T \int \frac{d^d q}{(2\pi)^d} \ln \left( 1 - e^{-\omega_q/T} \right) \right\}. \tag{10}$$

Applying the assumption of Ref. 10 for the singular part of the free energy for classical systems within the theory of finite size scaling to the case of quantum critical phenomena at finite temperature, the singular part of the free energy should scale like

$$F_d^{\text{sing.}}(T) \sim T^{1+d/z} \tilde{F} \left[ (r - r_c) T^{-\nu z} \right], \tag{11}$$

where the function $\tilde{F}$ is an universal scaling function, whose value at the quantum critical point is equivalent to the Casimir amplitude for temperature driven phase transitions in films. Such an idea, considering the inverse temperature as an additional dimension, has been developed for quantum critical points in Ref. 9. Notice however that for quantum systems this quantity may be
measured experimentally since it is related to the amplitude of the specific heat of the system at finite temperature.

For the model under consideration in the interval of interest i.e. dimensions $1 < d < 3$ and in the vicinity of the quantum critical point, the singular part of the free energy takes the scaling form

$$ F^{\text{sing.}}_d(T) = T^{1+d} g_d(x), \quad (12) $$

where

$$ g_d(x) = \frac{1}{2} x^{2d} - \frac{1}{2} \left( \frac{4\pi}{d+1} \right)^{(d+1)/2} \Gamma \left( -\frac{d+1}{2} \right) \alpha_{d+1} - \pi^{-(d+1)/2} \Gamma \left( -\frac{d+1}{2} \right) h_{d+1} \left( \alpha_{d}^2 \right), \quad (13) $$

is an universal scaling function with $\alpha_d$ the solution (6) to Eq. (3). It is worth mentioning that the scaling form (12) is in agreement with the scaling ansatz (11).

The behavior of the scaling function (13) for $d = 2$ is well known in the literature. Here we wish to check its dependence upon the dimensionality. We are primarily interested in the behavior of the amplitude $g_d(0)$ of the free energy at the quantum critical point, as this is tightly related to the "Casimir effect in time". For the particular case $d = 2$, it can be computed analytically resulting in

$$ g_2(0) = -\frac{2\zeta(3)}{5\pi}, \quad (14) $$

For arbitrary $d$ the behavior of $g_d(0)$ can be obtained by numerical means. This is graphed in FIG. 2. It is found that the scaling function has a maximum at $d = 2.9144$. We check our numerical results in the vicinity of $d = 3$, using an $\varepsilon = 3 - d$ expansion, taking into account the small $\varepsilon$ behavior of $\alpha_{3-\varepsilon}$, to get

$$ g_{3-\varepsilon}(0) = -\frac{\pi^2}{90} + \left[ \frac{\pi^2}{360} (7 - 2\gamma - 2 \ln \pi) + \frac{\zeta'(4)}{\pi^2} \right] \varepsilon - \frac{\pi^2}{9\sqrt{6}} \varepsilon^{3/2} + o(\varepsilon^{3/2}), \quad (15) $$

where $\gamma = 0.5772$ is the Euler–Mascheroni constant. Indeed, expression (15) exhibits a maximum at $d = 2.9818$. This maximum is shifted compared to the one obtained by numerical means due to the used approximation for $\varepsilon$.

At the borderlines $d \to 1^-$ and $d \to 3^+$, the values of $g_d(0)$ coincide with their counterparts of the Gaussian theory corresponding to $\alpha_d = 0$ i.e.

$$ g_{d}^{\text{Gauss.}}(0) = -\pi^{-(d+1)/2} \Gamma \left( -\frac{d+1}{2} \right) \zeta(d+1) $$

This can be seen in the inset of FIG. 2, where we present the behavior of

$$ \rho = g_d(0)/g_d^{\text{Gauss.}}(0). \quad (16) $$

which is related to the Zamolodchikov $C$-function extended to arbitrary dimensions and nonzero temperature (see Ref. 5 and references therein). Here, we would like to point out the similarity between the behavior of $\rho$ in FIG. 2 and the one obtained in Ref. 12 for the characteristic parameter of the corresponding conformal field theory in dimensions $2 < d < 4$.

Let us note, before closing this comment, that the gap equation [Eq. (3)] with l.h.s. equals zero is equivalent to the spherical constraint imposed on the quantum spherical model, see Refs. 8,9,13 where the finite-temperature scaling was studied in great details.
FIG. 2: The behavior of the Casimir amplitude $g_d(0)$ from Eq. (13). In the inset we graph the ratio $\rho$ defined in Eq. (16).

The consideration outlined in this comment remains valid also for systems with film geometry under periodic boundary conditions with temperature driven phase transition. This is due to the fact that the thickness of films is in some sense equivalent to the inverse temperature in a quantum system. This is a facet of the property known as temperature inversion symmetry discussed in the literature that leads to explicit conversion from Casimir force to Planck’s law of radiation.\textsuperscript{14,15} Very recently, in Refs. \textsuperscript{16} and \textsuperscript{17} using the $\varepsilon$ expansion and/or the limit $N \to \infty$ in the framework of the classical $O(N)$ symmetric $\varphi^4$ model with film geometry one obtains results for the amplitude of the correlation length and quantities related to the Casimir effect in a close vicinity of the upper critical dimension that can be conversed to the field of quantum paraelectric-ferroelectric phase transitions in particular and to quantum critical phenomena in general.

This work was supported by the Bulgarian Fund for Scientific Research Grant No. F-1517 (H.C.) and Grant No. BYX-308/2007 (N.T.).

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1. L. Pálová, P. Chandra, and P. Coleman, Phys. Rev. B \textbf{79}, 075101 (2009).
2. S. Sachdev, \textit{Quantum Phase Transitions} (Cambridge University Press, Cambridge, England, 1999).
3. M. Moshe and J. Zinn–Justin, Phys. Rep. \textbf{385}, 69 (2003).
4. V. Privman, ed., \textit{Finite size scaling and numerical simulations of statistical systems} (World Scientific, Singapore, 1990).
5. J. G. Brankov, D. M. Danchev, and N. S. Tonchev, \textit{The Theory of Critical Phenomena in Finite–Size Systems: Scaling and Quantum Effects}, vol. 9 of Series in Modern Condensed Matter Physics (World Scientific, Singapore, 2000).
6. S. Sachdev, Phys. Rev. B \textbf{55}, 142 (1997).
7. H. Chamati and N. S. Tonchev, J. Phys. A: Math. Gen. \textbf{33}, 873 (2000).
8 H. Chamati, E. S. Pisanova, and N. S. Tonchev, Phys. Rev. B 57, 5798 (1998).
9 H. Chamati, D. M. Danchev, and N. S. Tonchev, Eur. Phys. J. B 14, 307 (2000).
10 V. Privman and M. E. Fisher, Phys. Rev. B 30, 322 (1984).
11 A. V. Chubukov, S. Sachdev, and J. Ye, Phys. Rev. B 49, 11919 (1994).
12 A. C. Petkou and N. D. Vlachos, arXiv:hep-th/9809096 (1998).
13 M. H. Oliveira, E. P. Raposo, and M. D. Coutinho-Filho, Phys. Rev. B 74, 184101 (2006).
14 F. Ravndal and D. Tollefsen, Phys. Rev. D 40, 4191 (1989).
15 K. Fukushima and K. Ohta, Physica A 299, 455 (2001).
16 D. Grüneberg and H. W. Diehl, Phys. Rev. B 77, 115409 (2008).
17 H. W. Diehl and H. Chamati, Phys. Rev. B 79, 104301 (2009).