
EFFECTIVE FREE ENERGY OF GINZBURG-LANDAU MODEL

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It is argued that the presence of a nonanalytic term in the effective potential of the Ginzburg-Landau model is immaterial as far as the order of the superconductor-normal phase transition is concerned. To achieve agreement with the renormalization group, the effective potential has to be extended to include derivative terms, providing the theory with a low momentum scale which can be varied to probe the (possible) fixed point.

1 Prelude

This paper is dedicated to Professor Kleinert on the occasion of his 60th birthday with special thanks for the exciting years I had the good fortune to be his *Wissenschaftlicher Assistent* at the Freie Universität Berlin. It is an implementation of one of the many neat ideas he shared with me over the years. This particular one he told me about four years ago in the late summer of 1996.

It is a common belief that the order of an equilibrium phase transition can be inferred from the form of the effective potential at criticality. For example, the presence of a cubic term in the order parameter is taken as signalling a discontinuous transition, while the absence of such a term is taken as indicating a continuous transition. At the mean-field level, where fluctuations in the order parameter are ignored, this is certainly true [1]. However, the question about the order of a transition is settled in the full theory, and fluctuations may well change the mean-field result.

In a renormalization group (RG) approach, a continuous phase transition is associated with an infrared-stable fixed point in the space of coupling parameters characterizing the theory. Sufficiently close to the transition, such a fixed point acts as an attractor to which the couplings flow when one passes to larger length scales by integrating out field fluctuations of smaller length scales. When no infrared-stable fixed point is detected in this process, the transition is discontinuous.

It is important for our purposes to note that a fixed point is probed by changing a scale. For this, the effective potential evaluated at criticality in itself is inadequate as it lacks a scale. In this contribution we show that a scale can be introduced by extending the effective potential to include derivative terms. The resulting effective free energy contains the same information as that obtained in RG. Along the way we are able to implement Kleinert's idea of finding a fixed point without calculating flow functions first.

2 Cubic Term

To be concrete we consider the superconductor-normal phase transition described by the $O(n)$ Ginzburg-Landau model, which has been one of Kleinert's research topics for many years, and to which a large part of the first volume of his textbook [2] *Gauge Fields in Condensed Matter* is devoted. The model is specified by the free energy density (in the notation of statistical physics)

$$\mathcal{E} = |(\partial_\mu - ieA_\mu)\phi|^2 + m^2|\phi|^2 + \lambda|\phi|^4 + \frac{1}{4}F_{\mu\nu}^2 + \frac{1}{2\alpha}(\partial_\mu A_\mu)^2, \quad (1)$$

with a complex order parameter ϕ having an even number n of real field components:

$$\phi = \frac{1}{\sqrt{2}} \begin{pmatrix} \phi_1 + i\phi_2 \\ \vdots \\ \phi_{n-1} + i\phi_n \end{pmatrix}. \quad (2)$$

A conventional superconductor with Cooper pairing in the s-channel corresponds to $n = 2$. The parameters e and m are the electric charge and mass of the field, while λ is the coupling constant characterizing the 4th-order interaction term. We include a gauge-fixing term with parameter α , and $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ is the (magnetic) field strength. For convenience we will work in the gauge $\partial_\mu A_\mu = 0$, which is implemented by taking the limit $\alpha \rightarrow 0$. The mass term depends on the temperature T , and changes sign at the critical

temperature T_c . In the Ginzburg-Landau model, $m^2 = \xi_0^{-2}(T/T_c - 1)$, where ξ_0 is the length scale of fluctuations in the amplitude of the order parameter.

As a first step to investigate the effect of fluctuations on the mean-field picture, let us, following Halperin, Lubensky, and Ma [3], consider those in the vector field A_μ . Since (at least in the normal phase) the corresponding mode is gapless, it can have an important impact on the infrared behavior of the theory. The functional integral over A_μ is a simple Gaussian and leads to a contribution to the effective potential energy density in d dimensions

$$\mathcal{V}_{\text{eff}} = \frac{d-1}{2} \int \frac{d^d k}{(2\pi)^d} \ln(k^2 + 2e^2|\Phi|^2), \quad (3)$$

where we assume that the order parameter is a nonfluctuating background field denoted by Φ . In deriving this, we used that the combination

$$P_{\mu\nu}(k) = \delta_{\mu\nu} - \frac{k_\mu k_\nu}{k^2}, \quad (4)$$

which shows up in intermediate steps, is a projection operator satisfying $P^2 = P$, and that its trace gives the number of transverse components: $\text{tr } P = d-1$. The momentum integral is easily carried out using dimensional regularization, with the result

$$\mathcal{V}_{\text{eff}} = \frac{1}{(2\pi)^{d/2}} \frac{d-1}{d} \Gamma(1-d/2) e^d |\Phi|^d, \quad (5)$$

where $\Gamma(x)$ is the Gamma function. For $d = 3$, this leads to the cubic term in the effective potential mentioned in the introduction [3]. The 1-loop contribution is to be added to the mean-field potential $\mathcal{V}_0 = m|\Phi|^2 + \lambda|\Phi|^4$. It is often taken as indicating a discontinuous phase transition at a, what Kleiner [4] likes to call, precocious temperature T_1 above the mean-field critical temperature T_c ,

$$\frac{T_1}{T_c} = 1 + \frac{\xi_0^2}{18\pi^2} \frac{e^6}{\lambda}, \quad (6)$$

where the mass term is still positive, and the order parameter jumps from zero to the finite value $|\Phi|^2 = (1/18\pi^2)e^6/\lambda^2$ (see Fig. 1).

Since this result is obtained in perturbation theory, both e and λ are assumed to be small. This still leaves the ratio of the two, or the so-called Ginzburg-Landau parameter $\kappa_{\text{GL}}^2 = e^2/\lambda$, undetermined. This parameter separates type-II ($\kappa_{\text{GL}} > 1/\sqrt{2}$) superconductors, which have a Meissner phase where an applied magnetic field can penetrate the sample in the form

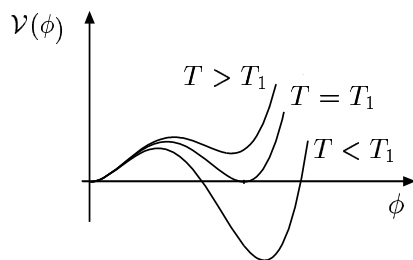


Figure 1. Sketch of the 1-loop effective potential.

of quantized flux tubes, and type-I ($\kappa_{GL} < 1/\sqrt{2}$) superconductors, for which these flux tubes, become unstable. Neglecting fluctuations in the order parameter, as is done here, is valid in the type-I regime, where κ_{GL} is small. (In the opposite limit of deep type-II superconductors where κ_{GL} is large, fluctuations in the vector field can be neglected instead.) This leads to the conclusion that type-I superconductors undergo a discontinuous phase transition [3]. It should, however, be noted that fluctuations in the order parameter produce also a cubic term in the effective potential at criticality, meaning that type-II superconductors, too, should undergo such a transition according to this argument.

As the result discussed in this section is independent of the number of field components, it should be valid for any n , including large numbers. This opens the possibility to check it using a $1/n$ expansion.

3 $1/n$ Expansion

The $1/n$ expansion can be used when the number n of field components is large, so that its inverse provides the theory with a small parameter. Contributions are then ordered not according to the number of loops, as in the loop expansion, but according to the number of factors $1/n$. The leading contribution in $1/n$ due to fluctuations in the vector field is obtained by dressing its correlation function with arbitrary many bubble insertions, and summing the entire set of Feynman diagrams [5]. The resulting series is a simple geometrical one, which leads to the following change in the correlation

function:

$$\frac{P_{\mu\nu}(k)}{k^2} \rightarrow \frac{P_{\mu\nu}(k)}{k^2 + bne^2 k^{d-2}}, \quad (7)$$

where $b = c/(d-1)$, with c the 1-loop integral

$$c(d) = \int \frac{d^d k}{(2\pi)^d} \frac{1}{k^2(k+q)^2} \Big|_{q^2=1} = \frac{\Gamma(2-d/2)\Gamma^2(d/2-1)}{(4\pi)^{d/2}\Gamma(d-2)}. \quad (8)$$

Below $d = 4$, the infrared behavior is now less singular. Instead of the effective potential (3), we now obtain

$$\mathcal{V}_{\text{eff}} = \frac{d-1}{2} \int \frac{d^d k}{(2\pi)^d} \ln(k^2 + be^2 k^{d-2} + 2e^2 |\Phi|^2). \quad (9)$$

For large fields, $|\Phi| > (be^{d-2})^{1/(4-d)}$, the main contribution to the integral comes from large momenta, where $k^2 + be^2 k^{d-4} \approx k^2$, so that in this limit we recover the result (5) obtained in the loop expansion: $\mathcal{V}_{\text{eff}} \propto |\Phi|^d$. In the limit of small fields, on the other hand, the main contribution comes from small momenta, where $k^2 + be^2 k^{d-4} \approx be^2 k^{d-4}$. We then find $\mathcal{V}_{\text{eff}} \propto |\Phi|^{2d}$ instead, implying that, in $d = 3$, the $1/n$ expansion no longer gives a cubic term in the effective potential. [This argument captures only those terms in the Taylor expansion of the logarithm in the effective potential (9) which diverge in the infrared. These are the important ones for our purposes as they can produce nonanalytic behavior. The first terms in the expansion may be infrared finite, depending on the dimensionality d , and have to be treated separately. But they always lead to analytic terms and are therefore of no concern to us here.]

The $1/n$ expansion calls into question the validity of the result obtained in the loop expansion as it corresponds to large field values. It is not clear that this is still in the realm of perturbation theory.

In the next section, we show that by extending the calculation of the effective potential to that of the effective free energy, which includes derivative terms, things become consistent and in agreement with RG.

4 Effective Free Energy

When computing the effective free energy, we not only consider fluctuations in the vector field, but also include those in the order parameter. To this end, we set

$$\phi(x) = \Phi(x) + \tilde{\phi}(x), \quad (10)$$

with $\Phi(x)$ being a nonfluctuating background field, and integrate out the fluctuating field $\tilde{\phi}(x)$. The main difference with the previous calculation of the effective potential is that the background field is no longer assumed to be constant, but can vary in space. Therefore, we also have to analyze the derivative terms in the effective theory.

Because of gauge invariance, the results will depend solely on the absolute value $|\Phi|$. Without loss of generality we can thus assume that the background field Φ has only one nonzero component, say the first one, $\Phi = (v, 0, \dots, 0)/\sqrt{2}$. For convenience we will work at criticality and set the mass parameter m to zero.

A straightforward calculation yields in the gauge $\partial_\mu A_\mu = 0$ the 1-loop effective free energy

$$F_{\text{eff}}[v] = \frac{1}{2} \text{Tr} \ln \left(1 + 3\lambda \frac{1}{p^2} v^2 \right) + \frac{n-2}{2} \text{Tr} \ln \left(1 + \lambda \frac{1}{p^2} v^2 \right) \quad (11)$$

$$+ \frac{1}{2} \text{Tr} \ln \left[\begin{pmatrix} 1 & 0 \\ 0 & \delta_{\mu\rho} \end{pmatrix} + \frac{1}{p^2} \begin{pmatrix} 1 & 0 \\ 0 & P_{\mu\nu}(p) \end{pmatrix} \begin{pmatrix} \lambda v^2 & e\partial_\nu v \\ e\partial_\rho v & e^2 v^2 \delta_{\nu\rho} \end{pmatrix} \right],$$

where we ignored an irrelevant constant. The trace Tr denotes the trace tr over discrete indices as well as the integration over momentum and space. More precisely,

$$\text{Tr} \ln[1 + K(x, p)] = \text{tr} \int d^d x \int \frac{d^d k}{(2\pi)^d} e^{-ik \cdot x} \ln[1 + K(x, p)] e^{ik \cdot x}, \quad (12)$$

with $p_\mu = -i\partial_\mu$ the derivative operating on everything to its right. Since the background field is space-dependent, the integrals in Eq. (11) cannot be evaluated in closed form, but only in a derivative expansion [6].

The first step in this scheme is to expand the logarithm in a Taylor series. Each term of the series contains powers of the derivative p_μ , which in the second step are shifted to the left using the identity

$$f(x)p_\mu g(x) = (p_\mu - i\partial_\mu)f(x)g(x), \quad (13)$$

where $f(x)$ and $g(x)$ are arbitrary functions. The symbol ∂_μ in the last term denotes the derivative which, in contrast to p_μ , operates *only* on the next object to its right. The next step is to repeatedly integrate by parts, until all p_μ derivatives operate to the left. They then simply produce factors of k_μ as only the function $\exp(-ik \cdot x)$ appears at the left. In shorthand, for an

arbitrary function $h(k)$, we have

$$\begin{aligned} \int \frac{d^d k}{(2\pi)^d} e^{-ik \cdot x} h(p) f(x) &= \int \frac{d^d k}{(2\pi)^d} e^{-ik \cdot x} h(-\bar{p}) f(x) \\ &= \int \frac{d^d k}{(2\pi)^d} e^{-ik \cdot x} h(k) f(x), \end{aligned} \quad (14)$$

ignoring total derivatives. In this way, all occurrences of the derivative operator p_μ are replaced with a mere integration variable k_μ . The function $\exp(ik \cdot x)$ at the right can now be moved to the left where it is annihilated by the function $\exp(-ik \cdot x)$. The momentum integration can then, in principle, be performed and the effective free energy takes the form of a spatial integral over a local density $F_{\text{eff}} = \int d^d x \mathcal{E}_{\text{eff}}$.

Applied to the formal expression (11), the derivative expansion yields the following quadratic terms in the effective free energy density:

$$\begin{aligned} \mathcal{E}_{\text{eff}}(|\Phi|) &= -e^4(d-1) \int \frac{d^d k}{(2\pi)^d} \frac{1}{k^2} \frac{1}{(k-i\partial)^2} |\partial_\mu \Phi|^2 \\ &\quad - (n+8)\lambda^2 \int \frac{d^d k}{(2\pi)^d} \frac{1}{k^2} \frac{1}{(k-i\partial)^2} |\Phi|^2 |\Phi|^2 \\ &\quad - e^2 \int \frac{d^d k}{(2\pi)^d} \frac{1}{k^2} P_{\mu\nu}(k) \frac{1}{(k-i\partial)^2} P_{\nu\mu}(k-i\partial) |\Phi|^2 |\Phi|^2. \end{aligned} \quad (15)$$

Assuming that the order parameter carries a momentum κ , we can replace all occurrences of the derivative $-i\partial_\mu$ with κ_μ .

It is important to note that infrared divergences are absent here, because κ_μ acts as an infrared cutoff. Without such a cutoff, as in the effective potential (3), the individual terms in the Taylor expansion cannot be integrated because of infrared divergences, and the entire series has to be summed, which can lead to nonanalytic contributions. From the perspective of RG, the presence of the momentum scale κ_μ is crucial as it allows studying the fixed point by letting that scale approach zero.

With the tree contribution $\mathcal{E}_{\text{tree}}$ added, we obtain after carrying out the integrals over the loop momentum

$$\begin{aligned} \mathcal{E}_{\text{tree}} + \mathcal{E}_{\text{eff}} &= [1 - c(d-1)\hat{e}^2] |\partial_\mu \Phi|^2 \\ &\quad + \left\{ \hat{\lambda} - c \left[(n+8)\hat{\lambda}^2 + d(d-1)\hat{e}^4 \right] \right\} \kappa^{4-d} |\Phi|^4, \end{aligned} \quad (16)$$

where $\hat{\lambda} = \lambda \kappa^{d-4}$ and $\hat{e}^2 = e^2 \kappa^{d-4}$ are the rescaled dimensionless coupling

constants. As an aside, by evaluating the integrals in fixed dimension $2 < d < 4$, and not in an ϵ expansion close to the upper critical dimension $d = 4$, we implement in effect Parisi's approach to critical phenomena [7]. The factor in front of the kinetic term in Eq. (16) amounts to a field renormalization. It can be absorbed by introducing the renormalized field $\Phi_r = Z_\phi^{-1/2} \Phi$, with Z_ϕ the field renormalization factor

$$Z_\phi = 1 + c(d-1)\hat{e}^2. \tag{17}$$

The effective free energy density then becomes

$$\mathcal{E}_{\text{tree}} + \mathcal{E}_{\text{eff}} = |\partial_\mu \Phi_r|^2 + \lambda_r |\Phi_r|^4, \tag{18}$$

where λ_r is the renormalized coupling

$$\frac{1}{\lambda} = \frac{1}{\lambda_r} - c \left[(n+8) - 2(d-1) \frac{\hat{e}_r^2}{\lambda_r} + \frac{1}{4} d(d-1) \frac{\hat{e}_r^4}{\lambda_r^2} \right]. \tag{19}$$

It was Kleinert's idea to put this equation in this form. The reason being that the critical point is approached by letting the momentum scale approach zero. Since the original coupling constant λ is fixed, the left side tends to zero when $\kappa \rightarrow 0$. The resulting quadratic equation then determines the value of $\hat{\lambda}_r$ at the critical point, provided we know the value of \hat{e}_r^2 there. This procedure is equivalent to finding the root of the flow equation for $\hat{\lambda}_r$ in conventional RG [8].

To obtain the value of \hat{e}_r^2 at criticality, we rescale the vector field $A_\mu \rightarrow A_\mu/e$ and consider it instead of the order parameter to be the background field. The 1-loop effective free energy, obtained after integrating out the scalar fields, reads:

$$F_{\text{eff}}[A] = \frac{n}{2} \text{Tr} \ln \left[1 + \frac{1}{p^2} (2p_\mu A_\mu - A_\mu^2) \right], \tag{20}$$

where we again ignored an irrelevant constant and used the gauge $\partial_\mu A_\mu = 0$. The second term in the expansion of the logarithm yields the first nonzero contribution

$$\mathcal{E}_{\text{eff}}(A) = n \int \frac{d^d k}{(2\pi)^d} \frac{k_\mu (k_\nu - i\partial_\nu)}{k^2 (k - i\partial)^2} A_\mu A_\nu. \tag{21}$$

If we assume that the vector field carries the same momentum κ_μ as does the order parameter, we obtain after carrying out the momentum integral for the

sum of the tree and the 1-loop contribution

$$\mathcal{E}_{\text{tree}} + \mathcal{E}_{\text{eff}} = -\frac{1}{2e_r^2} \partial^2 A_\mu A_\mu, \quad (22)$$

where e_r^2 is the renormalized coupling constant,

$$\frac{1}{\hat{e}_r^2} = \frac{1}{\hat{e}^2} + \frac{n}{2} \frac{c}{d-1}. \quad (23)$$

Keeping e fixed and letting $\kappa \rightarrow 0$ so as to approach the critical point, we see that the renormalized coupling tends to a constant value

$$\hat{e}_r^{*2} = \frac{2}{n} \frac{d-1}{c}. \quad (24)$$

When this constant is substituted in Eq. (19) with the left side set to zero, the resulting quadratic equation in $\hat{\lambda}_r$ has two real solutions

$$\hat{\lambda}_r^* = \frac{1}{2n(n+8)} \frac{1}{c} [n + 4(d-1)^2 \pm \Delta_d], \quad (25)$$

provided that the determinant

$$\Delta(d) := \sqrt{n^2 - 4(d-2)(d-1)^2(d+1)n - 16(d-1)^3(d+1)} \quad (26)$$

is real. For fixed dimensionality, this condition is satisfied only for a sufficient number of field components n . Specifically, the minimum number in $d = 2, 3$, and 4 is $n_c(2) = 4\sqrt{3} \approx 6.9$, $n_c(3) = 16(2 + \sqrt{6}) \approx 71.2$, and $n_c(4) = 12(15 + 4\sqrt{15}) \approx 365.9$. The plus sign in Eq. (25) corresponds to the infrared-stable fixed point, while the minus sign corresponds to the tricritical point, where the continuous phase transition changes to a discontinuous one. For a fixed number of field components n , this 1-loop result shows that continuous behavior is favored when $d \rightarrow 2$, while in the opposite limit, $d \rightarrow 4$, discontinuous behavior is favored.

5 Conclusions

For a conventional 3-dimensional superconductor corresponding to $n = 2$, the 1-loop result fails to give an infrared-stable fixed point. It should, however, be kept in mind that there are infinitely many loop diagrams, and that the values of the coupling constants at criticality are not particular small to justify low-order perturbation theory. For example, $\hat{e}_r^{*2} = 32/n$ according to Eq. (24)

with $d = 3$, which only for large n is small. Different approaches are therefore required to investigate the presence of a fixed point.

One of these is the dual approach [2,9,10], which is a formulation in terms of magnetic vortex loops. Monte Carlo simulations of the dual model led to the conclusion that 3-dimensional type-II superconductors undergo a continuous phase transition belonging to the XY universality class with an inverted temperature axis [11]. Using this approach, Kleinert [12] predicted the presence of a tricritical point at a value of the Ginzburg-Landau parameter $\kappa_{\text{tri}} \approx 0.8/\sqrt{2}$.

Another approach within the framework of the Ginzburg-Landau model itself was put forward in Ref. [13], where – in our language – the vector field was assumed to carry not the same momentum κ_μ as the order parameter, but κ_μ/x instead. The charged fixed points for $n = 2$ and $d = 3$ are then located at $\hat{e}_r^{*2} = 16/x$ which becomes small for large x , facilitating the existence of an infrared-stable fixed point. The free parameter x was determined by matching κ_{tri} with Kleinert's estimate or Monte Carlo simulations [14] which gave $\kappa_{\text{tri}} \approx 0.42/\sqrt{2}$. From Eqs. (24) and (25) one obtains, with the parameter x included [15],

$$\kappa_{\text{tri}}^2 = (8 + x + \sqrt{x^2 + 16x - 176})/40. \quad (27)$$

The resulting values for the critical exponents are consistent with the expected (inverted) XY universality class.

Also resummation techniques applied to results obtained to second order in the loop expansion [16] predict the existence of an infrared-stable fixed point in the Ginzburg-Landau model [17].

In conclusion, by extending the effective potential to include derivative terms, we achieved agreement with RG as they provide the theory with a low momentum scale which can be varied to probe the fixed point. The presence of a nonanalytic term in the effective potential at criticality is argued to be immaterial as far as the order of the phase transition is concerned.

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References

- [1] L.D. Landau and E.M. Lifshitz, *Statistical Physics*, Part 1 (Pergamon, New York, 1986).
- [2] H. Kleinert, *Gauge Fields in Condensed Matter*, Vol. I: *Superflow and Vortex Lines* (World Scientific, Singapore, 1989).
- [3] B.I. Halperin, T.C. Lubensky, and S.-K. Ma, *Phys. Rev. Lett.* **32**, 292 (1974).
- [4] H. Kleinert, *Phys. Lett. B* **128**, 69 (1983).
- [5] T. Appelquist and U. Heinz, *Phys. Rev. D* **25**, 2620 (1982).
- [6] C.M. Fraser, *Z. Phys. C* **28**, 101 (1985).
- [7] G. Parisi, Lectures presented at the Cargèse Summer School 1973 (unpublished); *J. Stat. Phys.* **23**, 23 (1980).
- [8] A.M.J. Schakel, *Boulevard of Broken Symmetries*, Habilitationsschrift, Freie Universität Berlin, eprint: cond-mat/9805152.
- [9] T. Banks, B. Meyerson, and J.B. Kogut, *Nucl. Phys. B* **129**, 493 (1977); M.E. Peskin, *Ann. Phys. (N.Y.)* **113**, 122 (1978); P.R. Thomas and M. Stone, *Nucl. Phys. B* **144**, 513 (1978).
- [10] M. Kiometzis and A.M.J. Schakel, *Int. J. Mod. Phys. B* **7**, 4271 (1993); M. Kiometzis, H. Kleinert, and A.M.J. Schakel, *Phys. Rev. Lett.* **73**, 1975 (1994); *Fortschr. Phys.* **43**, 697 (1995).
- [11] C. Dasgupta and B.I. Halperin, *Phys. Rev. Lett.* **47**, 1556 (1981).
- [12] H. Kleinert, *Lett. Nuovo Cim.* **35**, 405 (1982).
- [13] I.F. Herbut and Z. Tešanović, *Phys. Rev. Lett.* **76**, 4588 (1996).
- [14] J. Bartholomew, *Phys. Rev. B* **28**, 5378 (1983).
- [15] C. de Calan, A.P.C. Malbouisson, F.S. Nogueira, and N.F. Svaiter, *Phys. Rev. B* **59**, 554 (1999).
- [16] J. Tessmann, Diplomarbeit, Freie Universität Berlin (1984); S. Kolnberger and R. Folk, *Phys. Rev. B* **41**, 4083 (1990).
- [17] R. Folk and Yu. Holovatch, *J. Phys. A* **29**, 3409 (1996).