Z. Phys. B – Condensed Matter 73, 271–275 (1988)

Condensed Matter
Zeitschrift für Physik B

Mean relaxation time approximation for dynamical correlation functions in stochastic systems near instabilities

III. The mean field n-vector model

W. Nadler
Arthur Amos Noyes Laboratory of Chemical Physics,*
California Institute of Technology, Pasadena, California, USA

Received June 20, 1988

The linewidth factor of the order parameter autocorrelation function for the mean field n-vector Ginzburg-Landau model is determined numerically for $n>2$. This generalizes results for the single mode laser ($n=2$) obtained in Part II [Nadler, W., Schulten, K.: Z. Phys. B – Condensed Matter].

The time-dependent mean field n-vector Ginzburg-Landau model for phase transitions, given by the Langevin equation.

$$\dot{\boldsymbol{\varphi}}(t)=a\boldsymbol{\varphi}(t)-\varphi(t)^2\boldsymbol{\varphi}(t)+\boldsymbol{\zeta}(t), \tag{1}$$

with $\varphi(t)^2=|\boldsymbol{\varphi}(t)|^2$, the fluctuating forces $\boldsymbol{\zeta}(t)$ being Gaussian with white spectrum

$$\langle\zeta_i(t)\,\zeta_j(t')\rangle=2\delta_{ij}\,\delta(t-t'), \tag{2}$$

describes the fluctuations of an n-component order parameter $\boldsymbol{\varphi}(t)=(\varphi_i(t);\ i=1,\ldots,n)$. Equations (1) and (2) are the zero-dimensional version of the general time-dependent Ginzburg-Landau model [1], and provide its leading order description (in a system size expansion) for dimension $d>4$ [2]. For values of the control parameter $a<0$ the equilibrium distribution of $\boldsymbol{\varphi}$ is peaked around zero. For $a>0$ this symmetry is broken, and the distribution of order parameters is peaked around nonzero values for $|\boldsymbol{\varphi}|$. In this regime the dominant slow fluctuations of the order parameter are angular fluctuations of the $\boldsymbol{\varphi}$ for $n>1$, whereas barrier crossing processes are the dominant slow fluctuations for $n=1$. Apart from being a generic description of phase transitions, the above model has also some particular physical realizations for different values of n. For example, the case $n=1$ also describes diffusion in a one-dimensional bistable potential, a model of interest in chemical reaction kinetics [3, 4]. The case $n=2$ also describes the fluctuations of the field amplitude in the single mode laser [3, 4], whereas the case $n=4$ describes those fluctuations in the polarization symmetric two-mode laser [5].

A quantity of particular interest for the above model is its autocorrelation function

$$C(t)=\langle\boldsymbol{\varphi}(t)\cdot\boldsymbol{\varphi}(0)\rangle. \tag{3}$$

The time scale of the relaxation of $C(t)$ is given by its *mean relaxation time*

$$\tau=\int_0^\infty \mathrm{d}t\, C(t)/C(0), \tag{4}$$

or, equivalently, by the linewidth factor

$$\alpha=C(0)/\tau. \tag{5}$$

Equation (4) gives rise to a single-exponential approximation

$$C(t)\approx C(0)\,\mathrm{e}^{-t/\tau} \tag{6}$$

for the correlation function (3), the *mean relaxation time approximation.* This approximation is, in a sense, the best single-exponential description of $C(t)$, since it provides an interpolation between the correct short-time (high-frequency) behavior and the correct long-time (low-frequency) behavior [6, 7]. In Parts I and II [6, 7] this approximation was determined for various stochastic models exhibiting phase transition-like

* Contribution No. 7796

instabilities, among them the cases $n=1$ and $n=2$ of the above model. In this communication the results for the mean relaxation time τ, or, equivalently, the linewidth factor α, obtained in Parts I and II are generalized to the case $n>2$. This paper concludes the series of papers [6, 7] on applications of the mean relaxation time approximation.

I will review briefly the previous work on the dynamics of the above model. For $n=1$ Dekker and van Kampen [8] have determined numerically the lowest eigenvalues for the Fokker-Planck operator equivalent to the Langevin Eq. (1) and (2). Bernstein and Brown [9] have used an analytical variational approximation for the lowest eigenvalue, based on the supersymmetry of the Fokker-Planck equation. Note here that the mean relaxation time τ is related to the (nonzero) eigenvalues $-\lambda_n$ of the Fokker-Planck operator via [6]

$$\tau=\sum_{n=1}^{\infty} c_n \lambda_n^{-1}, \tag{7}$$

where the c_n are the (positive) expansion coefficients of the autocorrelation function $C(t)$ in a spectral expansion. The sum in (7) is often dominated by the contributions due to the lowest eigenvalue. For the single-mode laser equivalent case, $n=2$, Risken [4, 10] has determined the lowest eigenvalue of the Fokker-Planck operator numerically. Grossmann [11] has determined an analytical approximation for the linewidth factor based on a mode-coupling approximation. For $n=4$, the polarization symmetric two-mode laser, Grossmann and Krauth [5] have determined an analytical approximation based on a second order continued fraction expansion. The case of general n was treated by Ziegler and Horner [12], employing a perturbation expansion approach. They derive selfconsistently an approximate expression for the linewidth factor α, using a partial summation of the perturbation expansion (corresponding to a random phase approximation) which is equivalent to an $1/n$ expansion. I will compare particularly their analytical result, which has the form

$$\alpha_{zH}=n-\frac{1}{\left(1+\frac{n}{\langle\varphi^2\rangle^2}\right)\left(1+\frac{3n}{2\langle\varphi^2\rangle^2}\right)} \tag{8}$$

in my notation, with my calculations. I would like to note that for the case $n=4$ the result of (8) is numerically almost indistinguishable from Grossmann and Krauth's [5] approximation.

A description equivalent to the Langevin Eq. (1) and (2) is provided by the Fokker-Planck equation

$$\frac{\partial}{\partial t} P(\boldsymbol{\varphi}, t)=\mathbf{L}(\boldsymbol{\varphi})\, P(\boldsymbol{\varphi}, t) \tag{9}$$

for the probability distribution $P(\boldsymbol{\varphi}, t)$, with the Fokker-Planck operator $\mathbf{L}(\boldsymbol{\varphi})$ given by

$$\mathbf{L}(\boldsymbol{\varphi})=\nabla_{\boldsymbol{\varphi}}\cdot\{\nabla_{\boldsymbol{\varphi}}+[\nabla_{\boldsymbol{\varphi}} U(\boldsymbol{\varphi})]\}. \tag{10}$$

$\nabla_{\boldsymbol{\varphi}}$ is the gradient with respect to $\boldsymbol{\varphi}$, and the potential $U(\boldsymbol{\varphi})$ is given by

$$U(\boldsymbol{\varphi})=U(\varphi)=-\tfrac{1}{2}a\varphi^2+\tfrac{1}{4}\varphi^4, \tag{11}$$

with $\varphi^2=|\boldsymbol{\varphi}|^2$ as before. The stationary distribution of (9) is the Boltzmann distribution

$$p_0(\boldsymbol{\varphi})\propto\exp[-U(\boldsymbol{\varphi})]. \tag{12}$$

Using the adjoint Fokker-Planck operator

$$\mathbf{L}^+(\boldsymbol{\varphi})=\{\nabla_{\boldsymbol{\varphi}}-[\nabla_{\boldsymbol{\varphi}} U(\boldsymbol{\varphi})]\}\cdot\nabla_{\boldsymbol{\varphi}}, \tag{13}$$

the mean relaxation time can be written in terms of a matrix element of its inverse [6, 7],

$$\tau=-\langle\boldsymbol{\varphi}[\mathbf{L}^+(\boldsymbol{\varphi})]^{-1}\boldsymbol{\varphi}\rangle/\langle\varphi^2\rangle, \tag{14}$$

where $\langle\ \rangle$ denotes the average with respect to $p_0(\boldsymbol{\varphi})$ and has the properties of an inner product on the space of functions. The identity $C(0)=\langle\varphi^2\rangle$ was employed in (14).

For the case $n=1$ it was shown in Part I, using results of [13], that the matrix element in (14) can be determined analytically in terms of an integral expression. This result is reproduced, for completeness, in the Appendix of the present paper. In order to determine the matrix element in (14) for $n>1$ an auxiliary vector function $\boldsymbol{\mu}_{-1}(\boldsymbol{\varphi})$ is defined through

$$\boldsymbol{\mu}_{-1}(\boldsymbol{\varphi})=-[\mathbf{L}^+(\boldsymbol{\varphi})]^{-1}\boldsymbol{\varphi}. \tag{15}$$

$\boldsymbol{\mu}_{-1}(\boldsymbol{\varphi})$ is, in effect, the right hand side function in the scalar product that contributes to the matrix ele-

ment. This auxiliary function can be determined as the solution of the equation

$$\mathbf{L}^{+}(\boldsymbol{\varphi})\,\boldsymbol{\mu}_{-1}(\boldsymbol{\varphi}) = -\boldsymbol{\varphi} \tag{16}$$

with reflective boundary conditions [13, 14]. In order to solve (16) I make the ansatz

$$\boldsymbol{\mu}_{-1}(\boldsymbol{\varphi}) = \mu_{-1}(\varphi)\begin{pmatrix}\varphi_1/\varphi\\ \vdots\\ \varphi_n/\varphi\end{pmatrix}. \tag{17}$$

This ansatz leads to the one-dimensional equation

$$\left[\mathbf{L}_0^{+}(\varphi) - \frac{n-1}{\varphi^2}\right]\mu_{-1}(\varphi) = -\varphi \tag{18}$$

for the radial part $\mu_{-1}(\varphi)$. The radial part $\mathbf{L}_0^{+}(\varphi)$ of the adjoint Fokker-Planck operator can be written as

$$\mathbf{L}_0^{+}(\varphi) = \frac{1}{\varphi^{n-1}p_0(\varphi)}\frac{\mathrm{d}}{\mathrm{d}\varphi}\varphi^{n-1}p_0(\varphi)\frac{\mathrm{d}}{\mathrm{d}\varphi}. \tag{19}$$

Equation (18) has to be supplemented with reflective boundary conditions for $\varphi = 0$ and $\varphi \to \infty$, see [13, 14]. The differential equation (18) can be solved very easily numerically by discretizing the one-dimensional state space for φ, employing the methods of [14]. In this discretization scheme the singular nature of the reactive term $\propto 1/\varphi^2$ gives no problems since the singularity lies on the (lower) boundary of the state space. The resulting linear equation is of tridiagonal form and can, therefore, be solved directly using the Gaussian elimination scheme [15]. In an actual calculation one has to introduce an upper limit for the state space, and the independence of the numerical results from this upper limit, as well as from the actual value of the discretization length, has to be checked. The matrix element is finally determined from the auxiliary function $\mu_{-1}(\varphi)$ through

$$-\langle\varphi[\mathbf{L}^{+}(\varphi)]^{-1}\varphi\rangle = \int_0^\infty \mu_{-1}(\varphi)\,p_0(\varphi)\,\varphi^n\,\mathrm{d}\varphi, \tag{20}$$

where $p_0(\varphi)$ is considered to be normalized so that $\int_0^\infty p_0(\varphi)\,\varphi^{n-1}\,\mathrm{d}\varphi = 1$.

The case $n=2$ was analyzed using the above algorithm already in Part II [7], and the reader is referred to that reference. For the cases $n=3$, $n=4$, and $n=10$, the results for the linewidth factor, (5), are shown in Fig. 1. The presented data are the first numerically exact results for the linewidth factor for $n>2$. α interpolates in a sigmoidal curve between $\alpha=n$ for $a\ll 0$, and $\alpha=n-1$ for $a\gg 0$. This corresponds to the "freezing out" of the radial degree of freedom by the phase transition. In Fig. 1 the exact results are also compared with the approximation of Ziegler and Horner, (8). As it is to be expected from the derivation of (8), an $1/n$ expansion, the approximation becomes increasingly better for increasing values of n. For $n=4$ the maximal relative error of α_{ZH} is $<1\%$, and becomes about 10^{-3} for $n=10$.

According to (7) the linewidth factor can be given alternatively by an expansion in the eigenvalues of the Fokker-Planck operator. As was demonstrated in Part II, for $n=2$ the linewidth factor is dominated by the contribution of the lowest nonzero eigenvalue, but in the transition regime and for $a>0$ other eigenvalues also contribute. A relatively simple way to evaluate qualitatively the contribution of higher eigenvalues is the *long-time relaxation time*

$$\tau' = \frac{\int_0^\infty \mathrm{d}t\,t\,C(t)/C(0)}{\int_0^\infty \mathrm{d}t\,C(t)/C(0)} = -\frac{\langle\boldsymbol{\varphi}[\mathbf{L}^{+}(\boldsymbol{\varphi})]^{-2}\boldsymbol{\varphi}\rangle}{\langle\boldsymbol{\varphi}[\mathbf{L}^{+}(\boldsymbol{\varphi})]^{-1}\boldsymbol{\varphi}\rangle}. \tag{21}$$

For a single-exponential behavior of $C(t)$ the relaxation times τ and τ' are equal, whereas they will differ in case $C(t)$ shows contributions from several eigenvalues. Note that $\tau' \geqq \tau$ holds. τ' is easily calculated from the auxiliary function $\mu_{-1}(\varphi)$ using (20) and

$$\langle\varphi[\mathbf{L}^{+}(\varphi)]^{-2}\varphi\rangle = \int_0^\infty [\mu_{-1}(\varphi)]^2\,p_0(\varphi)\,\varphi^{n-1}\,\mathrm{d}\varphi. \tag{22}$$

In Fig. 2 the ratio τ/τ' is shown for various values of n. Although small ($<3\%$), the deviation of $C(t)$ from a single-exponential behavior is strongest around $a=3$. Figure 2 also demonstrates that for the increasing n the relaxation of $C(t)$ is increasingly dominated by one single eigenvalue.

To summarize, I have presented here the first numerically exact results for the linewidth factor in the time-dependent mean field n-vector model for $n>2$. The results show that the approximation by Ziegler and Horner [12], Eq. (8), can be employed with sufficient accuracy ($<1\%$ error) for $n>3$.

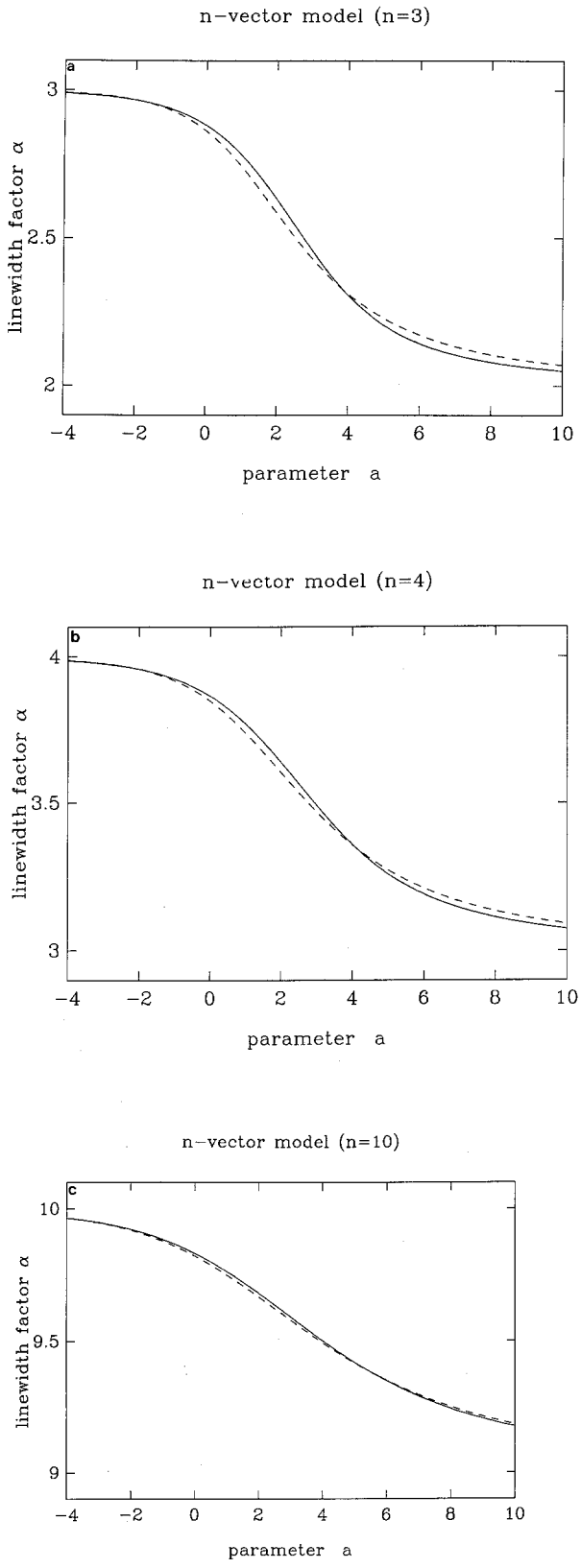

Fig. 1a–c. Linewidth factor α vs. control parameter a for (top) $n=3$, (middle) $n=4$, and (bottom) $n=10$; (solid line) is our result from a numerical solution of (19) and (20); (dashed) is the result of Ziegler and Horner's analytical approximation [12], (8)

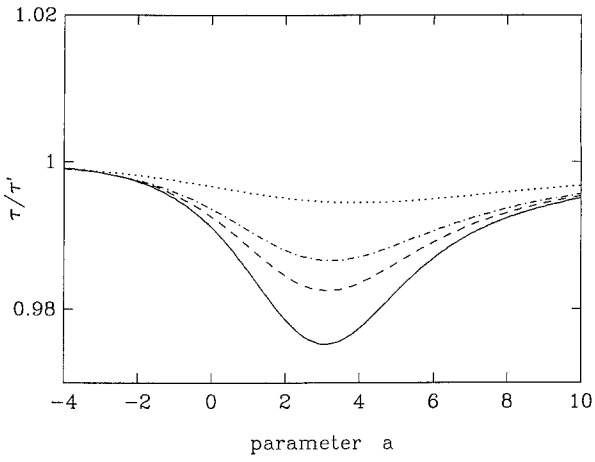

Fig. 2. Ratio of relaxation times τ, (14), and τ', (21), vs. control parameter a. (solid line) $n=2$, (dashed) $n=3$, (dashed-dotted) $n=4$, (dotted) $n=10$

This work has been supported by a grant from the National Science Foundation. The author is pleased to acknowledge also Prof. R.A. Marcus for his support.

Appendix

For the case $n=1$ the matrix element in (14) is given analytically by the integral expression [6]

$$-\langle\varphi[\mathbf{L}^{+}(\varphi)]^{-1}\varphi\rangle = 2\int_0^\infty \exp[U(x)]\,I(x)\,dx \Big/ \int_0^\infty \exp[-U(x)]\,dx, \quad \text{(A1)}$$

where $I(x)$ is

$$I(x)=\left|\int_x^\infty y\exp[-U(y)]\,dy\right|^2, \quad \text{(A2)}$$

with the potential $U(x)$ given by (11). In Part I it was demonstrated that the resulting mean relaxation time is numerically very close to the inverse of the lowest nonzero eigenvalue of the Fokker-Planck operator which was determined numerically by Dekker and van Kampen [8]. For a zero value of the control parameter a the integrals in (A1) and (A2) can be evaluated analytically (see Part I) and give for the linewidth factor α the result

$$\alpha(a=0)=\frac{1}{\sqrt{2}}\left(\frac{\Gamma(3/4)}{\Gamma(5/4)}\right)^2\frac{1}{\pi-\ln\left(\frac{2+\sqrt{2}}{2-\sqrt{2}}\right)}. \quad \text{(A3)}$$

For other values of a (A 1) and (A 2) have to be evaluated numerically [15]. However, as it was demonstrated in Part I, for values of $a > 2$ the approximation

$$\alpha_K = \frac{1}{\pi} \frac{a}{\sqrt{2}} \exp(-a^2/4) \langle \varphi^2 \rangle, \tag{A 4}$$

based on the Kramers rate for barrier crossing [3, 4], is a very good numerical description of the line-with factor. Note that $\langle \varphi^2 \rangle \approx a$ holds in this regime (which is also true asymptotically for all values of n). Ziegler and Horner's approximation, (8), fails to describe correctly the slowing down due to the barrier crossing processes. Their leading order contribution for large values of a is

$$\alpha_{ZH} \approx \frac{5}{2} \langle \varphi^2 \rangle^{-2} \approx \frac{5}{2a^2}, \tag{A 5}$$

and does not give the correct exponential slowing down, see (A 4). This failure of α_{ZH} for $n = 1$ is to be expected, since (8) was based on an $1/n$ expansion, and for $n = 1$ the character of the slow fluctuations is qualitatively different from $n > 1$.

References

1. Hohenberg, P.C., Halperin, B.I.: Rev. Mod. Phys. **49**, 435 (1977)
2. Diehl, H.W.: Z. Phys. B – Condensed Matter **66**, 211 (1987)
3. van Kampen, N.G.: Stochastic processes in physics and chemistry. Amsterdam: North-Holland 1981
4. Risken, H.: The Fokker-Planck equation. Berlin, Heidelberg, New York: Springer 1984
5. Grossmann, S., Krauth, W.: Phys. Rev. A **35**, 2523 (1987). There is a typographical error in (31) of this paper: the expression under the square root should read $1 + 16(a_3/\langle I \rangle)/(b_3/a_3 + \lambda_u^{(0)})^2$. I thank Prof. Grossmann for correspondence clarifying this point
6. Nadler, W., Schulten, K.: Z. Phys. B – Condensed Matter **59**, 53 (1985)
7. Nadler, W., Schulten, K.: Z. Phys. B – Condensed Matter **72**, 535 (1988)
8. Dekker, H., van Kampen, N.G.: Phys. Lett. **73** A, 374 (1979)
9. Bernstein, M., Brown, L.S.: Phys. Rev. Lett. **52**, 1933 (1984)
10. Risken, H.: Z. Phys. **191**, 302 (1966)
11. Grossmann, S.: Phys. Rev. A **17**, 1123 (1978)
12. Ziegler, K., Horner, H.: Z. Phys. B – Condensed Matter **37**, 339 (1980); note that this paper also discusses the problems arising from an inappropriate renormalization of the perturbation expansion
13. Nadler, W., Schulten, K.: J. Chem. Phys. **82**, 151 (1985)
14. Nadler, W., Schulten, K.: J. Chem. Phys. **84**, 4015 (1986)
15. Press, W.H., Flannery, B.P., Teukolsky, S.A., Vetterling, W.T.: Numerical recipes. Cambridge: Cambridge Universtiy Press 1986

Walter Nadler
Arthur Amos Noyes Laboratory of Chemical Physics
California Institute of Technology
Pasadena, CA 91125
USA