BROWNIAN MOTION OF SOLITONS IN THE $\Phi^4$ MODEL

F. ALDABE

International Center for Theoretical Physics
P.O. Box 586, 34100 Trieste, Italy

January 9, 2022

ABSTRACT

We derive an expression for the correlation function of the random force on a soliton which is consistent with the constraints needed to integrate out the zero modes which appear due to the broken translational symmetry of the soliton solution. It is shown that when the constraint does not commute with the operator which defines the correlation function, i.e. when the operator is not physical, only low frequency phonons contributions may be considered. On the contrary, when the correlation function of the random force on the soliton is constructed with physical operators one may also include in a correct manner the contributions from the optical phonons.

\footnote{E-mail: aldabe@ictp.trieste.it}
1 Introduction

Although the $\phi^4$ is not an adequate model to describe solitons and their motion in polyacetylene because it does not include retardation effects, it is a model simple enough to make possible the study of soliton diffusion [1]. In this model, the soliton is taken as the classical solution of a non-linear differential equation. This solution is stable because it is possible to define a topological charge which commutes to leading order with the Hamiltonian describing the soliton. It is then impossible to deform the soliton solution to a trivial solution in a continuous manner. The quantum fluctuations about the soliton are then the phonons of the model. Since the Hamiltonian is non-linear, there are interactions between the soliton and the phonons.

One may then consider how these phonons give rise to a Brownian motion of the soliton. The observable which measures how the Brownian motion takes place is the diffusion operator. The diffusion operator has a diffusion constant which is proportional to the square of the phonon number. Thus, at zero temperature we expect the soliton to undergo a mild Brownian motion due to quantum effects. As temperature increases, soft frequency phonons will contribute to the diffusion of the soliton. As temperature increases even more, optical phonons will come into the picture and contribute to the Brownian motion of the soliton. Thus, in order to describe soliton diffusion at high temperature in a correct manner it is necessary to take into account the contribution of optical phonons. Experimental values of the extension of the soliton are of the order of the wavelength of optical phonons. It is thus important that the information of the profile of the soliton entering the correlation function for the random force be in agreement with that of the classical solution.

The problem of soliton diffusion has been studied in [4], were used was made of the formalism presented in [3] to calculate the contribution to the diffusion of the soliton due to phonons. However, the analysis done in [4] does not take into account in a proper manner the shape of the soliton. Thus, the contribution from the optical
phonons to the correlation function used in [4] is incorrect. This follows from the
analysis done below were we show that the correlation function as defined by Mori [4]
is constructed from an unphysical operator. This operator is not physical in soliton
models because these systems have zero modes associated to the loss of translational
invariance of the classical solution. In order to integrate out this zero mode and obtain
a theory free of infrared singularities we must introduce a collective coordinate. In
doing so we enlarge the phase space, and to recover the physical theory we must make
use of a constraint which appear in the definition of the collective momentum. That
is, the collective momentum is not the time derivative of the collective coordinate.
Rather, it is a function of the fluctuations and classical solution. This relation imposes
a constraint. And this constraint does not commute with the collective coordinate.
Thus, the collective coordinate is not physical. This can alternatively be understood
by looking at the original phase space. This space is embedded in a large space which
also contains the collective coordinate which was not present in the original theory.
Despite subtleties which involve certain transformations among the variables in the
enlarged phase space, the collective coordinate is an artificial operator which is not
physical.

The reason is that one cannot simply measure the position of the soliton. The best
one can do is to measure the energy density of the soliton. Thus, one can effectively
measure the classical soliton solution. Where the solution vanishes we define the
position of the soliton. In fact, if one expands the soliton solution in a Taylor series
in the collective coordinate, she or he will find that the leading term is nothing but
the collective coordinate. However, the soliton solution is not physical either. To be
physical one must add the fluctuations about the soliton. Thus, one must replace
the collective coordinates appearing in the correlation function of the random forces
which act on the soliton defined in [5] by the field appearing in the theory.

When such a replacement is made, we find that the information entering the
correlation function of the random forces acting on the soliton will contain all the
information of the soliton profile and not just the first term in the Taylor series in
the collective coordinate. Retaining only the first term is equivalent to assuming
that the energy density of the soliton is evenly distributed throughout the polymer.
Thus, low frequency phonons will not see the shape of the soliton but neither will
the optical phonons. While the soft phonon have wavelength much larger than the
measured extension of the soliton and thus do not effectively see the soliton, this is
not the case for optical phonons whose wavelength is of the order of the extension of
the energy density of the soliton. Thus by keeping only the first term in the Taylor
series, e.i. the collective coordinate, the contribution of the optical phonons to the
correlation function of the random forces acting on the soliton is incorrect. Only when
we retain the remaining terms in the expansion will the contribution of these phonons
be correct. Thus, conclusions regarding soliton diffusion at high temperatures using
the diffusion equation in [4] must be reconsidered and effects from optical phonons
recalculated.

2 The Model

We consider the propagation of a soliton in a box of length $L$. The Lagrangian is

$$L(\Phi, \Psi) = L(\Phi) + L(\Psi) + L_{int}$$

and it is invariant under translations. The first, second and third terms on the
r.h.s refer to the bosonic term, fermionic term and interaction term between them,
respectively. The fermions will not play a role in our discussion. We thus concentrate
on the bosonic sector. The Lagrangian for this sector reads

$$L = \int dx (\dot{\Phi}^2 - \Phi'^2 + \Phi^2 - \frac{1}{2\lambda^2} \Phi^4 - \frac{\lambda^2}{2})$$

The classical equation of motion for this system is

$$\ddot{\phi} - \phi'' + V_1(\phi) = 0.$$
where $V_n = \partial^n V / \partial \phi^n$. Static solutions to this equations can be classified according their translational invariance. For example, the constant solution

$$\phi_{co} = \lambda$$

(4)

has translational invariance, and vanishing topological charge. The Solution without translational invariance

$$\phi_c = \lambda \tanh \left( \frac{x}{\sqrt{2}} \right),$$

(5)

satisfies

$$\phi_c(x) \to \phi_c(x + X) \neq \phi(x).$$

(6)

The solution $\phi_c$ is stable since it has topological charge equal to one and cannot decay without changing this value.

The loss of translational invariance of the classical solutions lead to the appearance of zero modes in the spectrum of the fluctuations. The spectrum of the fluctuations $\hat{q}$ with

$$\Phi = \phi_c + \hat{q}.$$  

(7)

is obtained from the linearized equation of motion for the fluctuations

$$-\ddot{\hat{q}} + \hat{q}'' + V_2|\phi_c|\hat{q}^2 = 0.$$  

(8)

Expanding the fluctuations in normal modes

$$\hat{q} = \sum_n \frac{i}{\sqrt{2\omega_n}}(\psi_n a_n^+ + h.c.),$$

(9)

we see that among the solutions $\psi_n$ to (8) there is a normalized solution

$$\psi_1 = \frac{\phi'_c}{\sqrt{M}}$$

(10)

where $M$ is the mass of the soliton. The eigenfrequency of this solution is $\omega_1 = 0$. This is the zero mode. In doing a perturbative treatment of an observable we will
encounter infrared divergences coming from the contributions of this zero mode. In order to integrate out these zero modes and obtain an infrared divergent free theory we must make use of collective coordinates.

The solutions $\psi_n$ to the equation (8) satisfy

$$\delta(x - y) = \sum_n \psi_n(x)\psi_n^*(y) \quad (11)$$

$$\int \psi_n\psi_m^* = \delta_{nm} \quad (12)$$

With the help of these relations we can write the quadratic Hamiltonian in the form

$$H = \sum_n \omega_n(a_n^+a_n + \frac{1}{2}) + (p^{(1)})^2 \quad (13)$$

where the summation in the first term excludes the zero mode and the last term depends only on the zero mode creation and annihilation operators $a_1^+$ and $a_1$

$$p^{(1)} = \psi_1\sqrt{\frac{\omega_1}{2}}(a_1 + a_1^+) \quad (14)$$

### 3 The Collective Coordinates

We gauge the translational invariance [3]. We do this by raising the parameter $X$ to a dynamical variable $X(t)$ which we will refer to as collective coordinate. The field will have a dependence on $X(t)$

$$\Phi(x) \rightarrow \Phi(x + X(t)) \quad (15)$$

Considering this dependence in the Lagrangian we find that we recover the equation of motion for $\Phi$. In going to the Hamiltonian formalism, the conjugate of $\Phi$ is

$$\Pi := \frac{\partial L}{\partial \dot{\Phi}} = \hat{\pi} \quad (16)$$

where $[\hat{\pi}(x), \hat{q}(y)] = -i\delta(x - y)$. We also acquire an additional equation which follows from the definition of the collective momentum.

$$P := \frac{\partial L}{\partial X} = \int \Phi' \hat{\pi} \quad (17)$$
This is a constraint which allows us to integrate the zero mode without encountering infrared divergences. The constraint is best put in the form

$$f = \int \phi' \dot{c} + \dot{q}' \pi - P$$  \hspace{1cm} (18)

Standard treatment of systems with collective coordinates requires that physical operators commute with the constraint and that physical states be annihilated by the constraint. The reason for this requirement is simple. We have embedded our theory, which was defined in a phase space which contains $\Phi$ and its conjugate only, into a larger phase space which also includes the collective coordinate and its conjugate. The embedding is performed by the gauge transformations whose generator is $f$. We require that physical operators, those which were defined in the original theory, be independent of the collective coordinate before the embedding. This is equivalent to requiring that the operator commute with the constraint after the operator has been embedded.

Examples of operators which are physical are the Hamiltonian $H$ and the field $\Phi$ for which it holds

$$[H, f] = 0, \quad [\Phi, f] = 0.$$  \hspace{1cm} (19)

Operators which are not physical are the fluctuations $\hat{q}$ and the collective coordinate $X$ since the commutators

$$[f, X] = -i \quad [f, \hat{q}(x)] = -i \Phi'(x)$$  \hspace{1cm} (20)

do not vanish. To determine if $\dot{X}$ is a physical operator we first write the Hamiltonian after integrating out the zero mode. The infrared free collective Hamiltonian can be written as

$$H_{\text{coll}} = \frac{1}{2} \left\{ (P - \int \dot{q}' \pi)^2, \frac{1}{2M(1 + \frac{\phi' \phi}{M})^2} \right\}_+. \hspace{1cm} (21)$$

Using the definition

$$\dot{X} = \frac{\partial H}{\partial P},$$  \hspace{1cm} (22)
we obtain an expression for $\dot{X}$

$$\dot{X} = \frac{1}{2} \left\{ (P - \int \dot{q}' \pi), \frac{1}{M(1 + \frac{2q}{M})^2} \right\} + .$$  \hfill (23)

It is a simple exercise to check that the commutator

$$[f, \dot{X}] \neq 0.$$  \hfill (24)

Thus, the operator $\dot{X}$ does not have a physical meaning. A similar exercise for $\ddot{X}$ shows that neither this operator is physical.

4  The Diffusion Equation

The Fourier transform of the correlation function of the random force on the soliton was written in [4] as

$$\Gamma(\omega) = \int \frac{<\dot{X}(t)\dot{X}(0)>}{<\dot{X}(t)\dot{X}(0)>} e^{-i\omega t} dt.$$  \hfill (25)

Equation (25) is related to the diffusion equation for the soliton

$$D(\omega) = \frac{\alpha}{i\omega + \Gamma(\omega)}.$$  \hfill (26)

Where $\alpha$ is the thermal average of the square of the soliton velocity. For adiabatic phonons, equation (25) is a good approximation. The reason for this follows from the fact that the operator $X$ and its time derivatives are not physical operator. Thus the equations (25) and (26) do not have a physical meaning.

The natural question which arises is which is the minimal operator that must be added to the operator $X$ to have a physical operator. To leading order, the constraint implies

$$P = \int \phi' \pi$$  \hfill (27)

Since $P$ is the conjugate of $X$ it follows that

$$X(t) = \frac{\int \phi' \dot{q}}{M}.$$  \hfill (28)
The operator in the r.h.s. of (28) is unphysical and the minimal operator which includes the r.h.s of (28) and is physical at the same time is

\[ \phi = \phi_c + \hat{q}_{re} + \psi_1 X(t) = \phi_c + \hat{q}_{re} + \psi_1 \int \psi_1 \hat{q} = \phi_c + \hat{q}. \]  

(29)

where in the second term use was made of (12) and

\[ q_{re}(x) = \sum_{n \neq 1} \psi_n(x) \int \psi_n^* \hat{q}. \]  

(30)

The equation (29) is a sensible choice because the equation (26) refers to the diffusion of the soliton and not of the collective coordinate of the soliton. However, the collective coordinate is a good but unphysical approximation to the soliton. To see that this is an approximation we write the equation (25) in terms of the soliton field

\[ \Gamma(\omega) = \int \frac{<\hat{\Phi}(t)\hat{\Phi}(0)>}{<\Phi(t)\Phi(0)>} e^{-i\omega t} dt. \]  

(31)

When we associate \( X \) with \( \Phi \) we have that

\[ \dot{X} = \dot{\Phi} \]  

(32)

which to leading order yields after use of (23)

\[ \dot{X} = \frac{P}{M} \phi'_c \]  

(33)

The equality holds exactly when

\[ \phi_c(x) = x \]  

(34)

which is the expansion of the soliton field about the kink position. Thus when we use (25) we are taking (34) to be the solution of the field at arbitrary distances of the kink position, rather than the solution (5).

Using the identity [6]

\[ <P'|\phi_c(x + X)|P> = \int dz \phi_c(z - x) e^{i\Delta P'^* z} e^{i\Delta E_{P'} t} = \phi_c(\Delta P') e^{i\Delta E_{P'} t} \]  

(35)
where $\Delta P' = P - P'$ and $\Delta E_{P'} = \frac{P^2 - P'^2}{2M}$, we see that the equation (31) becomes for the forward term

$$\Gamma_f(w) = \int dt \int \frac{dP'}{\Delta E_{P'}^2} \frac{\phi_c(\Delta P')}{|\phi_c(\Delta P')|^2} e^{i\Delta E_{P'} t} \theta(t) e^{-i\omega t}$$  \hspace{1cm} (36)$$

The backwards component reads

$$\Gamma_b(w) = \int dt \int \frac{dP'}{\Delta E_{P'}^2} \frac{\phi_c(\Delta P')}{|\phi_c(\Delta P')|^2} e^{i\Delta E_{P'} t} \theta(-t) e^{-i\omega t}$$  \hspace{1cm} (37)$$

It follows from the construction of $\Gamma(w)$ that the equation (26) for the soliton diffusion is mediated by phonons whose wavelength is $\Delta P$. \[3\]

We know that soft acoustic phonons will not see the soliton profile because their wavelength is much larger then the soliton extension. On the other hand, we see that the equations (37) and (36) depend on the soliton profile. Thus if we replace $\phi_c$ by $X$ we must impose a cutoff on the integrals over the momenta $P', P''$. The cutoff should be such that the smallest wavelength is much larger than the soliton extension. However, if we do not make such a replacement, we may safely integrate over the phonon spectrum, optical phonons included.

To see the difference between using the classical solution (5) and using the collective coordinate in the diffusion equation (26) it is convenient to write (26) as \[4\]

$$D_P(\omega) = \int dt < P|\dot{\Phi}(t)\dot{\Phi}(0)|P > e^{-i\omega t}.$$  \hspace{1cm} (38)$$

If we replace the collective coordinate of the soliton with the soliton field in (38) we obtain

$$D_P(\omega) = \int dt < P|\Phi(t)\Phi(0)|P > e^{-i\omega t}.$$  \hspace{1cm} (39)$$

which after using the integral representation for the Heavy-side function and integrating in time takes the form

$$D_P(\omega) = \frac{1}{i\pi} \int_{P_c}^{P_c} dP' \frac{\Delta E_{P'}^3 |\phi'_c(\Delta P')|^2}{\Delta E_{P'}^2 - \omega^2}.$$  \hspace{1cm} (40)$$

We may then study how equation (40) behaves for different profiles as a function of the cutoff. First we note that since we are interested in the contribution of optical
phonons and as pointed out in [1], only the leading order term in the $\omega$ expansion represent the contribution from the optical phonons, we may discard terms which depend on $\omega$. Unfortunately, we cannot get an analytical expression for the profile (5). However, assuming that $P = 0$, we may study how $D_0(0) \equiv D$ behaves as a function of the cutoff, $P_c$, in the integral (40). The behaviour is plotted in Figure 1.

We find that the diffusion equation saturates for high values of $P_c$ and it is independent of $P_c$ for large $P_c$ allowing us to carry the integration of $D$ to arbitrary large $P_c$.

Next we investigate the behaviour for the profile $\Phi = X$. It will give us a taste of how sensible is the diffusion equation (39) to the profile of the soliton. In this case the contribution from the optical phonons is obtained analytically

$$D \sim \int_{-P_c}^{P_c} dP' \sin^2\left(\frac{1}{2}LP'\right)$$

(41)
where $L >> 1$ is the length of the box in which the soliton is confined. Evaluation of the integral as a function of the cutoff shows that $D$ grows like

$$D \sim P_c$$  \hspace{1cm} (42)

This dependence was expected and shows that an improper treatment of the collective coordinates leads to a diffusion equation which is ill defined. We also conclude that $D$ is quite sensible to different profiles which lead to different contribution from the optical phonons. For the soliton profile we see that the contribution of optical phonons saturates for large momenta. However for the profile $X$, $D$ continues to increase linearly in $P_c$. Define as cutoff the value of momenta for for which $D$ saturates when considering the correct soliton profile. Then this must be the cutoff imposed on the profile $X$ to have a sensible theory. Thus for acoustic phonons the diffusion equation is not sensible to the profile. However, for optical phonons the diffusion equation is very sensitive to the profile.

### 5 Conclusions

The existence of a constraint in the system we have considered is a consequence of the broken translational symmetry of the vacuum, e.i. by our choice of classical solution. It has been shown that the operators defining the diffusion equation for the soliton must commute with the constraint. Because the operators defining the diffusion equation in [4] are not physical because they do not commute with the constraint it follows that this diffusion equation does not have a physical meaning. In order to have only the contributions from the physical sector of the theory we must replace the operators used in [4] to define the soliton diffusion by physical ones. The canonical operator which is physical and contains the information of the soliton position is the soliton field. We have also shown that using the collective coordinate as the operator defining the soliton profile is not only unphysical but it is also a good approximation to the soliton profile if we consider the contribution of the acoustic phonons only. On
the other hand, the contribution from the optical phonons, as we have shown, is very sensitive to the soliton profile. One must therefore use the exact profile of the soliton and not just the linear term in the expansion of the soliton profile when considering the contribution of the optical phonons to the diffusion of the soliton.

Acknowledgements

It is a pleasure for me to thank Yu Lu for many interesting and helpful conversations.
References

[1] Y. Wada, “Soliton Diffusion”, Prog. Theo. Phys. Sup. 113 (1993) 1.

[2] F. Aldabe, Phys. Lett. B351 (1995) 257;
   M. Henneaux and C. Teitelboim, Quantization of Gauge Systems. Princeton University Press, New Jersey (1992).

[3] J.L. Gervais, A. Jevicki and B. Sakita, Phys. Rev. D12 (1975) 1038;
   E. Tomboulis, Phys. Rev. D12 (1975) 1678.

[4] M. Ogata, A Terai, and Y Wada, J. Phys. Soc. Jnp 55 (1986) 2296.

[5] H. Mori, Prog. Theor. Phys. 33 (1965) 423.

[6] K. Ohta, Nucl.Phys. A511 (1991) 620.