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Renormalized perturbation theory for a toy model of fluctuating nonlinear hydrodynamics of supercooled liquids

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ABSTRACT

We study the field theoretic renormalized perturbation theory for a toy model of fluctuating nonlinear hydrodynamics (FNH) of compressible liquids. The toy model contains a density-like and a momentum-like variable without any spatial dependence. We present a detailed derivation of a set of coupled equations among correlation and response functions for these variables. In particular, we focus on how the static limit of the correlation and response functions can be achieved in the renormalized perturbation theory. Numerical methods of solving these equations at a given order of the loop expansion are explained and the results for the one-loop theory are given in detail. The simple nature of the toy model enables us to compare the static limit obtained from the exact solution with that of the one-loop order. This shows explicitly the range of validity of the one-loop theory in the field theoretic formulation.

1. Introduction

Understanding the slow dynamics of supercooled liquids within a field theoretic framework [1–10] has many advantages including the possibility of a systematic improvement. However, there have been more subtle issues than one might first expect in the development of a consistent renormalized perturbation theory for the dynamics of glass forming liquids. The nonlinear feedback mechanism of density fluctuations in the so-called fluctuating nonlinear hydrodynamics (FNH) of compressible fluids was studied by Das and Mazenko (DM) [1] within the field theoretic renormalized perturbation theory. They find that the system remains ergodic at all temperatures or densities without a sharp ergodic-to-nonergodic (ENE) transition predicted in the standard mode coupling theory (MCT) [11–14]. Recently, another version of field theory for glass forming liquids was developed by Andreanov, Biroli and Lefèvre (ABL) [4] where the dynamical action is invariant under a set of linear time-reversal transformations. The field theory by ABL was later modified for the case of interacting Brownian particles by Kim and Kawasaki (KK) [7], where the standard MCT result was recovered at the one-loop order of perturbation theory. This modified method was then applied to the FNH [10] with results indicating a sharp ENE transition at the one-loop order with the nonergodicity parameter satisfying the standard MCT result. In response to these developments, DM reexamined their work and showed [15] in a nonperturbative analysis that the sharp ENE transition is not present in the FNH after all. This conclusion is also supported by the recent direct numerical integration of the generalized Langevin equations of the FNH [16].

In Ref. [17], in order to clarify these subtle points in the field theoretic formulations for glass forming liquids, a simple toy model for the FNH has been studied. In the toy model, there are no spatial degrees of freedom in the dynamical field variables which consist simply of a density-like variable and a single-component momentum-like variable. The two types of field theories were formulated for the toy model, namely the original DM-type field theory and the one by ABL and KK. The simple nature of the toy model enables one to see directly that a major difference between the two formulations lies in the way of treating the density nonlinearities present in FNH within the renormalized perturbation theory [17].

In the original treatment of FNH by DM [1], the density feedback mechanism was studied via a single equation for the density autocorrelation function obtained at the one-loop order in the hydrodynamic limit. For the toy model [17], without resorting to the hydrodynamic limit, a set of coupled self-consistent equations among all the independent correlation and response functions involved was obtained at the one-loop order and solved numerically. This program of considering the coupled equations can in principle be generalized for the field theory of FNH with full spatial dependences at a given order of the loop expansion. In order to carry out this program, it will be necessary to handle certain technical issues arising in the construction of the coupled equations in such a field theory, which involve short-time singularities appearing in some of the correlation and self-energy functions. In this paper, we clarify these issues by presenting a detailed construction of the self-consistent equations obtained in Ref. [17] for the correlation and response functions in the renormalized field theory of the toy model. In particular, we show how to manage the short-time singularities mentioned above and how to set up the self-consistent equations ready for the numerical calculations. We also show that this

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task is closely related to taking static limits of the correlation and response function, which are determined self-consistently at a given order of the loop expansion. Since the static limit for the present toy model can be calculated exactly, by comparing with the one-loop result, we will be able to obtain explicitly the range of validity of the one-loop approximation.

In the next section, we summarize key features of the toy model introduced in Ref. [17], and its field theoretic formulation according to the DM prescription. In Section 3, we study the renormalized perturbation theory using the Schwinger–Dyson equations. We focus on how the static limit can be taken within this formulation. In Section 4, we present in detail a set of coupled equations for the correlation and response functions in the DM field theory at the one-loop order and their numerical solutions. In the final section, we summarize our results with discussion.

2. Model

In this section we present the toy model studied in Ref. [17]. It is a zero-dimensional version of the FNH of compressible fluids developed by Das and Mazenko [1]. The dynamical variables consist of a time-dependent density-like variable $\rho(t)$ and a single-component momentum-like variable $g(t)$ without any spatial degrees of freedom. The equations of motion for these variables are constructed in Ref. [17] with respect to the effective free energy F, where the equilibrium distribution for the system at temperature T is given by $\exp(-F/T)$. The free energy is written as $F=F_K+F_U$ where $F_K[\rho,g]$ is the kinetic energy and the potential energy part $F_U[\rho]$ is assumed to depend only on ρ. We take the usual form for the kinetic part, and the simple Gaussian form for the potential energy part:

$$F_K = \frac{g^2}{2\rho}, \quad F_U = \frac{A}{2}(\delta\rho)^2, \tag{1}$$

for some constant A and the fluctuation $\delta\rho=\rho-\rho_0$ and the average value ρ_0. Despite the simple form for F_U, the nonlinearity in the form of $1/\rho$ in F_K plays an important role in the following discussion. The equation of motion for the variable $\rho(t)$ is in the form of a zero-dimensional version of the continuity equation, namely

$$\dot{\rho}(t) + Jg(t) = 0 \tag{2}$$

for some constant J, where the dot indicates the time derivative. The equation of motion for $g(t)$ has the dissipative part described by the coefficient Γ in addition to the reversible part as follows:

$$\dot{g}(t) + J\left(\frac{g^2}{2\rho}\right) - JA\rho(\delta\rho) + TJ + \Gamma\left(\frac{g}{\rho}\right) = \theta, \tag{3}$$

where the Gaussian white noise θ has the variance $\left\langle\theta(t)\theta\left(t'\right)\right\rangle = 2\Gamma T\delta(t-t')$.

In this paper we study this toy model using the renormalized field theory. The field theory for this purpose can be obtained by using the standard Martin–Siggia–Rose (MSR) procedure [18], where the hatted fields $\hat{\rho}$ and $\hat{g}$ are introduced to enforce the equations of motion for ρ and g respectively. Following DM [1], we introduce an auxiliary velocity-like field $V(t)$ such that the condition $g(t)=\rho(t)V(t)$ is enforced through a delta-function

$$\begin{aligned} 1 &= \int\mathcal{D}V(t)\,\delta(\rho(t)V(t)-g(t)) \\ &= \int\mathcal{D}V(t)\int\mathcal{D}\hat{V}(t)\exp\left[-i\hat{V}(t)(g(t)-\rho(t)V(t))\right]. \end{aligned} \tag{4}$$

The first equality holds up to a Jacobian. This Jacobian was shown in Ref. [19] to have no effect on the correlation and response functions and will be neglected in the following analysis. Using this identity, we obtain the generating functional Z as a functional integral over the fields $\psi_i(t)=\delta\rho(t),g(t),V(t)$ and $\hat{\psi}_i(t)=\hat{\rho}(t),\hat{g}(t),\hat{V}(t)$. We can write

$$Z = \int\prod_i \mathcal{D}\psi_i\mathcal{D}\hat{\psi}_i\,\exp\left(-S\left[\psi,\hat{\psi}\right]\right), \tag{5}$$

where

$$\begin{aligned} S = \int dt\Big[&\Gamma T\hat{g}^2(t) + i\hat{\rho}(t)\{\dot{\rho}(t) + Jg(t)\} \\ &+ i\hat{g}(t)\{\dot{g}(t) - JA\rho_0\delta\rho(t) + \Gamma V(t) + TJ \\ &+ \frac{J\rho_0}{2}(V(t))^2 + \frac{J}{2}\delta\rho(t)(V(t))^2 - JA(\delta\rho(t))^2\} \\ &+ i\hat{V}(t)\{g(t)-\rho_0V(t)-\delta\rho(t)V(t)\}\Big]. \end{aligned} \tag{6}$$

We use $\Psi(t)$ to represent any one of the six variables $\{\psi_i, \hat{\psi}_i\}$ in our model, and denote the two-point correlation function between arbitrary two variables $\Psi(t)$ and $\Psi'(t')$ by

$$G_{\Psi\Psi'}(t-t') = \left\langle\Psi(t)\Psi'(t')\right\rangle. \tag{7}$$

(For the subscripts, we will use ρ instead of $\delta\rho$ for simplicity.) Note that among the correlation functions those between two hatted variables vanish due to causality, that is $G_{\hat{\psi}_i\hat{\psi}_j}=0$. It follows that $iTJ\hat{g}(t)$ term in the action Eq. (6) has no effect on the correlation functions and will be neglected in the following. The causality also requires that $G_{\psi_i\hat{\psi}_j}(t)=0$ for $t<0$.

There are some nonperturbative relations among the correlation functions which will be useful in later discussion. We have

$$\dot{G}_{\rho\psi}(t) + JG_{g\psi}(t) = 0, \tag{8}$$

and

$$\dot{G}_{\rho\hat{\psi}}(t) + JG_{g\hat{\psi}}(t) = -i\delta_{\hat{\psi}\hat{\rho}}\delta(t). \tag{9}$$

There exist fluctuation–dissipation relations (FDR) that relate linearly the correlation functions to response functions. Assuming the time-reversal properties of the fields as $\rho(-t)=\rho(t)$, $g(-t)=-g(t)$ and $V(-t)=-V(t)$, we can derive the FDR for $\psi=\rho,g$ and V as

$$G_{\psi\hat{g}}(t) = -\frac{i}{T}\Theta(t)G_{\psi V}(t), \tag{10}$$

where $\Theta(t)=1$ for $t>0$ and vanishes for $t<0$. The detailed derivation of the nonperturbative relations and the FDR closely follows the one given in Ref. [1]. Since $\hat{\psi}_i$ is a real field, we can show that the correlation function between unhatted and hatted variables is a pure imaginary number, that is

$$G^*_{\psi_i\hat{\psi}_j}(t) = -G_{\psi_i\hat{\psi}_j}(t). \tag{11}$$

From the time-reversal properties of the variables, it also follows that

$$G_{\rho g}(-t) = -G_{\rho g}(t) = G_{g\rho}(t), \tag{12}$$

$$G_{\rho V}(-t) = -G_{\rho V}(t) = G_{V\rho}(t), \tag{13}$$

$$G_{gV}(-t) = G_{gV}(t) = G_{Vg}(t). \tag{14}$$

3. Renormalized perturbation theory

In this section, we develop a self-consistent renormalized perturbation theory for the field theoretic approach introduced in