Dynamic scaling analysis of Binary fluid model

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Abstract

This paper examines the dynamic scaling behavior of the binary fluid model, and hence show that the static scaling hypothesis breaks down. Mode-coupling method is examined in detail. By following Kandanoff and Swift's method, we show that the transport coefficients diverge near the vicinity of the critical region. We also find that the scaling law of the transport coefficients, $\eta\lambda^* \propto \xi^{4-d-\eta}$.

1 Introduction

In this paper, we investigate the dynamic property of binary-fluid model. Mode coupling succeeds in predicting critical exponents and scaling functions in $3d$. However, this method does not work quite well for general d. Therefore, RG comes into play and proves to be a great success in finding scaling relations and its critical exponents.

First, we will illustrate why static scaling behavior fails because of the dynamic property of binary fluid model.We will derive the expression of for thermal and viscous diffusion constant. With the expressions of thermal and viscous diffusion constant, we use dimensional analysis to find the scaling form of the relaxation rate. Hence, we show that static scaling behavior breaks down because of the relaxation rate. Second, we will work out the mode coupling method by introducing Liouville equation, which is the realization of continuity equation in quantum mechanics. We can retrieve the scaling function presented in Kadanoff and Swift's paper, where the transport coefficient $\lambda\bar{\eta}$ diverges as $\xi^{4-d-\eta}$.

2 The breakdown of static scaling

Binary fluid model exhibits a segregation of the gas and the liquid gas. We can denote the gas state by state 1 and the liquid state by state 2. The order parameter that describes the difference of the two different states is defined by ψ. We define the current that passes between the two states by $\vec{j}^{\psi}$. The conservation law states that $d\psi/dt = -\nabla \cdot \vec{j}^{\psi}$. If the external force is absent, the current depends on the gradient of chemical potential which determines the concentration difference. Therefore,

$$\vec{j}^{\psi} = -\lambda \nabla \mu = -\lambda \frac{\partial \psi}{\partial \mu}|_{T,P} \nabla \psi = -\frac{\lambda}{\chi_{\psi}} \nabla \psi \tag{2.1}$$

where we define the relation $\frac{\partial \psi}{\partial \mu}$ by the susceptibility of the order parameter χ_{ψ} and λ is the transport coefficient. The negative sign shows that the particles move from the high density state to the low density state. We can find the dispersion relation by combing Equation (2.0.1) with the conservation law, in which we expand the order parameter in Fourier series, $\psi(\vec{r}) = \int_{\vec{k}} e^{i\vec{k}\cdot\vec{r} - i\omega_{\psi} t} \psi_{\vec{k}}$.

$$\omega_{\psi} = D_c k^2 \tag{2.2}$$

where the diffusion constant D_c is $\frac{\lambda}{\chi_{\psi}}$. Likewise, we can obtain the relation for the thermal constant.

$$D_T = \frac{\lambda}{C_p} \tag{2.3}$$

$$D_{\nu} = \frac{\bar{\eta}}{\rho} \tag{2.4}$$

where λ_T is the thermal conductivity, and C_p is the constant pressure specific heat. [1]η is the shear viscosity.

Next, we present a heuristic argument for the failure of static scaling theory in binary fluid model. Static scaling theory gives the expressions of the susceptibility of χ_{ψ} and the correlation length, ξ.

$$\chi_{\psi} \propto \xi^{2-\eta} \tag{2.5}$$

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[1] Let's define the thermal current density $j_Q = -\lambda_T \nabla T$. Based on the conservation law, $-\nabla j_Q = \frac{dE}{dt} = \frac{dE}{dT}|_p \frac{dT}{dt} = C_p \frac{dT}{dt}$. So, $D_t = \frac{\lambda_T}{C_p}$. Similary, for D_{ν}, use Navier-Stoke's equation.

where ξ is the correlation length and diverges near the critical point T_c, $\xi \propto (T - T_c)^{-\nu}$.[2]

Let's find the scaling form of the relaxation rate, ω_ψ. We have two conditions; the wavelength is larger than ξ and the wavelength is shorter than ξ. If the wavelength is larger than ξ, the relaxation rate vanishes. Combine Equation (2.0.2) with the definition of the diffusion constant, $D_\lambda = \lambda/\chi_\psi$. We have the following relation,

$$\omega_\psi \propto \xi^{-z}(k\xi)^2 \tag{2.6}$$

where $z = 4 - \mu$.

If the wavelength is shorter than the correlation length ξ, χ_{psi} should be decay as $k^{-2+\eta}$.[3] So, the relaxation rate is

$$\omega_\psi \propto k^z \tag{2.7}$$

Combine the case of $k < \xi$ and the case of $k > \xi$.

$$\omega_\psi(k) = k^z \Omega(k\xi) \tag{2.8}$$

Note that if $k\xi \ll 1$, $\Omega(k\xi) = (k\xi)^{-z+2}$. And if $k\xi \gg 1$, $\Omega(k\xi) = 1$. However, the exponent z is smaller than $4 - \mu$ according to Hohenberg and Halperin. The static scaling theory fails. The transport coefficient diverges in the vicinity region of the critical point.

3 Coupling mode method

In this section, we will introduce the building block of the coupling mode method. Due to the influence of the relaxation rate, the theory can be stated in the context of non-equilibrium statistical mechanics. Therefore, the state of the system should be time dependent. We can describe the system of N particles as

$$\langle \vec{p}_1 \vec{p}_2 \dots \vec{p}_N, \vec{r}_1 \vec{r}_2 \dots \vec{r}_N | t \rangle = \langle p, r, N | t \rangle \tag{3.1}$$

Since the state of the system is time dependent, the time evolution of the system can be described by Liouville theorem

$$\left(\frac{\partial}{\partial t} + L \right) |t\rangle = 0 \tag{3.2}$$

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[2] In class, ,we show that $\chi \propto t^{-\gamma}$ and $\xi \propto t^{-\nu}$. Combine this with Fischer scaling law, $\nu(2 - \eta) = \gamma$.

[3] Note that $[k] = L^{-1}$.

This is a fancy version of the total time derivative of the state. We can find the matrix element of L,

$$\langle p', r', N'|L|p, r, N\rangle = \sum_{\alpha=1}^{N}[\frac{\partial \vec{r}_\alpha}{\partial t}\frac{\partial}{\partial \vec{r}_\alpha} + \frac{\partial \vec{p}_\alpha}{\partial t}\frac{\partial}{\partial \vec{p}_\alpha}] \tag{3.3}$$

$$= \sum_{\alpha=1}^{N}[\frac{\partial H}{\partial \vec{p}_\alpha}\frac{\partial}{\partial \vec{r}_\alpha} - \frac{\partial H}{\partial \vec{r}_\alpha}\frac{\partial}{\partial \vec{p}_\alpha}] \times \langle p', r', N|p, r, N\rangle \tag{3.4}$$

with the orthonormal relation that

$$\langle p'r', N'|p, r, N\rangle = \delta_{N,N'}\prod_{\alpha=1}\delta(\vec{p}_\alpha - \vec{p}'_\alpha)\delta(\vec{r}_\alpha - \vec{r}'_\alpha) \tag{3.5}$$

The equilibrium state is described by the canonical ensemble equilibrium distribution[4]. If L act on the equilibrium state, we have

$$L|\rangle = 0, \quad \text{and} \quad \langle L = 0 \tag{3.6}$$

Any physical quantity X in this state is given by the time average over the grand canonical ensemble, where the matrix element is X_{op}.

Now, we can apply the notion in fluid dynamics to the quantum state. The continuity equation is

$$\frac{\partial A}{\partial t} = -\nabla \cdot \vec{j}^{A}_{op}(\vec{r}) = [L, A_{op}(\vec{r})] \tag{3.7}$$

So, we may define the following quantities and their related current. Define the number operator as $n_{op}(\vec{r})$, the momentum density as $g_{op}(\vec{r})$, and the energy density as $\epsilon_{op}(\vec{r})$. We can also define their currents, $\vec{j}(\vec{r})$, $\vec{j}^\epsilon$ and $\tau_{ij}(\vec{r})$ for number density, energy and momentum, respectively. The correlation function of the currents and the momentum are shown

$$\beta\langle g_i(\vec{r})j_k(\vec{r'})\rangle_q = \delta(\vec{r} - \vec{r'})n_{op}(\vec{r})\delta_{ik} \tag{3.8}$$

$$\beta\langle g_i(\vec{r})j^\epsilon_k(\vec{r'})\rangle_q = \delta(\vec{r} - \vec{r}')[\epsilon_{op} + p_{op}(\vec{r})] \tag{3.9}$$

$$\beta\langle g_i(\vec{r}\tau(\vec{r'}))\rangle_q = 0 \tag{3.10}$$

The above equations can be verified by applying the commutator relations shown before. Note that the second equation indicates the Galilean invariance of the energy current. We need to introduce a parameter that describes the fluctuation of the system, $s_{op}(\vec{r})$. s_{op} is the entropy density, where

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[4] Grand canonical ensemble is $\exp\{-\beta[H(p, r) - \mu N]\}/[h^3 NZ(\beta, \mu)]$.

$s_{op}(\vec{r}) = \frac{1}{T}[\epsilon_{op} - \langle j^\epsilon v\rangle n_{op}]$ and $\langle j^\epsilon v\rangle$ is $\langle \epsilon + p\rangle / \langle n\rangle$. Therefore, the entropy current is

$$\vec{j}^\epsilon_{op} = \frac{1}{T}[\vec{j}^\epsilon_{op} - \frac{\langle\epsilon\rangle + \langle p\rangle}{\langle n\rangle}\vec{j}_{op}] \tag{3.11}$$

Now, consider how the equilibrium state can be described by the entropy density so that we can monitor the local property of the system. The quantum state can be described as

$$|i, \vec{q}\rangle = a_i(\vec{q})|\rangle \ \ \langle i, \vec{q}| = \langle|a_i(-\vec{q}) = q^2\lambda(\vec{q}, s) \tag{3.12}$$

where we introduced a set of operators that are orthogonal to each other.

$$a_1(\vec{q}) = \frac{s_{op}(\vec{q})}{[k_B\rho C_p(\vec{q})]^{1/2}} \tag{3.13}$$

$$a_2(\vec{q}) = \frac{(\rho\beta)^{1/2}}{\langle n\rangle}c(\vec{q})n_{op}(\vec{q}) + \left(\frac{1}{k_B\rho}[\frac{1}{C_V(\vec{q})} - \frac{1}{C_p(\vec{q})}]\right)^{1/2} s_{op}(\vec{q}) \tag{3.14}$$

$$a_3(\vec{q}) = g_x(\vec{q})(\beta/\rho)^{1/2} \tag{3.15}$$

$$a_4(\vec{q}) = g_y(\vec{q})(\beta/\rho)^{1/2} \tag{3.16}$$

$$a_4(\vec{q}) = g_z(\vec{q})(\beta/\rho)^{1/2} \tag{3.17}$$

Note that the operators carry out the thermodynamic quantities and they agree with the dimensional analysis in which the $[a_i(\vec{q})] = O(1)$.

It is natural to ask the following question.What is the L's eigenvalue of $|i, \vec{q}\rangle$? This relates to the transport process of the system. Suppose a system with the following relation, $|\rangle_t = e^{-st}|\rangle$, where s is the relaxation rate. The transport state can be obtained by setting the relaxation time to be infinite, and its eigenvalue is s_ν.

$$s_\nu|\nu, \vec{q}\rangle_R = L|\nu, \vec{q}\rangle_R \tag{3.18}$$

Let's take the inner product of the transport state and other "local" state, $\langle i, \vec{q}|$.

$$\langle i\vec{q}|L|\nu, \vec{q}\rangle = \langle i, \vec{q}|L|\nu, \vec{q}\rangle_R \tag{3.19}$$

$$= \sum_j \langle i, \vec{q}|L|j, \vec{q}\rangle\langle j, \vec{q}|\nu, q\rangle_R + \langle i, \vec{q}|L(1 - \sum_j |j, \vec{q}\rangle\langle j, \vec{q}|)|\nu, \vec{q}\rangle_R \tag{3.20}$$

where we define the projection operator, $P = 1 - \sum_j |j, \vec{q}\rangle\langle j, \vec{q}|$. We can find the expression for $P|\nu, \vec{q}\rangle = \frac{1}{s_\nu - PLP}\sum_i PL|j, \vec{q}\rangle\langle j, \vec{q}|\nu, \vec{q}\rangle_R$ by applying the iteration method. Note that L and P is commutable to each other. So, Equation (3.20) becomes

$$\sum_j [s_\nu \delta_{ij} - L_{ij}(\vec{q} - U_{ij}(\vec{q}s_\nu)]\langle j, \vec{q}|\nu, \vec{q}\rangle_R = 0 \tag{3.21}$$

where $L_{ij}(\vec{q}) = \langle i, \vec{q}|L|j, \vec{q}\rangle$ and $U_{ij} = \langle i, \vec{q}|LP\frac{1}{s - PLP}PL|j, \vec{q}\rangle$. By linear algebra, we know that the determinant of the matrix $s\delta_{ij} - L_{ij} - U_{ij}$ is 0 in order to have a non-trivial solution of the state $\langle j, \vec{q}|\nu, \vec{q}\rangle$.

It is important to note that the matrix element U_{ij} entails the previously defined thermodynamic quantities. U_{ij} is very important in our later calculations.

4 Perturbation theory and critical exponents

In this section, we will use the matrix element U_{ij} to find the critical exponents of the transport coefficient. Let's further expand the matrix element U_{ij}.

$$U_{ij)}(\vec{q}, s) = \langle i, \vec{q}|LP\frac{1}{s - PLP}PL|j, \vec{q}\rangle \tag{4.1}$$

$$= \langle a_i(-\vec{q})LP\frac{1}{s - PLP}PLa_j(\vec{q})|\rangle \tag{4.2}$$

$$= \langle|[a_i(-\vec{q}), L]P\frac{1}{s - PLP}[a_j(-\vec{q}), L]\rangle \tag{4.3}$$

$$= -\vec{q}^2\langle|\vec{j}_i(-\vec{q})P\frac{1}{s - PLP}P\vec{j}_k(\vec{q})|\rangle \tag{4.4}$$

where $\vec{j}_i$ is the corresponding current of a_i. There are $25 = 5 \times 5$ U_{ij}s. Some terms can be eliminated by the argument that $\vec{j}_{3,4,5}$ is proportional to the momentum density $g(\vec{q}_i)$. The correlation function of such currents is 0. Consider the following the matrix element,

$$-\langle|s_{op}(-\vec{q})LP\frac{1}{PLP - s}PLs_{op}(\vec{q})|\rangle/k_B \tag{4.5}$$

where we apply the fact $s_v\delta_{ij} = \lambda q^2/\rho$.[6] And the matrix index, i, j must be the same. Therefore, we can set the operator a_i to be proportional to $s_{op}(\vec{q})/[k_B\rho C_p(\vec{q})]^{1/2}$. Compare Equation (4.4) with Equation (4.5), we have

$$U_{11} = q^2\lambda(\vec{q}, s) \tag{4.6}$$

For the viscosity, we do the same thing. Based on the dispersion relation of η. we have the following relation,

$$-q^2\eta(\vec{q}, s) = \langle |g_y(-\vec{q})LPXPLg_\nu(\vec{q})|\rangle\beta \tag{4.7}$$

where X is $1/(PLP - s)$.

We can apply perturbation theory to this expression. We can expand the relaxation rate around a wave vector,

$$s'_\nu(\vec{q}) = s_{\nu 1}(\vec{q}') + s_{\nu 2}(\vec{q} - \vec{q}') \tag{4.8}$$

where $\vec{q}$ and $\vec{q} - \vec{q}'$ are the two different transport processes. Expand the operator L,

$$L = \sum_{r'} \int \frac{d^3q'}{(2\pi)^3} |\nu', \vec{q}'\rangle_R s_{\nu'}(\vec{q}')_L\langle \nu'\vec{q}'| \tag{4.9}$$

Note the index R and L are the eigenstates of the operator L, in which they have an orthonormal solution, ${}_R\langle \nu, \vec{q}|\nu', \vec{q}'\rangle_R = \delta_{\nu,\nu'}\delta(\vec{q} - \vec{q}')(2\pi)^3$. Hence, we can write down the representation for X_q. We find the projection operator eliminates the transport states. So, $(\langle (PLP - s)\rangle_{\nu\vec{q}})^{-1} = s_\nu - s$[7]. Hence we can write down the representation of X_q.

$$X_q = \sum_{\nu'=6}^{\infty} \frac{|\nu', \vec{q}\rangle_{RL}\langle \nu'\vec{q}|}{s'_\nu(\vec{q}) - s} \tag{4.10}$$

By applying Equation (4.10) to Equation (4.7), we have

$$-q^2\eta_{TT}(\vec{q}, s) = \frac{1}{2}\beta \int \frac{d^3q'}{(2\pi)^3} \frac{\langle |g_\nu(-\vec{q})La_1(\vec{q}')a_1(\vec{q} - \vec{q}')\rangle \langle |a_1(\vec{q}' - \vec{q})a_1(-\vec{q})Lg_y(\vec{q})|\rangle}{s_T(\vec{q}') + s_T(\vec{q} - \vec{q}') - s} \tag{4.11}$$

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[6] This is the modification of the dispersion relation of Equation (2.3).

[7] Based on the definition of P, $P = 1$ if $\nu > 5$

This form is analogous to the one loop expansion of Feynman diagram. A factor of $\frac{1}{2}$ avoids the over-counting of the exchanging terms. With the definition that $a_1(\vec{q}) = \dfrac{s_{op}}{[k_B \rho C_p]^{1/2}}$, we have

$$q^2 \eta_{TT} = \frac{\beta}{2k_B^2} \int \frac{d^3q'}{(2\pi)^3} \frac{|M_{q,q'}|^2}{[\rho C_q(\vec{q}')\rho C_p(\vec{q}-\vec{q}')][s_T(\vec{q}' + s_T(\vec{q}-\vec{q}')) - s]} \tag{4.12}$$

where $M_{\vec{q},\vec{q}'} = \langle | g_y(-\vec{q}) L s_{op}(\vec{q}') s_{op}(\vec{q}-\vec{q}') | \rangle$. It's not hard to evaluate this matrix. We follow the formalism of Equation (4.1) – (4.4). We will get

$$M_{q,q'} = \langle | g_y(-\vec{q})(-i\vec{q}')\dot{\vec{j}}^s_{op}(\vec{q}') s_o p(\vec{q}-\vec{q}') | \rangle + \langle | g_y(-\vec{q})[i(\vec{q}-\vec{q}')] \cdot \vec{j}^s_{op}(\vec{q}-\vec{q}') s_{op}(\vec{q}') | \rangle \tag{4.13}$$

Now we replace j^s_{op} by $j^\epsilon(\vec{r}) = [\vec{j}^\epsilon - \dfrac{\langle \epsilon + p \rangle}{\langle n \rangle} \vec{j}(\vec{r})]/T$. Furthermore, using the correlation functions of Equation (3.11), we find that

$$M_{q,q'} = (-i\vec{q}'_y)\beta^{-1} \langle | [s_{op}(\vec{q}-\vec{q}') + (1/T)p_{op}(\vec{q}'-\vec{q})] s_{op}(\vec{q}-\vec{q}') | \rangle \tag{4.14}$$

$$+ i(\vec{q}_y - \vec{q}'_y)\beta^{-1} \langle | [s_{op}(-\vec{q}') + (1/T)p_{op}(-\vec{q}')] s_{op}(\vec{q}') | \rangle \tag{4.15}$$

where p_{op} is the pressure operator, $p_{op} = (\langle n \rangle_{op} - n)\frac{\langle \epsilon + p \rangle}{\langle n \rangle}$. Based on the Kandanoff and Swift's argument that the entropy operator is an artificial product so that its correlation with pressure vanishes. So, the matrix element $M_{q,q'}$ becomes

$$M_{q,q'} = [i\vec{q}'_y C_p(\vec{q} - \vec{q}' + i(\vec{q}'_y - \vec{q}) C_p(\vec{q}')] \rho k_B^2 T \tag{4.16}$$

We now can reduce the formula for the viscosity to

$$q^2 \eta_{TT}(\vec{q}, s) = \frac{1}{2\beta} \int \frac{d^3q'}{(2\pi)^3} (\vec{q}_y)^2 \frac{[C_p(-\vec{q}+\vec{q}') - C_p(\vec{q}')]^2}{C_p(-\vec{q}'+\vec{q}) C_p(\vec{q}')} \tag{4.17}$$

$$\frac{1}{s_T(\vec{q}') + s_T(\vec{q}-\vec{q}') - s} \tag{4.18}$$

In the static limit, where the wave vector and the relaxation time go to 0. So, the expression in the bracket of Equation $(4, 17)$ can be written as a derivative form.

$$\eta_{TT}(\vec{0}, 0) = \frac{1}{8\beta} \int \frac{d^3q'}{(2\pi)^3} (q'_y)^2 \frac{[\frac{\partial}{\partial q'_x} C_p(\vec{q}')]^2}{s_T(\vec{q})[C_p(\vec{q}')]^2} \tag{4.19}$$

Now, scaling law and dimensional analysis come into play. Based on scaling-law analysis, the wave vector is measured under the scale of the correlation length in the vicinity region near the critical point. Therefore, we can set the integration limit to be ξ. By the same method, we can estimate the derivative of C_p and the relaxation rate $s_T(\vec{q}')$ in the critical region.

$$\frac{\partial}{\partial q'_x} C_p(\vec{q}') \propto \frac{q'_x}{(q')^2} C_p(\vec{q}') \tag{4.20}$$

$$s \propto \frac{\lambda(\vec{q}, s) q^2}{\rho C_p(\vec{q})} = (\lambda/\rho C_p)\xi^2 \tag{4.21}$$

The first equation is based on the assumption that the heat capacity near the critical region is estimated by scaling law, which is related to the expression of the correlation length. So, $\frac{\partial}{\partial q'_x} C_p(\vec{q}') \propto \frac{C_p(\vec{q}')}{\xi^{-1}}(\frac{q'_x}{q'})$. Note that $\frac{q'_x}{q'}$ is the scale approximation which estimates the value of the C_p in the critical region. Furthermore, the relaxation rate can be estimated as a fixed value in the critical region. $s*_T = (\lambda/\rho C_p)\xi^{-2}$. We can evaluate the integral based on dimensional analysis and above approximations.

$$\text{Integral} \propto \text{Constant} * \int^{\xi^{-1}} dq'(q')^2 \propto \text{Constant}\, \xi^{-3} \tag{4.22}$$

where the constant is $\frac{1}{\beta}\frac{\rho C_p}{\lambda *}\xi^2$. So, we find that

$$\eta_{TT}(\vec{q}, s) \propto \frac{1}{\beta}\frac{\rho C_p}{\lambda^*}\xi^{-1} \tag{4.23}$$

We proceed to find the critical exponent with the notion that $C_p \propto t^{-\gamma}$ and $\xi \propto t^{-\nu}$, where $t = (T - T_c)/T_c$.

$$\eta_{TT}(\vec{0}, 0)\lambda^* \propto t^{-\gamma+\nu} \propto \xi^{1-\eta} \tag{4.24}$$

Since Kandanoff studied the $3d$ case, we may write a general scaling law for the transport coefficient without proof.

$$\eta\lambda^* \propto \xi^{4-d-\eta} \tag{4.25}$$

This relation indicates that at least one of the transport coefficients must diverge in the critical region. Thus, we show that the transport coefficients diverges near the vicinity of the critical region, which is contradictory to the result from the static scaling hypothesis.

5 Summary

In this paper, we revisit the mode-coupling method introduced by Kadanoff and Swift and show that the transport coefficient is indeed diverges near the critical region. Kadanoff and Swift applied the operator formalism in quantum mechanics and examined the critical behavior of the transport coefficients of the binary fluid model. However, this method only works successfully well in the $3d$ case. For higher dimension case, we should employ $\epsilon = 4 - d$ expansion that is commonly used in RG analysis, and get the recursion relation to find the critical exponents.

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