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Density fluctuation of the ^{3}He reaction–diffusion model in nonextensive statistical mechanics

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In this paper the time-space correlation of density fluctuation of the ^{3}He reaction–diffusion model is investigated where the equilibrium distribution is described by the generalized Maxwell–Boltzmann distribution in the framework of Tsallis statistics. By using the density operator technique, the nonextensive pressure effect is introduced into the master equation and thus the generalized master equation is derived for the nonextensive system. This paper uses the ^{3}He reaction–diffusion model to analyse the effect of nonextensive pressure on the fluctuation and finds that the nonextensive parameter q plays a very important role in determining the characteristics of the fluctuation waves.

Keywords: nonextensive statistics, ^{3}He reaction–diffusion model, density fluctuation
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1. Introduction

The spatial correlation of fluctuation for a reaction–diffusion system is usually investigated by introducing the term for diffusion in the master equation within the description of mean-field and phase space.[1] However, for a gas reaction–diffusion system, when the inhomogeneous pressure drives particles to flow from one area with high pressure to another with low pressure, the pressure effect, as that in the case of diffusion, can also introduce the spatial correlation of fluctuation.[2] In particular, for the systems having long-range inter-particle interactions, which behave nonextensively, the inhomogeneity of pressure may play more significant role in the spatial correlation of the density fluctuation. In this case, we should introduce the nonextensive effect into consideration in the master equation in the framework of nonextensive statistical mechanics.

To analyse the nonextensive pressure effect on the reaction–diffusion systems with long-range interactions, we need to know the equation of state of the gas. On the assumption that the matter is in the state of an ideal gas in the Maxwellian sense, the gas pressure is given by $P = Nk_{\rm B}T$, where P is pressure, T is temperature, N is particle density, and $k_{\rm B}$ is Boltzmann constant. However, the systems whose equation of state may be regarded as that one of an ideal gas are usually extensive, this property holds for systems with short-range inter-particle forces. In other words, the equation of state of an ideal gas cannot correctly describe the nonextensive system. Recently, the equilibrium distribution for the nonextensive systems with long-range interactions can be described by the generalized Maxwell–Boltzmann distribution in the framework of Tsallis statistics,[3−8] which, in the light of Du's theory[5−8] and the present understanding, can be reasonably applied to the statistical description of the nonequilibrium system being in the stationary state. Thus, when treating the nonextensive and nonequilibrium reaction–diffusion systems, we should replace the conventionally used equation of state of an ideal gas by that of the nonextensive gas. In the q-ensemble theory,[9] the nonextensive gas pressure is defined as

$$P = C(q)Nk_{\rm B}T, \tag{1}$$

where $C(q) = [1 + S_q(1-q)/k_{\rm B}]$ and S_q is the nonextensive entropy. In the q-kinetic theory, the nonextensive gas pressure is[6]

$$P = \frac{2}{5-3q}Nk_{\rm B}T, \tag{2}$$

if the expectation value of square velocity is dependent on the escort average, or it is also presented[10] by

$$P = \frac{2}{7-5q}Nk_{\rm B}T, \tag{3}$$

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if the expectation value of square velocity is dependent on the standard average, where q is the nonextensive parameter whose deviation from unity measures the degree of nonextensivity of the system. It is clear that the equation of state of an ideal gas can be correctly recovered from Eqs.(1), (2) or (3) if we let $q = 1$. The nonextensivity has been considered in varieties of interesting problems where the systems are known to need nonextensive statistics due to the long-range interactions, the spatial inhomogeneity or the non-additivity.[5−19]

In this paper, we will investigate the time-space correlation of density fluctuation in a nonextensive reaction–diffusion system. In Section 2, we introduce the nonextensive pressure effect into the master equation for the characteristic function by using the density operator equation for the system. In Section 3, we take ^{3}He reaction–diffusion model as an example to analyse the nonextensive pressure effect on the density fluctuation. Finally, we present our conclusion and discussion in Section 4.

2. The generalized master equation for characteristic function

The reaction–diffusion equation for a reaction–diffusion system is expressed with the density operator, $\hat{N}(r,t)$,[20] as

$$\frac{\partial}{\partial t}\hat{N}(r,t) = R(\hat{N}) + D\nabla^2\hat{N}(r,t) + \hat{F}(r,t), \qquad (4)$$

where R is the reaction term, D is the diffusion coefficient, and $\hat{F}$ is the quantum random force, satisfying the conditions,

$$\langle\hat{F}(r,t)\rangle = 0, \quad \langle\hat{F}(r,t)\hat{N}(r,t)\rangle = 0. \qquad (5)$$

For a gas system with chemical reactions in it, if the inhomogeneous pressure leads to a flow taking place in the system with a velocity, $v(r,\, t)$, then Eq.(4), after introducing this effect,[21] becomes

$$\frac{\partial}{\partial t}\hat{N}(r,t) = -\nabla(v\hat{N}) + R(\hat{N}) + D\nabla^2\hat{N}(r,t) + \hat{F}(r,t), \qquad (6)$$

where the flow term satisfies Euler's equation, assuming v to be small, we obtain

$$\frac{\partial}{\partial t}(v\hat{N}) = -\frac{1}{m}\nabla\hat{P}, \qquad (7)$$

where the pressure should be considered as that one of the nonextensive gas, Eq.(1), which in combination with Eqs.(6) and (7) yields

$$\frac{\partial^2}{\partial t^2}\hat{N}(r,t) = \frac{\partial R(\hat{N})}{\partial t} + D\nabla^2\frac{\partial\hat{N}}{\partial t} + \frac{2k_{\rm B}T}{5-3q}\frac{1}{m}\nabla^2\hat{N} + \hat{F}'(r,t), \qquad (8)$$

where we may still assume the random term, $\hat{F}'$, to satisfy Eq.(5) based on the law of cause and effect.

According to the theory of nonequilibrium statistics, the generalized master equation satisfied by the characteristic function for particle density in reaction–diffusion systems can be derived by the density operator technique.[2] It is given by

$$\frac{\partial^2 G}{\partial t^2} = y\Big\langle\frac{\partial^2\hat{N}}{\partial t^2}\mathrm{e}^{y\hat{N}}\Big\rangle + y^2\Big\langle\Big(\frac{\partial\hat{N}}{\partial t}\Big)^2\mathrm{e}^{y\hat{N}}\Big\rangle, \qquad (9)$$

where $G(y,\, r,\, t)$ is the characteristic function of density, $\hat{N}$ is density operator, y is a parameter, $-1 \le y \le 0$, and $\langle\cdots\rangle$ denotes the statistical average. On the basis of this equation, the time–space correlation of fluctuation in reaction–diffusion systems can be generally analysed if the equation of density operator for the systems is presented. On the right hand side of Eq.(9), the second term may be neglected in comparison with the first one in the present case that y is very near zero because we will only interested in the behaviours near the point $y = 0$. Thus, substituting Eq.(8) into Eq.(9), we have

$$\frac{\partial^2 G}{\partial t^2} = y\Big\langle\frac{\partial R}{\partial t}\mathrm{e}^{y\hat{N}}\Big\rangle + yD\frac{\partial}{\partial t}\langle(\nabla^2\hat{N})\mathrm{e}^{y\hat{N}}\rangle + y\frac{2k_{\rm B}T}{5-3q}\frac{1}{m}\langle(\nabla^2\hat{N})\mathrm{e}^{y\hat{N}}\rangle. \qquad (10)$$

By using the formula,[16]

$$\langle(\nabla^2\hat{N})\mathrm{e}^{y\hat{N}}\rangle = G\nabla^2\frac{\partial}{\partial y}\ln G,$$

we find

$$\frac{\partial^2 G}{\partial t^2} = y\Big\langle\frac{\partial R}{\partial t}\mathrm{e}^{y\hat{N}}\Big\rangle + y\Big(D\frac{\partial}{\partial t} + \frac{2k_{\rm B}T}{5-3q}\frac{1}{m}\Big) \times\Big(G\nabla^2\frac{\partial}{\partial y}\ln G\Big). \qquad (11)$$

This is the generalized master equation of the nonextensive reaction–diffusion system. It is clear that the standard form for extensive systems is correctly recovered from Eq.(11) when $q = 1$.

3. The density fluctuation of the ^{3}He reaction–diffusion model

The ^{3}He reaction–diffusion model is from the p–pI nuclear reaction chain taking place inside stars, so it is the nonextensive reaction–diffusion system due to the long-range nature of the inter-particle interactions of gravitation and Coulombian forces. We consider this model as an example to analyse the nonextensive pressure effect. This model can be expressed by the reaction–diffusion equation,[22]

$$\frac{\partial Y}{\partial t} = K - k_3 Y^2 + D_Y \nabla^2 Y, \tag{12}$$

where K is regarded as a constant, k_3 is the reaction rate constant, Y is the particle density of ^{3}He, and D_Y is its diffusion coefficient. This equation is allowed to have the homogeneous stationary solution, $Y_0 = (K/k_3)^{1/2}$. If no nonextensive effect is considered, by analysing the fluctuation spectrum one can easily derived the dispersion relation,

$$\omega_k^{(\mathrm{s})} = -(2k_3 Y_0 + D_Y k^2)s, \quad s = 1, 2, \cdots, \tag{13}$$

for which we find that they are only decaying waves for all s and k, where k is the wave number.

When analysing the nonextensive effect, we consider the reaction terms in Eq.(12) as that one in the generalized master equation, Eq.(11). We find

$$\frac{\partial^2 G}{\partial t^2} = yK\frac{\partial G}{\partial t} - k_3 y(y+2)\frac{\partial^3 G}{\partial^2 y \partial t} + y\Big(D_Y\frac{\partial}{\partial t} + \frac{2k_{\mathrm{B}}T}{5-3q}\frac{1}{m}\Big)\Big(G\nabla^2\frac{\partial}{\partial y}\ln G\Big), \tag{14}$$

where we have used the birth-death expressions for the reaction terms. If let $G_0(y) = \exp\phi_0(y)$ be the homogeneous stationary solution of Eq.(14), satisfying the normalizing condition, $G_0(y=0) = 1$ or $\phi_0(y=0) = 0$, one has the following condition,

$$K - k_3(y+2)\Big(\frac{\partial^2\phi_0}{\partial y^2} + \Big(\frac{\partial\phi_0}{\partial y}\Big)^2\Big) = 0. \tag{15}$$

We let $G = G_0 + \delta G$ and take the perturbation about G_0 as

$$\delta G = G_0\tilde{\psi}_1 = G_0\phi_1\exp(\omega t + \mathrm{i}kr). \tag{16}$$

Then we derive

$$\frac{\partial^2\tilde{\psi}_1}{\partial t^2} = -k_3 y(y+2)\Big(\frac{\partial^3\tilde{\psi}_1}{\partial y^2\partial t} + 2\frac{\partial\phi_0}{\partial y}\frac{\partial^2\tilde{\psi}_1}{\partial y\partial t}\Big) + y\Big(D_Y\frac{\partial}{\partial t} + \frac{2k_{\mathrm{B}}T}{5-3q}\frac{1}{m}\Big)\nabla^2\frac{\partial\tilde{\psi}_1}{\partial y}, \tag{17}$$

where we have used condition, Eq.(15). Substituting Eq.(16) into Eq.(17) and using the small fluctuation approximation we find

$$\omega^2\phi_1(y) = y\Big(-2k_3(y+2)\omega\frac{\partial\phi_0}{\partial y} - \omega D_Y k^2 - \frac{2k_{\mathrm{B}}T}{5-3q}\frac{1}{m}k^2\Big)\frac{\mathrm{d}\phi_1}{\mathrm{d}y}. \tag{18}$$

According to the theory of ordinary differential equations, the solutions of Eq.(18) can be expanded near the singular point $y = 0$ as $\phi_1 \sim y^s\sum_{m=0}^{\infty} b_m y^m$. For a fixed $k \neq 0$, only the solutions for $s = 1, 2, 3, \cdots$. are allowed to be the physical ones. Thus, the coefficient equation for the lowest order power of y yields the dispersion relation,

$$\omega^2 + s(2k_3Y_0 + D_Y k^2)\omega + \frac{2k_{\mathrm{B}}T}{5-3q}\frac{1}{m}sk^2 = 0 \quad (s = 1, 2, 3, \cdots), \tag{19}$$

for which we find

$$\omega_{\pm}(k,s) = -\frac{1}{2}(2k_3Y_0 + D_Y k^2)s \pm\frac{1}{2}\Big((2k_3Y_0 + D_Y k^2)^2 s^2 - \frac{8k_{\mathrm{B}}T}{5-3q}\frac{1}{m}sk^2\Big)^{1/2}. \tag{20}$$

These relations recover as the cases for the extensive system when $q = 1$. From these relations we come to the conclusions as follows.

(a) There are tow branches of purely decaying waves if

$$(2k_3Y_0 + D_Y k^2)^2 > \frac{8k_{\mathrm{B}}T}{(5-3q)m}k^2, \tag{21}$$

which is basically equivalent to the case of no nonextensive pressure effect.

(b) There are still tow branches of decaying waves for $s = 1$ if

$$(2k_3Y_0 + D_Y k^2)^2 < \frac{8k_{\mathrm{B}}T}{(5-3q)m}k^2. \tag{22}$$

But the nonextensive pressure effect can lead to the density oscillations, which will propagate in space in the form of fluctuation waves with the phase speeds given by

$$V = \frac{1}{2}\Big(\frac{8k_{\mathrm{B}}T}{(5-3q)m}s - (2k_3Y_0/k + D_Y k)^2 s^2\Big)^{1/2}. \tag{23}$$

In particular, it is shown that the phase speeds can be more than the sound speed, $(k_{\mathrm{B}}T/m)^{1/2}$, if the nonextensive parameter q is near 5/3.

(c) The dispersion relation Eq.(13) is recovered from Eq.(20) for $s = 1$ if

$$(2k_3Y_0 + D_Y k^2)^2 = \frac{8k_{\mathrm{B}}T}{(5-3q)m}k^2. \tag{24}$$

It is clear that in all the three cases, Eqs.(21), (22) and (24), the nonextensive parameter q plays a very important role. To some degree, its value determines which of the three cases will take place in the system. In particular we find from Eq.(20) that there must be one branch of purely growing wave if q is more than 5/3, which means that the reaction–diffusion system is unstable.

The study of the physical meaning for the nonextensive parameter q different from one has now made some important progress. For instance, when the long-range interactions in the system are Coulombian forces,[7] it is found that $k_{\rm B}\nabla T-(1-q)e\nabla\varphi=0$, where e is the electronic charge and φ is the electric field potential. When the long-range interactions in the system are the gravitational forces,[5] it is found that

$$1-q=-\frac{k_{\rm B}}{\mu m_{\rm H}}\frac{{\rm d}T}{{\rm d}r}\Big/\frac{GM(r)}{r^2},$$

where G is the gravitational constant, $M(r)$ is the mass interior to a sphere of radius r, $m_{\rm H}$ is the mass of hydrogen atom, and μ is the mean molecular weight. This fine formula has led to the key experiment test of nonextensive statistics by using the helioseismological measurements.[8]

4. Summary and conclusion

In summary, we have investigated the time-space correlation of density fluctuation in the nonextensive reaction–diffusion system where the equilibrium distribution can be described by the generalized Maxwell–Boltzmann distribution in the framework of nonextensive statistical mechanics. By using the density operator technique, we introduce the nonextensive pressure effect into the master equation and thus derive the generalized master equation, Eq.(11), by which we can investigate the nonextensive effect on the density fluctuation in a nonextensive reaction–diffusion system.

In order to analyse the nonextensive effect on the density fluctuation in a reaction–diffusion system, as an example we have investigated the ^{3}He reaction–diffusion model. This model is from the p–pI nuclear reaction chain that is taking place inside stars, so it can be considered as the nonextensive reaction–diffusion system due the long-range nature of the inter-particle interactions of gravitation and Coulombian forces. We find that the characteristics of the spectrum for fluctuation waves have been changed after the nonextensive pressure effect is taken into account. Equation (13) shows that, for every order of fluctuation waves, the frequencies $\omega_k^{(s)}$ are proportional to their order $s=1,2,3,\cdots$ if the nonextensive pressure effect is unconsidered. But in Eq.(20) this characteristics of the fluctuation spectrum have been changed where the nonextensive pressure effect is considered.

In all the three cases discussed in Eqs.(21), (22) and (24), the nonextensive parameter q plays a very important role in determining which of the three cases will take place in the system. In particular we find that there must be one branch of purely growing wave if q is more than 5/3, which means that the reaction–diffusion system is unstable. It is also worth notice that the phase speeds can be more than the sound speed, $(k_{\rm B}T/\ m)^{1/2}$, if the nonextensive parameter q is near 5/3.

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