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DAMPING OF COLLECTIVE MODES AS OPEN QUANTUM SYSTEMS

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In the framework of the Lindblad theory for open quantum systems the following results are obtained: a generalization of the fundamental constraints on quantum mechanical diffusion coefficients which appear in the corresponding master equations, a generalization of the Hasse pure state condition and a generalized Schrödinger type nonlinear equation for an open system. Also, the Schrödinger, Heisenberg and Weyl-Wigner-Moyal representations of the Lindblad equation are given explicitly. Based on these representations, one shows that various master equations for the damped quantum oscillator used in the literature for the description of the damped collective modes in DIC are particular cases of the Lindblad equation and that the majority of these equations are not satisfying the constraints on quantum mechanical diffusion coefficients.

The investigation has been performed at the Laboratory of Nuclear Reactions, JINR.

Затухание коллективных мод как эффект открытых квантовых систем

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В рамках теории Линдблада для открытых квантовых систем были получены следующие результаты: обобщение соотношения для ограничения коэффициентов диффузии, обобщенное условие для существования чистых состояний и обобщенное уравнение типа Шредингера для открытых систем. Были получены также в явном виде представления Шредингера, Гейзенберга и Вайла-Вигнера-Мойала уравнения Линдблада. На основе этих представлений было показано, что многие уравнения для гармонического осциллятора с диссипацией энергии, использованные в литературе для описания затухания коллективных мод, представляют собой частные случаи уравнения Линдблада и большинство этих уравнений не выполняет соотношения для ограничения коэффициентов диффузии, вытекающих из принципа неопределенности.

Работа выполнена в Лаборатории ядерных реакций ОИЯИ.

The only systems for which we can study experimentally the dynamics of nuclear matter are the deep inelastic collisions (DIC). In the last years a large body of experimental data has been accumulated in this field [1] which allows a vivid discussion between the two extreme theoretical approaches; the transport theories which view this process as being due to independent particle propagation thus stressing the stochastic, random walk nature of the relaxation phenomenon [2] and the quantum mechanical collective theories which view this process as being due to large scale collective modes thus stressing the coherent nature of the relaxation phenomenon [3].

It is now widely admitted that the description of the friction in quantum mechanics is far from trivial. Perhaps, the greatest difficulty arises from the fact that in classical mechanics the dissipation of the energy is directly related to the presence of a nonzero momentum (the friction force is proportional to the velocity). On the other hand it is known that such systems with forces proportional to the velocities cannot be described by the standard Hamiltonian mechanics and that the Liouville theorem is not valid. Such forces, which cause a decrease in the phase space volume, are more suitable described in the frame of the theory of stochastic processes.

In order to prevent the fall in time of any finite volume in phase space into a volume smaller than $(\hbar/2)^n$ a diffusion process (stochastic process) which increases the volume in phase space is needed. An equilibrium state is a state in which these two opposite tendencies balance. It follows that in order to obtain a quantum theory for systems with friction forces it is necessary to understand how such quantum diffusion processes arise which balance the friction forces and prevent the violation of the uncertainty relations.

In the literature there are an enormous number of papers which try to solve this problem by introduction, in addition to the friction forces, of some diffusion coefficients, using quite different and contradictory arguments.

In the present paper, we extend our previous work [4] on the dynamics of charge equilibration in damped heavy ion collisions as a large scale collective mode by describing the corresponding collective mode as an open quantum system. We adopt the Lindblad axiomatic way of introducing dissipation in quantum mechanics [5,6] based on completely positive dynamical semigroups with bounded generators.

We succeeded to obtain: a generalization of the fundamental constraints on quantum mechanical diffusion coefficients which appear in the corresponding master equation, a generalization of the Hasse pure state condition and a generalized Schrödinger type nonlinear and nonhermitic equation for an open system. Based on the Schrödinger, Heisenberg and Weyl-Wigner-Moyal representations of the Lindblad master equations we show that various master equations for the damped quantum oscillator used in the literature for the description of the damped collective modes in DIC are particular cases of the Lindblad equation and that the majority of these equations are not satisfying the constraints on quantum mechanical diffusion coefficients.

The Lindblad master equations are of the following form:

$$\frac{d\rho}{dt} = L(\rho(t)) = -\frac{i}{\hbar}[H, \rho(t)] + \frac{1}{2\hbar}\sum_{j=1}^{N}([V_j\rho(t), V_j^*] + [V_j, \rho(t)V_j^*]), \tag{1}$$

where $\rho(t)$ is the density matrix and V_j the corresponding bounded operators.

Also Lindblad proposed a model for the damped quantum harmonic oscillator with unbound V_j of the form $V_j = a_j p + b_j q$, $j = 1,2$, where a_j, b_j are complex numbers; and q and p the usual operators with the commutation relation $[q, p] = i\hbar$. For this model eq. (1) becomes

$$\frac{d\rho}{dt} = L(\rho(t)), \tag{2}$$

where

$$L(\rho) = -\frac{i}{\hbar}[H_0, \rho] - \frac{i(\lambda-\mu)}{2\hbar}[\rho, pq + qp] - \frac{i\lambda}{\hbar}[q, p\rho - \rho p] -$$

$$-\frac{D_{pp}}{\hbar^2}[q,[q,\rho]] - \frac{D_{qq}}{\hbar^2}[p,[p,\rho]] + \frac{(D_{pq}+D_{qp})}{\hbar^2}[p,[q,\rho]] \tag{3}$$

and $H_0 = \frac{1}{2m}p^2 + \frac{m\omega^2}{2}q^2$, $\quad H = H_0 + \frac{\mu}{2}(pq + qp)$.

Here we denoted by D_{pp}, D_{qq}, D_{pq}, and D_{qp} the diffusion coefficients and by λ the friction constant, all the parameters being real and related to the complex numbers a_j and b_j by the relations

$$D_{qq} = \frac{\hbar}{2}\sum_{j=1}^{2}|a_j|^2; \qquad D_{pp} = \frac{\hbar}{2}\sum_{j=1}^{2}|b_j|^2;$$

$$D_{pq} = D_{qp} = -\frac{\hbar}{2} \mathrm{Re} \sum_{j=1}^{2} \bar{a}_j b_j ; \qquad \lambda = -\mathrm{Im} \sum_{j=1}^{2} \bar{a}_j b_j , \tag{4}$$

where $\bar{a}_j$ means the complex conjugate of a_j.

Thus, the following constraints for the quantum mechanical diffusion coefficients result:

$$D_{qq} \geq 0; \qquad D_{pp} \geq 0 ; \qquad D_{qq} D_{pp} - D_{pq}^2 \geq \frac{\lambda^2 \hbar^2}{4} , \tag{5}$$

the last inequality being a consequence of the Schwartz inequality

$$(\mathrm{Re} \sum_{j=1}^{2} \bar{a}_j b_j)^2 + (\mathrm{Im} \sum_{j=1}^{2} \bar{a}_j b_j)^2 \leq \sum_{j=1}^{2} |a_j|^2 \sum_{j=1}^{2} |b_j|^2 . \tag{5'}$$

In the Heisenberg representation the master eq.(1) is:

$$\frac{dA(t)}{dt} = \tilde{L}(A(t)) = \frac{i}{\hbar} [H, A(t)] + \frac{1}{2\hbar} \sum_j (V_j^* [A(t), V_j] + [V_j^*, A(t)] V_j). \tag{6}$$

If the time evolution of the operator $M = \sum_j V_j^* V_j$ is considered we obtain from the 2-positivity of the dynamical semigroup generated by (6) that

$$M(t) \geq \sum_j V_j(t)^* V_j(t). \tag{7}$$

From this relation an inequality for mean values of M, V_j^*, and V_j follows immediately if we observe that the map $A \to \mathrm{Tr}\,\rho A$ is also 2-positive.

$$\mathrm{Tr}\,\rho M(t) \geq \sum_j \mathrm{Tr}(\rho V_j(t)^*) \,\mathrm{Tr}(\rho V_j(t)). \tag{8}$$

By the duality $\mathrm{Tr}\,\rho(A(t)) = \mathrm{Tr}\,\rho(t) A$ rel.(8) becomes:

$$\mathrm{Tr}(\rho(t) \sum_j V_j^* V_j) \geq \sum_j \mathrm{Tr}(\rho(t) V_j^*) \,\mathrm{Tr}(\rho(t) V_j). \tag{9}$$

This inequality is a generalization of the inequality (11) from ref. /6/ to all Markovian master equations.

For the damped quantum harmonic oscillator, the above inequality becomes:

$$D_{qq} \sigma_{pp}(t) + D_{pp} \sigma_{qq}(t) - 2 D_{pq} \sigma_{pq}(t) \geq \lambda \frac{\hbar^2}{2} , \tag{10}$$

where we have used the notations

$$\sigma_q = Tr(\rho(t)q); \quad \sigma_p = Tr(\rho(t)p); \quad \sigma_{qq} = Tr(\rho(t)q^2) - \sigma(t)^2$$

$$\sigma_{pp} = Tr(\rho(t)p^2) - \sigma_p(t)^2; \quad \sigma_{pq}(t) = Tr(\rho(t)(\frac{pq+qp}{2})) - \sigma_p(t)\sigma_q(t). \tag{11}$$

The equality in rel.(9) is a necessary and sufficient condition for $\rho(t)$ to be a pure state for all time $t > 0$. Indeed, the condition $\rho^2(t) = \rho(t)$ which is a necessary and sufficient condition for $\rho(t)$ to be a pure state /7-9/ gives $Tr\rho(t)^2 = 1$ for all $t > 0$. This implies:

$$\frac{d}{dt} Tr(\rho(t)^2) = Tr\rho(t)L(\rho(t)) = 0 \qquad t > 0, \tag{12}$$

or by using the explicit form of $L(\rho(t))$ given by eq.(1)

$$Tr(\rho(t)L(\rho(t)) = \frac{1}{2\hbar}\sum_j (Tr(\rho(t)V_j\rho(t)V_j^*) - Tr(\rho(t)^2 V_j^* V_j)) \tag{13}$$

and the conditions $\rho^2(t) = \rho(t)$ and $\rho(t)A\rho(t) = Tr(\rho(t)A)\rho(t)$ we have

$$Tr(\rho(t)\sum_j V_j^* V_j) = \sum_j Tr(\rho(t)V_j)Tr(\rho(t)V_j^*). \tag{14}$$

This equality is a generalization of the Hasse pure state condition /7-9/ to all Markovian master equations.

The condition $\rho^2(t) = \rho(t)$ implies firstly that $\rho(t)\phi = (\psi(t),\phi)\psi(t)$ for any wave function ϕ and secondly that its derivative

$$\frac{d\rho(t)}{dt} = \frac{d\rho(t)^2}{dt} = L(\rho(t))\rho(t) + \rho(t)L(\rho(t)) \tag{15}$$

is equivalent with the following Schrödinger type nonlinear and nonhermitic equation:

$$\frac{d\psi}{dt} = -\frac{i}{\hbar}(H + i\sum_j (\psi(t), V_j^*\psi(t))V_j - \\ - \frac{i}{2}(\psi(t), \sum_j V_j^* V_j \psi(t)) - \frac{i}{2}\sum_j V_j^* V_j)\psi(t). \tag{16}$$

This result is a generalization to all Markovian master equations of the results obtained for particular master equations in refs. /10/ and /7,8/.

For the damped quantum harmonic oscillator the new "Hamiltonian" is

$$H+\lambda(\sigma_p(t)q-\sigma_q(t)p)+$$

$$+i\{\lambda\hbar-\frac{D_{qq}}{\hbar}((p-\sigma_p(t))^2+\sigma_{pp}(t))-\frac{D_{pp}}{\hbar}((q-\sigma_q(t))^2+\sigma_{qq}(t))+ \quad (17)$$

$$+\frac{D_{pq}}{\hbar}((p-\sigma_p(t))(q-\sigma_q(t))+(q-\sigma_q(t))(p-\sigma_p(t))+2\sigma_{pq}(t))\}.$$

It is interesting to remark that the mean value of this new "Hamiltonian" is equal to the mean value of the original Hamiltonian H if the equality is valid in the inequality (10). In this last case the new "Hamiltonian" is equal to

$$H+\lambda(\sigma_p(t)q-\sigma_q(t)p)-\frac{i}{\hbar}\{D_{qq}(p-\sigma_p(t))^2+D_{pp}(q-\sigma_q(t))^2+$$

$$+D_{pq}((p-\sigma_p(t))(q-\sigma_q(t))+(q-\sigma_q(t))(p-\sigma_p(t))-\frac{\hbar^2\lambda}{2}\}. \quad (18)$$

This result, from the physical point of view, is quite natural since the average value of the new "Hamiltonian" of the nonlinear and nonhermitic Schrödinger equation describing the open system must give the energy of the open system.

Another possible representation of the Lindblad master equation is the Weyl-Wigner-Moyal representation. This is a phase-space representation of the quantum mechanics. Roughly speaking such a representation is a mapping from the Hilbert space operators to the functions on the classical phase space in such a way that if A is mapped into $f_A(x,y)$ and ρ is mapped onto $f_\rho(x,y)$, then

$$\mathrm{Tr}(\rho A)=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}f_\rho(x,y)f_A(x,y)\,dx\,dy. \quad (19)$$

This representation can be easily obtained by using Wigner mapping of the density operators $\rho(t)$ from the Hilbert space onto the functions $f_{\rho(t)}(x,y)$ on the classical phase space

$$f(x,y,t)=f_{\rho(t)}(x,y)=\frac{1}{(2\pi h)^2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}e^{-\frac{i}{\hbar}(x\eta-y\xi)}\mathrm{Tr}(\rho(t)W(\xi,\eta))d\xi d\eta, \quad (20)$$

where $W(\xi,\eta)$ is the Weyl operator.

Indeed, taking the time derivative of the Wigner function (20), using the master equation in the Heisenberg representation (6) and the explicit action of the dynamical semigroup on the Weyl operators we obtain:

$$\frac{\partial f(x,y,t)}{\partial t} = -\frac{y}{m}\frac{\partial f(x,y,t)}{\partial x} + m\omega^2 x \frac{\partial f(x,y,t)}{\partial y} + (\lambda-\mu)\frac{\partial x f(x,y,t)}{\partial x} +$$

$$+(\lambda+\mu)\frac{\partial y f(x,y,t)}{\partial y} + D_{qq}\frac{\partial^2 f(x,y,t)}{\partial x^2} + D_{pp}\frac{\partial^2 f(x,y,t)}{\partial y^2} + 2D_{pq}\frac{\partial^2 f(x,y,f)}{\partial x \partial y}. \tag{21}$$

This equation looks very classical, like an equation of the Fokker-Planck type, but we must be very careful with the initial function $f(x,y,0)$ on the phase space which must be a Wigner transform of a density operator in order to keep the quantum mechanical properties of the system.

Because the most frequently choice for $f(x,y,0)$ is a Gaussian function and because eq.(21) preserves this Gaussian type, i.e., $f(x,y,t)$ is also a Gaussian function, the differences between the quantum mechanics and classical mechanics are completely lost in this representation of the master equation. This is a possible explanation for the frequently occurred ambiguities on this subject in the literature.

In the following we show that various master equations for the damped quantum oscillator used in the literature for the description of the damped collective modes in DIC are particular cases of the Lindblad équation and that the majority of these equations are not satisfying the constraints on quantum mechanical diffusion coefficients.

Indeed, in the form (3) a direct comparison with eq.(1) from refs.[7,10-12] is possible. It follows that this master equation supplemented with the fundamental constraints (5) is a particular case of eq.(3), when $\mu = \lambda$.

Also a particular case of eq.(3) is the master equation (12) considered in ref.[13] for $\lambda = \gamma(\omega)/2m = \mu$; $D_{qq} = 0$; $D_{pp} = \gamma(\omega)T^*(\omega)$; and $D_{pq} = 0$. Evidently the constraints (5) are not satisfied.

Analogously, the master equation (A.36) considered in ref.[9] is a particular case of eq.(3) for $\lambda = \mu = \gamma/2$; $D_{pp} = D$; $D_{qq} = 0$; $D_{pq} = D_{qp} = -d/2$ and $H_0 = p^2/2m + \frac{1}{2}m(\omega^2 - \bar{k}^2)q^2$. Again the constraints (5) are not satisfied.

In the form (21) a direct comparison with two kinds of quantum master equations, written for the Wigner transform of the density matrix, obtained recently in ref.[14] is possible.

The first master equation (see eq.(5.1) of ref.[14]) is a particular case of eq. (21) for $\lambda = \mu = \Gamma/2$; $D_{pp} = D/2$; $D_{qq} = 0$; $D_{pq} = D_{qp} = B/2$ and $H = H_0 - \frac{Am\omega}{2}q^2 + f(t)q$. Evidently the constraints (5) are not satisfied.

The second master equation (see eq. (5.6) of ref.[14]) is also a particular case of eq. (21) for $\mu = 0$; $\Gamma_p^{II} = \Gamma_R^{II} = \lambda$; $D_{pp} = \frac{1}{2} D_p^{II}$; $D_{qq} = \frac{1}{2} D_R^{II}$; $D_{pq} = 0$ and $H = H_0 - A^{II} \frac{m\omega}{2} q^2 - \frac{A^{II}}{2m\omega} p^2 + f(t)q$. This equation satisfies the fundamental constraints (5).

Finally we should like to stress that the collective fluctuations have not been revealed with clarity by experiment. Now it is clear that, due to the similarity of the equations and solutions in both extreme theoretical approaches: transport theories and quantum collective theories, the effects are similar. We consider that it is premature to conclude, like the majority of the recent papers[1], that the present data suggest that the dynamical evolution of the dinuclear system may be seen as an independent particle exchange process constrained by the underlying potential energy surface (PES).

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