Записки научных
семинаров ПОМИ
Том 251, 1998 г.

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EFFECTIVE POTENTIAL AND QUANTUM DYNAMICAL CORRELATORS

Abstract. A new approach to calculating properties of quantum dynamical systems by means of calculation of classical type is presented. It is based on the Mori theory and on projection technique.

§1. Approach to quantum dynamical correlators

In recent years a large amount of work has been devoted to the investigation of a method that permits to determine, at least approximatively, the properties of quantum dynamical systems by means of calculations of classical type. This problem has been successfully solved for the static case by means of a variational procedure based on path integral formulation of statistical mechanics: the method leads to the construction of an effective potential that accounts completely for the quantum corrections of the quadratic part of the integration (*the harmonic oscillators*) and treats in a self-consistent one loop approximation the quantum effects due to nonlinear terms [1, 2, 3]. A Hamiltonian formulation of the procedure, hereby referred to as the PSCQHA [4, 5, 6], was obtained by recalling the Wigner and Weyl approaches [4] and has been extended the range of application of the method to a large number of dynamical systems, including spin systems [5]. The effective potential has proved to be a very powerful tool for concrete computations: in particular it has allowed the reduction of quantum Monte Carlo to classical Monte Carlo numerical calculations [6], with evident fruitful consequences [7].

A rigorous treatment of the dynamical problem is, as always, much more difficult. A success in such a program, however, is scientifically very remunerative. Indeed, for instance, it opens the way to a sound formulation of molecular dynamics for quantum systems. It permits, moreover, an easier calculations of correlation functionals and scattering cross sections. In perspective, then, it could also give a physically meaningful way of attacking the quantum chaos problem.

Using the effective potential obtained in [1, 2], some attempts of extending the treatment to a dynamical setting have been tried [8]. However, by admission of the aithors themselves, these attempts assume some *ad hoc* multiplicative relation in order to connect the "centroid molecular dynamics" to the quantum correlation function [8, 9].

In this paper we shall present a new approach, that, in our opinion, is more rigorous, suited to the problem and applicable to a large number of physical situations. It is based on the Mori theory and on projection techniques [10]. At lowest order, we recover the heuristic expressions of ref. [8], but within the framework of a consistent analysis.

2. Weyl-unified dynamics

The key points of our theory are:

i) the dynamics of classical and quantum oscillatots is the same; the only difference is the atatic amplitude factor determined by the initial conditions.

ii) the use of the Weyl representation [11] which translates quantum problems into a classical framework.

Starting from what we have learned in the theory of the effective potential and PSCQHA [4, 6], we develop a semiclassical calculation in the Weyl representation, that describes quantum mechanics in terms of the classical canonical variables q and p. A detailed treatment of the Weyl transform can be found, for instance in [4]. If we consider a dynamical system with a Hamiltonian H, the quantum equation of motion of an operator A, in the Weyl representation, reads [12]

$$\frac{d\Lambda_w}{dt} = \frac{2}{\hbar}\mathcal{H}_w \sin\frac{\hbar\Lambda}{2} A_w = i\mathcal{L}\, A_w . \tag{1}$$

Here A_w and $\mathcal{H}_w$ are the Weyl symbols of the corresponding quantum operators:

$$\mathcal{O}_w(x,p) = \int_{-\infty}^{\infty} d\zeta e^{ip\zeta} \langle\, x-\zeta|\mathcal{O}|x+\zeta\,\rangle, \tag{2}$$

and

$$\Lambda = \overleftarrow{\partial}_p \overrightarrow{\partial}_x - \overleftarrow{\partial}_x \overrightarrow{\partial}_p . \tag{3}$$

We call Liouvillian the operator $\mathcal{L}$ defined in Eq. (1). The average of a dynamical variable, can be written:

$$\mathrm{Tr}\,(\rho\mathcal{O}) = \langle\, \mathcal{O}\,\rangle = \int_{-\infty}^{\infty} dp\, dx\, \rho_w(p,x)\mathcal{O}_w(p,x). \tag{4}$$

The classical equation of motion, and the well known phase-space classical average is easily recovered for $\hbar \to 0$.

For sake of simplicity, we shall only consider a system with one degree of freedom and with a Hamiltonian

$$\mathcal{H} = \hbar\omega_0\, a^\dagger a + gV(a^\dagger, a), \tag{5}$$

where $a = p + iq$, $a^\dagger = p - iq$, and g is the quantum couplihg. In the following, when not necessary, we put $\hbar = 1$. The equation of motion for a_w can be put into the following form along the line of the projecton – Zwanzig-Mori theory [10]:

$$\frac{da_w(t)}{dt} = i\omega a_w(t) + \int_0^t d\tau M(\tau) a_w(t-\tau) + f_w(t). \tag{6}$$

This equation can be solved once the initial condition $a_w(0)$ is assigned. As it is well known, the term $f(t)$ describes the effect of the fluctuating forces and has the following expression:

$$f_w(t) = e^{it}(1-P)\mathcal{L}(1-P)\mathcal{L}\, a_w(0), \tag{7}$$

where P is the projection operator onto the direction of $a_w(0)$. The expkicit expression of P, as well as the memory kernel $M(t)$ are conveniently given in terms of a scalar product introduced by Mori [10]. The latter plays an important role in the theory and, for quantity with vanishing thermal averages, reads:

$$(a|b(t)) = \int_0^\beta d\lambda \langle\, a_w^*(0)\, b_w(t+i\lambda)\,\rangle. \tag{8}$$

It turns out that:

$$Pb(t) = (a|b)^{-1}(a|b(t)). \tag{9}$$

One realizes that this is just the Kubo function and reduces to be proportional to the correlation function in the classical limit.

The quantities of physical interest are the Fourier transforms $C(\omega)$ and $R(\omega)$ of the correlation function – probed by scattering experiments – and Mori product, respectively. They are connected by "detailed balance" principle:

$$C(\omega) = \frac{\omega}{1 - e^{-\beta\omega}}\, R(\omega). \tag{10}$$

The frequency ω is given by:

$$i\omega = (q_w|a_w)^{-1}(a_w|P\mathcal{L}a_w) \tag{11}$$

while the memory kernel $M(t)$ turns out to be

$$M(t) = (a_w|a_w)^{-1}(f_w(t)|f_w(0)). \tag{12}$$

Referring to Eq. (6), $M(\tau)$ can be written in the form

$$M(\tau) = \delta_1\,\Xi_1, \quad \Xi_1 = (f_w^{(1)}(0)|f_w^{(1)}(0))^{-1}(f_w^{(1)}(\tau)|f_w^{(1)}(0)) \tag{13}$$

where

$$\delta_1 = (a_w(0)|a_w(0))^{-1}(f_w^{(1)}(0)|f_w^{(1)}(0),$$
$$f_w^{(0)} \equiv a_w, \quad \omega_0 \equiv \omega, \quad P_0 \equiv P \quad \mathcal{L}^{(0)} \equiv \mathcal{L}; \tag{14}$$

the insertion of a new index will be necessary for the following, eventually together with the other definitions.

It can be seen that the factor δ_1 is defined only in terms of static quantities. We point out that the effective potential theory permits an appropriate (even though approximate) determination [6], which has been improved recently [13].

3. Continued fraction expansion

The equation of motion for

$$\Xi_0(\tau) = \frac{a_w|a_w(\tau)}{a_w(0)|a_w} \tag{15}$$

becomes:

$$\frac{d\Xi_0}{dt} = i\omega\Xi_0(t) + \delta_1\int_0^t d\tau\Xi_1(\tau)\Xi_0(t-\tau). \tag{16}$$

By means of the insertion of a set of projection operators P_j, Eq. (16) generates a hierarchy of equation with a reduced Liouvillian:

$$\mathcal{L}_j^{(j)} = (1 - P_j - P_{j-1} - \cdots - P_1 - P_0)\mathcal{L}^{(0)}. \tag{17}$$

Finally, the continued-fraction expansion for the Laplace transform $\Xi_0(z) = R(z)/R(t=0)$ is obtained [10]:

$$\Xi_j(z) = \frac{1}{z + i\omega_j + \delta_{j+1}\Xi_{j+1}(z)},$$

$$\omega_j = \frac{(f_w^{(j)}|\mathcal{L}_j f_w^{(j)})}{(f_w^{(j)}|f_w^{(j)})}, \quad \delta_{j+1} = \frac{(f_w^{(j+1)}|f_w^{(j+1)})}{(f_w^{(j)}|f_w^{(j)})}. \tag{18}$$

The quantities ω_j and δ_{j+1} are related to the first $2(j+1)$ moments of the time series expansion of $\Xi_0(t)$. While $(f_w^{(j)}|f_w^{(j)})$ with $j \neq 0$ can be expressed in terms of static correlation, the normalization quantity $(f_w^{(0)}|f_w^{(0)})$ required the direct evaluation of the Mori product, giving the static susceptibility.

Recently [13], using functional derivatives, all quantities are accessible by means the effective potential. As a matter of fact, we successed in evaluating the average of the imaginary time ordered products of operators that involve both momentum and displacement. If we introduce the two-component vector $\hat{z} =^t (\hat{p}, \hat{x})$, after some algebra, a useful general formula can be derived from the generating functional:

$$\Big\langle \mathcal{T}\Big[\prod_{\nu=1}^{N} \widehat{F}_\nu\big(\hat{z}_{i_\nu}(u_\nu)\big)\Big]\Big\rangle$$

$$= \mathcal{N}\int \frac{d\eta\, d\xi}{2\pi\hbar} e^{-\beta[\eta^2/2m + V_{\rm eff}]}\Big\langle\Big\langle \prod_{\nu=1}^{N} F_\nu\big(\rho_{i_\nu} + y_{i_\nu}(u_\nu)\big)\Big\rangle\Big\rangle. \tag{19}$$

Here ρ indicates the classical counterpart of the operator $\hat{z}$, while double braces denote the average over the Gaussian distribution of the variables $y_{i_\nu}(u_\nu)$, defined by the second moments,

$$\big\langle\big\langle \hat{y}_i(v)\, \hat{y}_j(u)\big\rangle\big\rangle = \Phi_{ij}(u-v). \tag{20}$$

For instance, by this expression, (19) the static average of a quantity $A(x)$ dependent on the coordinates only, turns out to be

$$\langle \widehat{A} \rangle = \mathcal{N}\sqrt{\frac{m}{2\pi\beta\hbar^2}} \int d\xi \langle\langle A(\xi) \rangle\rangle e^{-\beta V_{\rm eff}(\xi)}, \tag{21}$$

where

$$\langle\langle \widehat{A}(\xi) \rangle\rangle = (2\alpha\pi)^{-1} \int d\zeta A(\xi+\zeta) e^{-\zeta^2/(2\alpha)} \tag{22}$$

denotes the Gaussian spread of the variable $A(x)$ with moment

$$\alpha = \hbar/(2m\omega)(\coth f - 1/f). \tag{23}$$

The paramenetr $f = \beta\hbar\omega/2$, introduced by Feynman, determines the quantum character of the system.

We finally observe that the calculations of $\Xi(z)$ – and therefore of $C(\omega)$ – can be approached from the knowledge of the static quantities δ_j up to a sufficiently large number $j = J$, supported by some insight into long time behaviour of the continued fraction termination $\Xi_J(t)$ [14].

4. Effective potential dynamics

The expressions so far given are exact. We can also develop an approximation scheme along the same track that has proved so accurate in the treatment of the effective potential. This means that we can account exactly for the classical part as well as for the fully quantum contribution of the harmonic oscillators. The purely quantum effects of the nonlinear terms will then be calculated in a self consistent way at the level of one loop approximation. In particular, when operating on the nonlinear part $g\mathcal{H}_w^{nl}$, we shall be allowed to substitute at lowest order in the non linear quantum coupling:

$$(2\hbar)g\mathcal{H}_w^{nl}\sin(\hbar\Lambda/2) \sim g\mathcal{H}_w^{nl}\Lambda. \tag{24}$$

We therefore split the Liouvillian operator into the sum $\mathcal{L} = \mathcal{L}_0 + g\mathcal{L}_1$, where

$$\mathcal{L}_0 = 2\Omega\Big(a_w^*\, a_w + \frac{1}{2}\Big)\sin\frac{\hbar\Lambda}{2}, \quad g\mathcal{L}_1 = gW(a_w^*\, a_w)\Lambda. \tag{25}$$

It is apparent from Eq. (25) that the quadratic part is treated in fully quantum way, giving the quantum evolution of the "best" oscillator, while the non linearity causes a "ckassic" dynamics. As already done in the framework of the effective potential approach [1, 6], an one-loop renormalization of the coupling due to the quantum fluctuations only can give us a suitable "classic-like" term $W(a_w^*, a_w)$. The parameters Ω and W will be determined by physical requirements.

As a consequence of the splitting $\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_1$, at the lowest nonvanishing order in the coupling constant we have these important consequences. The quantum effects on dynamics refers to the imaginary part of the path $(0, i\beta)$. We take into account that the parameters of the effective potential are calculated at the average point of this path along which it is subjected be an harmonic potential. Therefore it is a consequence that Ω and W are exactly the same as defined by the effective potential for the static case!

The validity of the use of the effective potential is related to the quantum coupling g. At the first order the Definition 3 of $f_w(t)$ becomes:

$$f_w(t) = e^{-\lambda(1-P_0)\mathcal{L}_0} f_w(0) = e^{-\lambda(1-P_0)\mathcal{L}_0} f_w(0)(1-P)g\mathcal{L}_1\, a_w(0). \tag{26}$$

With the approcimate expression (26) of the fluctuating force, the integration on λ in the relaxation function can be easily performed. The result of this integration is cancelled out by the denominator in the expressions of Ξ_j, so that only correlation functions done by the rules given by Eqs. (19), (20), (21) are involved. Because also all the parameters δ's are calculated with the same receipt, $(a_w|a_w)$ included, we obtain now from (16) an hierarchy where the static parameters are always calculated consistently by the effective potential. Moreover, we can perform a further approximation, valid at lowest order, both in the quantum coupling g and in the quantum Gaussian fluctuations α, namely,

$$\langle\langle\, a_w(t)a_w\rangle\rangle = \langle\langle\, a_w(t)\rangle\rangle\langle\langle\, a_w\rangle\rangle. \tag{27}$$

At this level the equation of motion for $a_w(t)$ becomes

$$\frac{da_w(t)}{dt} = i\Omega a_w(t) + \delta_1 \int_0^1 d\tau \Xi_1(\tau) a_w(t-\tau) + f_w(t), \tag{28}$$

where $M(\tau) = \delta_1\Xi_1$, is given simply by a classical-like correlation functions. Therefore Eq. (28) represents a classical evolution of $a_w(t)$ where the frequency Ω and the potential W must be determined in such a way to reproduce the same static average values of the observables. At this approximation level, therefore, they must coincide with the quantum-renormalized frequency and with the effective potential parameter of the static case [4]. At this point the Mori product $\Xi_0(t)$ is nothing but its dynamical correlation function calculated by the classical-like effective potential. Finally, through the detailed balance principle, we can recover the spaectral shape as guessed in [8].

Our derivation indicates also how to improve the method. We can delay the decoupling procedure at later stage calculating consistently the related static parameters δ. In this way the classical-like dynamics can be used for the calculation of an (approximate) behaviour of the memory function. In this way, $\Xi_0(t)$ should have a greater number of well-calculated momenta. The iteration of the procedure is of course limited by the precision of the numerical computation of the parameters δ's.

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December 5, 1997

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