Purity and decoherence in the theory of a damped harmonic oscillator

A. Isar, 1,2,* A. Sandulescu, 1,2 and W. Scheid² ¹Department of Theoretical Physics, Institute of Atomic Physics, Bucharest-Magurele, Romania ²Institut für Theoretische Physik der Justus-Liebig-Universität, Giessen, Germany (Received 2 November 1998; revised manuscript received 2 August 1999)

For the generalized master equations derived by Karrlein and Grabert for the microscopic model of a damped harmonic oscillator, the conditions for purity of states are written, in particular for different initial conditions and different types of damping, including Ohmic, Drude, and weak coupling cases, and the Agarwal and Weidlich-Haake models. It is shown that the states which remain pure are the squeezed states with variances that are constant in time. For pure states, generalized nonlinear Schrödinger-type equations corresponding to these master equations are also obtained. Then the condition for purity of states of a damped harmonic oscillator is considered in the framework of Lindblad theory for open quantum systems. For a special choice of the environment coefficients, correlated coherent states with constant variances and covariance are shown to be the only states which remain pure all the time during the evolution of the considered system. In Karrlein-Grabert and Lindblad models, as well as in the particular models considered, expressions for the rate of entropy production are written, and it is shown that state which preserve their purity in time are also states which minimize entropy production and, therefore, are the most stable state under evolution in the presence of the environment, and play an important role in the description of decoherence phenomenon. [S1063-651X(99)00412-2]

PACS number(s): 05.30.-d, 03.65.Bz, 05.40.-a

I. INTRODUCTION

In the last two decades, more and more interest has arisen about the search for a consistent description of open quantum systems [1-5] (for a recent review, see Ref. [6]). Dissipation in an open system results from microscopic reversible interactions between the observable system and the environment. Because dissipative processes imply irreversibility and, therefore, a preferred direction in time, it is generally thought that quantum dynamical semigroups are the basic tools to introduce dissipation in quantum mechanics. In the Markov approximation and for weakly damped systems, the most general forms of the generators of such semigroups were given by Lindblad [7]. This formalism was studied for the case of damped harmonic oscillators [6,8–12], and applied to various physical phenomena, for instance, to the damping of collective modes in deep inelastic collisions in nuclear physics [13]. A phase space representation of open quantum systems within the Lindblad theory was given in Refs. [14,15]. Important progress beyond the limitations of the weak coupling approach was made in describing quantum dissipative systems by using path integral techniques [16,17].

In the present study we are also concerned with the observable system of a harmonic oscillator which interacts with the environment. We discuss under what conditions the open system can be described by a quantum mechanical pure state. In Sec. II we present the generalized uncertainty relations and the correlated coherent states, first introduced in Ref. [18], which minimize these relations. In Sec. III we consider generalized quantum master equations derived by Karrlein and Grabert in Ref. [17] for the microscopic model of a harmonic oscillator coupled to a harmonic bath [19] by using the path integral, and we obtain conditions for the purity of states, in particular for different initial conditions and different types of damping, including Ohmic, Drude, and weak coupling cases, and the Agarwal and Weidlich-Haake models. We show that the states which satisfy the conditions of purity are pure squeezed states with well-determined variances that are constant in time. For pure states, we also derive generalized Schrödinger-type nonlinear equations corresponding to these master equations. The Lindblad theory for open quantum systems is considered in Sec. IV. For the onedimensional harmonic oscillator as an open system, we show that for a special choice of the diffusion coefficients, the correlated coherent states, taken as initial states, remain pure for all time during the evolution. In some other simple models of a damped harmonic oscillator in the framework of quantum statistical theory [20,21], it was shown that Glauber coherent states remain pure during the evolution, and in all other cases the oscillator immediately evolves into mixtures. In this respect we generalize this result and also our previous result from Ref. [10] as well as the results of other authors [22], obtained by using different methods. In Sec. V we introduce the linear entropy; we present its role in the description of the decoherence phenomenon, and we derive expressions of the rate of entropy production. We show with Lindblad and Karrlein-Grabert models, respectively, that the correlated coherent states, and pure squeezed states, which fulfill the condition for purity of states, are also the most stable states under evolution in the presence of the environment, and make a connection with work done in this field by other authors [23–28]. Finally, a summary is given in Sec. VI.

II. GENERALIZED UNCERTAINTY RELATIONS

In the following we denote by $\sigma_{AA} = \langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2$ the dispersion of the operator \hat{A} , where $\langle \hat{A} \rangle \equiv \sigma_A = \text{Tr}(\hat{\rho}\hat{A})$, Tr $\hat{\rho}$

^{*}Electronic address: isar@theor1.theory.nipne.ro

= 1, and $\hat{\rho}$ is the statistical operator (density matrix). By $\sigma_{AB} = \frac{1}{2} \langle \hat{A} \hat{B} + \hat{B} \hat{A} \rangle - \langle \hat{A} \rangle \langle \hat{B} \rangle$ we denote the correlation (covariance) of the operators \hat{A} and \hat{B} . Schrödinger [29] and Robertson [30] proved that for Hermitian operators \hat{A} and \hat{B} and for pure quantum states the following generalized uncertainty relation holds:

$$\sigma_{AA}\sigma_{BB} - \sigma_{AB}^2 \geqslant \frac{1}{4} |\langle [\hat{A}, \hat{B}] \rangle|^2. \tag{1}$$

For the particular case of the operators of momentum \hat{p} and coordinate \hat{q} , the uncertainty relation (1) becomes

$$\sigma \equiv \sigma_{pp}\sigma_{qq} - \sigma_{pq}^2 \geqslant \frac{\hbar^2}{4}.$$
 (2)

This result was generalized for arbitrary operators (in general non-Hermitian) and for the most general case of mixed states in Ref. [18]. Inequality (2) can also be represented in the form

$$\sigma_{pp}\sigma_{qq} \geqslant \frac{\hbar^2}{4(1-r^2)},\tag{3}$$

where

$$r = \frac{\sigma_{pq}}{\sqrt{\sigma_{pp}\sigma_{qq}}} \tag{4}$$

is the correlation coefficient. The equality in relation (2) is realized for a special class of pure states, called correlated coherent states or squeezed coherent states, which are represented by Gaussian wave packets in the coordinate representation. These minimizing states, which generalize the Glauber coherent states, are eigenstates of an operator of the form

$$\hat{a}_{r,\,\eta} = \frac{1}{2\,\eta} \left[1 - \frac{ir}{(1-r^2)^{1/2}} \right] \hat{q} + i\,\frac{\eta}{\hbar}\,\hat{p}\,, \tag{5}$$

with real parameters r and η , |r| < 1, and $\eta = \sqrt{\sigma_{qq}}$. Their normalized eigenfunctions, denoted as correlated coherent states, have the form

$$\Psi(q) = \frac{1}{(2\pi\eta^2)^{1/4}} \exp\left\{-\frac{q^2}{4\eta^2} \left[1 - \frac{ir}{(1-r^2)^{1/2}}\right] + \frac{\alpha q}{\eta} - \frac{1}{2}(\alpha^2 + |\alpha|^2)\right\},\tag{6}$$

with α a complex number. If we set r=0 and $\eta = (\hbar/2m\omega)^{1/2}$, where m and ω are the mass and the frequency of the harmonic oscillator, respectively, state (6) becomes the usual Glauber coherent state. In Wigner representation, the state (6) has the form

$$\begin{split} W_{r,\eta}(p,q) &= \frac{1}{\pi \hbar} \exp \left[-\frac{(q-\sigma_q)^2}{2 \, \eta^2 (1-r^2)} - \frac{2 \, \eta^2}{\hbar^2} (p-\sigma_p)^2 \right. \\ &\quad \left. + \frac{2r}{\hbar (1-r^2)^{1/2}} (q-\sigma_q) (p-\sigma_p) \right], \end{split} \tag{7}$$

where σ_q and σ_p are the expectation values of coordinate and momentum, respectively. This is the classical normal distribution with the dispersions

$$\sigma_{qq} = \eta^2$$
, $\sigma_{pp} = \frac{\hbar^2}{4 \eta^2 (1 - r^2)}$, $\sigma_{pq} = \frac{\hbar r}{2(1 - r^2)^{1/2}}$ (8)

and the correlation coefficient r. The Gaussian distribution (7) is the only positive Wigner distribution for a pure state [31]. All other Wigner functions that describe pure states necessarily take on negative values for some values of p and q.

In the case of relation (1) the equality is generally obtained only for pure states. For any density matrix in the coordinate representation (normalized to unity) the following relation must be fulfilled:

$$\frac{1}{\nu} = \operatorname{Tr} \,\hat{\rho}^2 \le 1. \tag{9}$$

The quantity ν characterizes the degree of purity of the state: for pure states $\nu=1$ and for mixed states $\nu>1$. In the language of the Wigner function condition (9) has the form

$$\frac{1}{\nu} = 2\pi\hbar \int W^2(p,q) dp \, dq \le 1. \tag{10}$$

Let us consider the most general mixed squeezed states described by the Wigner function of the generic Gaussian form with five real parameters:

$$W(p,q) = \frac{1}{2\pi\sqrt{\sigma}} \exp\left\{-\frac{1}{2\sigma} \left[\sigma_{pp}(q-\sigma_q)^2 + \sigma_{qq}(p-\sigma_p)^2 - 2\sigma_{pq}(q-\sigma_q)(p-\sigma_p)\right]\right\}, \tag{11}$$

where σ is the determinant of the dispersion (correlation) matrix

$$egin{pmatrix} \sigma_{pp} & \sigma_{pq} \ \sigma_{pq} & \sigma_{qq} \end{pmatrix}.$$

Here σ is also the Wigner function area—a measure of the phase space area in which the Gaussian density matrix is localized. For Gaussian states of the form of Eq. (11), the coefficient of purity ν is given by

$$\nu = \frac{2}{\hbar} \sqrt{\sigma}.\tag{12}$$

Inequality (2) must be fulfilled actually for any states, not only Gaussian. Any Gaussian pure state minimizes relation (2). For $\sigma > \hbar^2/4$ function (11) corresponds to mixed quantum states, while in the case of the equality $\sigma = \hbar^2/4$ it takes the form of Eq. (7) corresponding to pure correlated coherent states.

The degree of the purity of a state can also be characterized by the quantum entropy (we put the Boltzmann's constant $k_B=1$):

$$S = -\operatorname{Tr}(\hat{\rho} \ln \hat{\rho}) = -\langle \ln \hat{\rho} \rangle. \tag{13}$$

For quantum pure states the entropy is identically equal to zero. It was shown [12,32] that for Gaussian states with the Wigner functions (11), the entropy can be expressed through σ only:

$$S = \frac{\nu+1}{2} \ln \frac{\nu+1}{2} - \frac{\nu-1}{2} \ln \frac{\nu-1}{2}, \quad \nu = \frac{2}{\hbar} \sqrt{\sigma}. \quad (14)$$

III. GENERALIZED QUANTUM MASTER EQUATIONS

In the framework of the standard microscopic model [19,32–35] for the damped harmonic oscillator, it was shown in Ref. [17] that in general there exists no exact master equation for the damped harmonic oscillator,

$$\frac{\partial}{\partial t}\rho(t) = \mathcal{L}\rho(t),\tag{15}$$

with a dissipative Liouville operator \mathcal{L} describing the dynamics of the oscillator and independent of the initial states. For specific initial preparations the time evolution is described exactly by a time-dependent Liouville operator, and the resulting master equation for the damped harmonic oscillator with the Hamiltonian

$$H_0 = \frac{1}{2M} p^2 + \frac{M \omega_0^2}{2} q^2, \tag{16}$$

corresponding to this Liouville operator [given by Eq. (40) of Ref. [17]], has the following general form ({,} denotes the anticommutator of two operators):

$$\dot{\rho}(t) = -\frac{i}{2M\hbar} [p^2, \rho(t)] - \frac{iM}{2\hbar} \gamma_q(t) [q^2, \rho(t)] - \frac{i}{2\hbar} \gamma_p(t)$$

$$\times [q, \{p, \rho(t)\}] + \frac{M}{\hbar^2} D_q(t) [p, [q, \rho(t)]]$$

$$-\frac{M^2}{\hbar^2} D_p(t) [q, [q, \rho(t)]]. \tag{17}$$

The dependence on ω_0 is included in the coefficients of commutators.

(a) For the so-called thermal initial condition [36], which can be used to describe initial states of the entire system (oscillator and bath) resulting from position measurements, $D_a(t)$ and $D_p(t)$ can be written as

$$D_q(t) = \gamma_q(t) \langle q^2 \rangle - \frac{\langle p^2 \rangle}{M^2}, \quad D_p(t) = \gamma_p(t) \frac{\langle p^2 \rangle}{M^2}. \quad (18)$$

Here $\gamma_q(t)$ and $\gamma_p(t)$ and the equilibrium variances $\langle q^2 \rangle$ and $\langle p^2 \rangle$ are given in terms of the equilibrium coordinate auto-correlation function $\langle q(t)q \rangle$.

We now derive the necessary and sufficient condition for $\rho(t)$ to be a pure state for all times. $\rho(t)$ is a pure state if and only if $\operatorname{Tr} \rho^2(t) = 1$. This is equivalent with $(d/dt)\operatorname{Tr} \rho^2(t) = 0$ for all times, i.e., with the condition $\operatorname{Tr}(\rho(t)\mathcal{L}\rho(t)) = 0$. With the explicit form of $\mathcal{L}\rho(t)$ given by the right-hand side of Eq. (17), and using the relations $\rho^2(t) = \rho(t)$ and $\rho(t)A\rho(t) = \operatorname{Tr}(\rho(t)A)\rho(t)$, we obtain the following condition for a state to be pure for all times:

$$M^2 D_p(t) \sigma_{qq}(t) - M D_q(t) \sigma_{pq}(t) - \frac{\hbar^2}{4} \gamma_p(t) = 0,$$
 (19)

and, by inserting expressions (18),

$$\gamma_{p}(t)\langle p^{2}\rangle\sigma_{qq}(t) - \left[M\gamma_{q}(t)\langle q^{2}\rangle - \frac{\langle p^{2}\rangle}{M}\right]\sigma_{pq}(t) - \frac{\hbar^{2}}{4}\gamma_{p}(t)$$

$$= 0. \tag{20}$$

(b) For factorizing initial conditions, that is, if the initial density matrix of the entire system factorizes in the density matrix of the oscillator and the canonical density matrix of the unperturbed heat bath [34,36–38], i.e., if the oscillator and bath are uncorrelated in the initial state, then the resulting master equation is equivalent to the result by Haake and Reibold [37], who derived it directly from microscopic dynamics and by Hu, Paz, and Zhang [39] from the path integral representation. The condition for purity of states for these master equations has also the form of Eq. (20), where now the coefficients are given by Eqs. (87) and (89) in Ref. [17].

For a pure state $\rho(t) = |\psi(t)\rangle \langle \psi(t)|$, from Eq. (17) we can obtain the evolution equation for the wave function $\psi(t)$ as an equation of the Schrödinger type:

$$\frac{d\psi(t)}{dt} = -\frac{i}{\hbar}H'\psi(t). \tag{21}$$

Taking into account the condition for purity of states [Eq. (19)], we find the non-Hermitian Hamiltonian

$$H' = \frac{p^{2}}{2M} + \frac{M}{2} \gamma_{q}(t) q^{2} + \frac{1}{2} \gamma_{p}(t) (qp + \sigma_{p}(t)q - \sigma_{q}(t)p)$$

$$+ \frac{iM}{\hbar} D_{q}(t) (p - \sigma_{p}(t)) (q - \sigma_{q}(t))$$

$$- \frac{iM^{2}}{\hbar} D_{p}(t) (q - \sigma_{q}(t))^{2}, \qquad (22)$$

which depends on the wave function $\psi(t)$ via the expectation values σ_q and σ_p , i.e., this Schrödinger-type equation is nonlinear.

The master equations considered up to now in this section are exact. We now consider particular types of damping for which the dynamics can be described in terms of approximate Liouville evolution operators, valid for arbitrary initial states [17]. Then the evolution operator is time independent, and the master equation for the density matrix obeys Eq. (17), where $D_q(t) = D_q$ and $D_p(t) = D_p$ read

$$D_q = \gamma_q \langle q^2 \rangle - \frac{\langle p^2 \rangle}{M^2}, \quad D_p = \gamma_p \frac{\langle p^2 \rangle}{M^2},$$
 (23)

with time-independent coefficients γ_q and γ_p [17].

(1) For strictly Ohmic damping, $\gamma_p = \gamma$ is the Laplace transform of the damping kernel [17,19] of the model and $\gamma_q = \omega_0^2$. In this case we do not have a well-defined Liouville operator since $\langle p^2 \rangle$, and, therefore, the coefficients D_q and D_p given by Eq. (23) are logarithmically divergent. The con-

dition for purity of states for this strictly Ohmic damping is similar to relation (20), only now the coefficients are constant:

$$\gamma \langle p^2 \rangle \sigma_{qq}(t) - \left(M \omega_0^2 \langle q^2 \rangle - \frac{\langle p^2 \rangle}{M} \right) \sigma_{pq}(t) - \frac{\hbar^2}{4} \gamma = 0. \tag{24}$$

(2) A more realistic case is the so-called Drude damping. For a sufficiently large Drude parameter ω_D and sufficiently high temperature $k_B T \gg \hbar \gamma$, the oscillator dynamics can be described by an approximate Liouville operator with the coefficients

$$\gamma_q = \alpha^2 + \eta^2, \quad \gamma_p = 2\alpha, \tag{25}$$

where α and η depend on γ , ω_0 , and ω_D , and then the condition for purity of states is

$$2\alpha \langle p^2 \rangle \sigma_{qq}(t) - \left[M(\alpha^2 + \eta^2) \langle q^2 \rangle - \frac{\langle p^2 \rangle}{M} \right] \sigma_{pq}(t) - \frac{\hbar^2}{2} \alpha = 0.$$
(26)

For a pure state, the Schrödinger equation (21) corresponding to the master equation with Ohmic damping has the Hamiltonian (22), with the coefficients given by Eq. (23) and with $\gamma_p = \gamma$ and $\gamma_q = \omega_0^2$. A similar result holds for the Drude damping, when we take the coefficients (25).

(3) In Ref. [17] it was shown that in the limit of weak damping the general master equation has the following form:

$$\dot{\rho}(t) = -\frac{i}{\hbar} \left[\frac{p^2}{2M} + \frac{M}{2} (\omega_0^2 + \omega_0 \gamma_s) q^2, \rho(t) \right] - \frac{i \gamma_c}{2\hbar} [q, \{p, \rho(t)\}] - \frac{K_s}{M\hbar \omega_0} \left[p, [q, \rho(t)] \right] - \frac{K_c}{\hbar} [q, [q, \rho(t)]].$$
 (27)

This equation is given in terms of four dissipation coefficients: γ_s leads to a frequency shift and may be absorbed by renormalizing ω_0 ; γ_c is the classical damping coefficient; the coefficients K_s and K_c depend on the temperature. K_s can be calculated analytically only in certain cases. One of these is the Drude model. The master equation (27) is a generalization of the Agarwal equation [40]

$$\dot{\rho}(t) = -\frac{i}{\hbar} \left[\frac{p^2}{2M} + \frac{M\omega_0^2}{2} q^2, \rho(t) \right] - \frac{i\kappa}{\hbar} [q, \{p, \rho(t)\}]$$

$$-\kappa \frac{M\omega_0}{\hbar} \coth\left(\frac{\hbar\omega_0}{2k_B T}\right) [q, [q, \rho(t)]], \qquad (28)$$

which was derived with the help of projection operator techniques from the same microscopic model using the Born approximation in conjunction with a short memory approximation. As a main difference, in Agarwal's equation the K_s term is absent. Here κ is a phenomenological damping coefficient

From Eqs. (27) and (28), we obtain the following conditions for purity of states:

$$K_c \sigma_{qq}(t) + \frac{K_s}{M\omega_0} \sigma_{pq}(t) - \frac{\hbar}{4} \gamma_c = 0$$
 (29)

and,

$$M\omega_0 \coth\left(\frac{\hbar\omega_0}{2k_BT}\right)\sigma_{qq}(t) = \frac{\hbar}{2}$$
 (30)

respectively. The corresponding Schrödinger-type equations for a pure state have the Hamiltonians

$$H' = \frac{p^2}{2M} + \frac{M}{2} (\omega_0^2 + \omega_0 \gamma_s) q^2 + \frac{1}{2} \gamma_c (qp + \sigma_p(t) q - \sigma_q(t) p)$$

$$-iK_c(q-\sigma_q(t))^2 - \frac{iK_s}{M\omega_0}(p-\sigma_p(t))(q-\sigma_q(t)) \quad (31)$$

and

$$H' = \frac{p^2}{2M} + \frac{M}{2}\omega_0^2 q^2 + \kappa(qp + \sigma_p(t)q - \sigma_q(t)p)$$
$$-i\kappa M\omega_0 \coth\left(\frac{\hbar\omega_0}{2k_BT}\right)(q - \sigma_q(t))^2. \tag{32}$$

respectively.

(4) All the above presented time-independent Liouville operators are not of Lindblad form. In Ref. [17] it is shown that in the weak coupling limit, further coarse graining will result in a Lindblad operator. Indeed, for weak damping, the master equation (27) simplifies and takes on the following form, written in terms of usual creation and annihilation operators a^{\dagger} and a:

$$\dot{\rho}(t) = -i \left(\omega_0 + \frac{\gamma_s}{2} \right) \left[a^{\dagger} a, \rho(t) \right] + \gamma_{\uparrow} \left(\left[a^{\dagger} \rho(t), a \right] \right)$$

$$+ \left[a^{\dagger}, \rho(t) a \right] + \gamma_{\downarrow} \left(\left[a \rho(t), a^{\dagger} \right] + \left[a, \rho(t) a^{\dagger} \right] \right),$$
(33)

where

$$\gamma_{\downarrow,\uparrow} = \frac{\gamma_c}{4} \left[\coth \left(\frac{\hbar \omega_0}{2k_B T} \right) \pm 1 \right].$$
 (34)

This equation, first derived by Weidlich and Haake [41] from a microscopic model for the damped motion of a single mode of the electromagnetic field in a cavity, is of Lindblad form, and can be obtained formally as a particular case of the general master equation (68) for the damped harmonic oscillator (see Sec. IV), if we take

$$D_{pp} = \frac{\hbar M \omega_0}{2} (\gamma_{\downarrow} + \gamma_{\uparrow}), \quad D_{qq} = \frac{\hbar}{2M\omega_0} (\gamma_{\downarrow} + \gamma_{\uparrow}),$$

$$D_{pq} = 0, \quad \lambda = (\gamma_{\downarrow} - \gamma_{\uparrow}), \quad \mu = 0.$$
(35)

From Eq. (33) we obtain the following condition for purity of states:

$$2 \coth \left(\frac{\hbar \omega_0}{2k_B T} \right) \sigma_{a\dagger a}(t) = 1, \tag{36}$$

or, in terms of coordinate and momentum,

$$\left(M\omega_{0}\sigma_{qq}(t) + \frac{\sigma_{pp}(t)}{M\omega_{0}}\right) \coth\left(\frac{\hbar\omega_{0}}{2k_{B}T}\right) = \hbar. \tag{37}$$

For a pure state, the Schrödinger-type equation corresponding to Eq. (33) has the Hamiltonian

$$\begin{split} H' = H + i\hbar \, \frac{\gamma_c}{2} \left(\, \sigma_{a \uparrow} a - \sigma_a a^\dagger + \frac{1}{2} \right) - i\hbar \, \frac{\gamma_c}{2} \, \mathrm{coth} \bigg(\frac{\hbar \, \omega_0}{2 k_B T} \bigg) \\ \times \left[\, (a^\dagger - \sigma_{a \dagger}) (a - \sigma_a) + \frac{1}{2} \right], \end{split} \tag{38}$$

with the notation $H = \hbar(\omega_0 + \gamma_s/2)a^{\dagger}a$. Taking into account condition (37), we see that the mean values of the two Hamiltonians H and H' are equal: $\langle H \rangle = \langle H' \rangle$.

In general, the dissipative systems cannot be described by pure states or by Schrödinger equations, because the environment produces transitions in any state basis. Nevertheless, we will show that this can happen in very limiting cases, corresponding to certain special states. In order to find in the general Karrlein-Grabert model the states which remain pure during the evolution of the system, we consider the equations of motion for the second order moments of coordinate and momentum. To obtain these equations, we first derive the evolution equation (17) with the coefficients (23) in a coordinate representation:

$$i\hbar \frac{\partial \rho}{\partial t} = -\frac{\hbar^2}{2M} \left(\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} \right) \rho + \frac{M \gamma_q}{2} (x^2 - y^2) \rho$$

$$-\frac{i\hbar \gamma_p}{2} (x - y) \left(\frac{\partial}{\partial x} - \frac{\partial}{\partial y} \right) \rho + M D_q (x - y)$$

$$\times \left(\frac{\partial}{\partial x} + \frac{\partial}{\partial y} \right) \rho - \frac{i}{\hbar} M^2 D_p (x - y)^2 \rho. \tag{39}$$

The first two terms on the right-hand side of this equation generate a purely unitary evolution (with a renormalized potential). The third term is the dissipative term, and the fourth is the so-called "anomalous diffusion" term, which generates a second derivative term in the phase space representation of the evolution equation, just like the ordinary diffusion term. The last term is the diffusive term, which is responsible for the process of decoherence. Since the considered dynamics is quadratic, we consider a density matrix solution of Eq. (39) of the form

$$\langle x|\hat{\rho}(t)|y\rangle = \left(\frac{1}{2\pi\sigma_{qq}(t)}\right)^{1/2}$$

$$\times \exp\left[-\frac{1}{8\sigma_{qq}(t)}(x+y)^2 + \frac{i\sigma_{pq}(t)}{2\hbar\sigma_{qq}(t)}(x^2 - y^2)\right]$$

$$-\frac{1}{2\hbar^2}\left(\sigma_{pp}(t) - \frac{\sigma_{pq}^2(t)}{\sigma_{qq}(t)}(x-y)^2\right], \tag{40}$$

which is the general form of Gaussian density matrices (with zero expectation values of coordinate and momentum). By direct substitution of ρ into Eq. (39), we obtain the following system of equations satisfied by dispersions of coordinate and momentum:

$$\frac{d\sigma_{qq}(t)}{dt} = \frac{2}{M}\sigma_{pq}(t),\tag{41}$$

$$\frac{d\sigma_{pp}(t)}{dt} = -2\gamma_p\sigma_{pp}(t) - 2M\gamma_q\sigma_{pq}(t) + 2M^2D_p,$$
(42)

$$\frac{d\sigma_{pq}(t)}{dt} = -M\gamma_q\sigma_{qq}(t) + \frac{1}{M}\sigma_{pp}(t) - \gamma_p\sigma_{pq}(t) + MD_q. \tag{43}$$

Introducing the notation

$$X(t) = \begin{pmatrix} m\sqrt{\gamma_q}\sigma_{qq}(t) \\ \sigma_{pp}(t)/m\sqrt{\gamma_q} \\ \sigma_{pq}(t) \end{pmatrix}, \tag{44}$$

and solving this system of equations with the method used in Refs. [6,9], we obtain the solution

$$X(t) = T(X(0) - X(\infty)) + X(\infty), \tag{45}$$

where the matrix T is

$$T = -2 \frac{e^{-\gamma_p t}}{\Omega^2} \begin{pmatrix} b_{11} & b_{12} & b_{13} \\ b_{21} & b_{22} & b_{23} \\ b_{31} & b_{32} & b_{33} \end{pmatrix}, \tag{46}$$

with time-dependent oscillating functions b_{ij} (i,j=1,2,3) given by $(\Omega^2=4\gamma_q-\gamma_p^2)$:

$$b_{11} = \left(\frac{\gamma_p^2}{2} - \gamma_q\right) \cos \Omega t - \gamma_p \frac{\Omega}{2} \sin \Omega t - \gamma_q, \qquad (47)$$

$$b_{12} = \gamma_a(\cos\Omega t - 1),\tag{48}$$

$$b_{13} = \sqrt{\gamma_q} (\gamma_p \cos \Omega t - \Omega \sin \Omega t - \gamma_p), \tag{49}$$

$$b_{21} = \gamma_q(\cos\Omega t - 1),\tag{50}$$

$$b_{22} = \left(\frac{\gamma_p^2}{2} - \gamma_q\right) \cos \Omega t + \gamma_p \frac{\Omega}{2} \sin \Omega t - \gamma_q, \qquad (51)$$

$$b_{23} = \sqrt{\gamma_q} (\gamma_p \cos \Omega t + \Omega \sin \Omega t - \gamma_p), \qquad (52)$$

$$b_{31} = -\sqrt{\gamma_q} \left(\frac{\gamma_p}{2} \cos \Omega t - \frac{\Omega}{2} \sin \Omega t - \frac{\gamma_p}{2} \right), \tag{53}$$

$$b_{32} = -\sqrt{\gamma_q} \left(\frac{\gamma_p}{2} \cos \Omega t + \frac{\Omega}{2} \sin \Omega t - \frac{\gamma_p}{2} \right), \tag{54}$$

$$b_{33} = -2\gamma_q \cos\Omega t + \frac{\gamma_p^2}{2}.$$
 (55)

The asymptotic values of variances and covariance have the following expressions:

$$\sigma_{qq}(\infty) = \frac{D_p + \gamma_p D_q}{\gamma_p \gamma_q}, \quad \sigma_{pp}(\infty) = \frac{M^2 D_p}{\gamma_p}, \quad \sigma_{pq}(\infty) = 0.$$
(56)

Introducing expressions (23) for the coefficients D_q and D_p , we obtain the following equilibrium asymptotic values of the dispersions:

$$\sigma_{qq}(\infty) = \langle q^2 \rangle, \quad \sigma_{pp}(\infty) = \langle p^2 \rangle, \quad \sigma_{pq}(\infty) = 0. \quad (57)$$

If the asymptotic state is a pure state, then

$$\sigma_{qq}(\infty)\sigma_{pp}(\infty) = \langle q^2 \rangle \langle p^2 \rangle = \frac{\hbar^2}{4},$$
 (58)

i.e., it is a squeezed state. Introducing the expressions of $\sigma_{qq}(t)$ and $\sigma_{pq}(t)$ given by Eq. (45) in the condition for purity of states [Eqs. (19) and (23)], we have shown, after a long but straightforward calculation, that this condition is fulfilled, for any time t, only if the initial values of dispersions are equal to their asymptotic values:

$$\sigma_{qq}(0) = \sigma_{qq}(\infty), \quad \sigma_{pp}(0) = \sigma_{pp}(\infty), \quad \sigma_{pq}(0) = \sigma_{pq}(\infty).$$
(59)

Then it follows from Eq. (45) that $X(t) = X(\infty)$; that is, the dispersions have constant values in time, given by Eq. (57). Therefore, the state which preserves its purity in time is given by the density matrix (40), i.e., it is a squeezed state, with the well-determined constant variances σ_{qq} and σ_{pp} [Eq. (57)]. The fluctuation energy has also a constant value in time:

$$E = \frac{1}{2M} \langle p^2 \rangle + \frac{M \omega_0^2}{2} \langle q^2 \rangle. \tag{60}$$

At the same time, the total energy of the open system is given by the mean value of the Hamiltonian (16),

$$\langle H_0 \rangle = \frac{1}{2M} \sigma_{pp}(t) + \frac{M \omega_0^2}{2} \sigma_{qq}(t) + \frac{1}{2M} \sigma_p^2(t) + \frac{M \omega_0^2}{2} \sigma_q^2(t), \tag{61}$$

and, since the expectation values of coordinate and momentum decay exponentially in time [19], the energy is dissipated and reaches the minimum value E. In the particular case of Agarwal model, the purity condition (30) shows that the variance of coordinate must also be constant in time:

$$\sigma_{qq}(t) = \frac{\hbar}{2M\omega_0 \coth\left(\frac{\hbar\omega_0}{2k_BT}\right)}.$$
 (62)

Using this condition, we find, from the equations of motion (41)–(43) written for the Agarwal model, when we have to take

$$D_p = \frac{\hbar \,\omega_0 \kappa}{M} \coth\left(\frac{\hbar \,\omega_0}{2k_B T}\right), \quad D_q = 0, \quad \gamma_p = \kappa, \quad \gamma_q = \omega_0^2,$$
(63)

that the dispersions have to satisfy the equalities

$$\sigma_{pp}(t) = \frac{\hbar M \omega_0}{2} \coth\left(\frac{\hbar \omega_0}{2k_B T}\right),$$

$$\sigma_{pp}(t) = M^2 \omega_0^2 \sigma_{qq}(t), \quad \sigma_{pq}(t) = 0. \tag{64}$$

Relations (62) and (64) are compatible only if $\coth(\hbar\omega_0/2k_BT)=1$, that is only when the temperature of the thermal bath is T=0. Then finally we obtain

$$\sigma_{qq} = \frac{\hbar}{2M\omega_0}, \quad \sigma_{pp} = \frac{\hbar M\omega_0}{2}, \quad \sigma_{pq} = 0, \quad (65)$$

and, therefore, in the particular case of the Agarwal model, the usual coherent state is the only state which remains pure for all times, if the temperature is T=0. In this case the fluctuation energy of the harmonic oscillator keeps all the time its minimum value $E_{\min} = \hbar \omega_0/2$. Relation (61) shows that in this case the total energy is also dissipated and reaches E_{\min} . The same results can be obtained for the model of Weidlich and Haake, described by the evolution equation (33). Indeed, this model is a particular case [cf. Eqs. (35)] of the Lindblad model considered in Sec. IV, and from the purity condition (37) it follows again that the coherent state is the only state which preserves its purity during the evolution in time of the system, for a zero temperature of the thermal bath. The importance of the states which preserve their purity in time will become evident in Sec. V, in the context of a discussion of the decoherence phenomenon.

IV. PURITY OF STATES IN THE LINDBLAD MODEL

We now consider the condition for purity of states in the Lindblad model for the damped harmonic oscillator, based on quantum dynamical semigroups [2,3,7,8]. The most general Markovian evolution equation preserving the positivity, hermiticity, and trace of $\hat{\rho}$ can be written as

$$\frac{d\hat{\rho}(t)}{dt} = -\frac{i}{\hbar} [\hat{H}, \hat{\rho}(t)] + \frac{1}{2\hbar} \sum_{j} ([\hat{V}_{j}\hat{\rho}(t), \hat{V}_{j}^{\dagger}] + [\hat{V}_{j}, \hat{\rho}(t)\hat{V}_{j}^{\dagger}]).$$
(66)

Here \hat{H} is the Hamiltonian operator of the system, and \hat{V}_j and \hat{V}_j^{\dagger} are operators on the Hilbert space \mathcal{H} of the Hamiltonian which model the interaction with the environment. In the case of an exactly solvable model for the damped harmonic oscillator we take the two possible operators \hat{V}_1 and \hat{V}_2 linear in \hat{p} and \hat{q} [6,8,9] and the harmonic oscillator Hamiltonian \hat{H} is chosen to be

$$\hat{H} = \hat{H}_0 + \frac{\mu}{2} (\hat{q}\hat{p} + \hat{p}\hat{q}), \quad \hat{H}_0 = \frac{1}{2m} \hat{p}^2 + \frac{m\omega^2}{2} \hat{q}^2. \quad (67)$$

With these choices the master equation (66) takes the following form [6,9]:

$$\frac{d\hat{\rho}}{dt} = -\frac{i}{\hbar} [\hat{H}_{0}, \hat{\rho}] - \frac{i}{2\hbar} (\lambda + \mu) [\hat{q}, \hat{\rho}\hat{\rho} + \hat{p}\hat{\rho}] + \frac{i}{2\hbar} (\lambda - \mu)
\times [\hat{p}, \hat{\rho}\hat{q} + \hat{q}\hat{\rho}] - \frac{D_{pp}}{\hbar^{2}} [\hat{q}, [\hat{q}, \hat{\rho}]] - \frac{D_{qq}}{\hbar^{2}} [\hat{p}, [\hat{p}, \hat{\rho}]]
+ \frac{D_{pq}}{\hbar^{2}} ([\hat{q}, [\hat{p}, \hat{\rho}]] + [\hat{p}, [\hat{q}, \hat{\rho}]]).$$
(68)

The quantum diffusion coefficients D_{pp} , D_{qq} , and D_{pq} and the dissipation constant λ satisfy the fundamental constraints [6,9]: $D_{pp} > 0$, $D_{qq} > 0$, and

$$D_{pp}D_{qq} - D_{pq}^2 \geqslant \frac{\hbar^2 \lambda^2}{4}.$$
 (69)

Relation (69) is a necessary condition that the generalized uncertainty inequality (2) is fulfilled.

By using the complete positivity property, it was shown in [9] that the relation

$$\operatorname{Tr}\left(\hat{\rho}(t)\sum_{j}\hat{V}_{j}^{\dagger}\hat{V}_{j}\right) = \sum_{j}\operatorname{Tr}(\hat{\rho}(t)\hat{V}_{j}^{\dagger})\operatorname{Tr}(\hat{\rho}(t)\hat{V}_{j}) \quad (70)$$

represents a necessary and sufficient condition for $\hat{\rho}(t)$ to be a pure state for all times $t \ge 0$. This equality is a generalization of the pure state condition [42–44] to all Markovian master equations (66). If $\hat{\rho}^2(t) = \hat{\rho}(t)$ for all $t \ge 0$, then there exists a wave function $\psi \in \mathcal{H}$ which satisfies a nonlinear Schrödinger equation with the non-Hermitian Hamiltonian

$$\hat{H}' = \hat{H} + i \sum_{j} \langle \psi(t), \hat{V}_{j}^{\dagger} \psi(t) \rangle \hat{V}_{j} - \frac{i}{2} \langle \psi(t), \sum_{j} \hat{V}_{j}^{\dagger} \hat{V}_{j} \psi(t) \rangle$$
$$- \frac{i}{2} \sum_{j} \hat{V}_{j}^{\dagger} \hat{V}_{j}. \tag{71}$$

For the damped harmonic oscillator the pure state condition (70) takes the form [9]

$$D_{pp}\sigma_{qq}(t) + D_{qq}\sigma_{pp}(t) - 2D_{pq}\sigma_{pq}(t) = \frac{\hbar^2 \lambda}{2}, \quad (72)$$

and Hamiltonian (71) becomes

$$\hat{H}' = \hat{H} + \lambda (\sigma_p(t)\hat{q} - \sigma_q(t)\hat{p}) - \frac{i}{\hbar} \left[D_{pp}(\hat{q} - \sigma_q(t))^2 + D_{qq}(\hat{p} - \sigma_p(t))^2 - D_{pq}((\hat{p} - \sigma_p(t))(\hat{q} - \sigma_q(t)) + (\hat{q} - \sigma_q(t))(\hat{p} - \sigma_p(t)) - \frac{\lambda \hbar^2}{2} \right].$$
 (73)

It is interesting to remark that the mean value of this Hamiltonian in the state $\hat{\rho}(t)$ is equal to the mean value of the Hamiltonian \hat{H} . From a physical point of view this result is quite natural, since the average value of the new Hamiltonian \hat{H}' describing the open system must give the energy of the open system.

In order to find the Gaussian states which remain pure during the evolution of the system for all times t, we consider the pure state condition (72) and the generalized uncertainty relation for pure states:

$$\sigma_{pp}(t)\sigma_{qq}(t) - \sigma_{pq}^2(t) = \frac{\hbar^2}{4}.$$
 (74)

By eliminating σ_{pp} between equalities (72) and (74), as in Ref. [45], we obtain

$$\left(\sigma_{qq}(t) - \frac{D_{pq}\sigma_{pq}(t) + \frac{1}{4}\hbar^{2}\lambda}{D_{pp}}\right)^{2} + \frac{D_{pp}D_{qq} - D_{pq}^{2}}{D_{pp}^{2}} \left[\left(\sigma_{pq}(t) - \frac{\frac{1}{4}\hbar^{2}\lambda D_{pq}}{D_{pp}D_{qq} - D_{pq}^{2}}\right)^{2} + \frac{1}{4}\hbar^{2}\frac{D_{pp}D_{qq} - D_{pq}^{2} - \frac{1}{4}\hbar^{2}\lambda^{2}}{(D_{pp}D_{qq} - D_{pq}^{2})^{2}} D_{pp}D_{qq}\right] = 0.$$
(75)

Since the diffusion and dissipation coefficients satisfy inequality (69), we obtain from Eq. (75) the following relations which have to be fulfilled at any moment of time:

$$D_{pp}D_{qq} - D_{pq}^2 = \frac{\hbar^2 \lambda^2}{4},\tag{76}$$

$$D_{pp}\sigma_{qq}(t) - D_{pq}\sigma_{pq}(t) - \frac{\hbar^2\lambda}{4} = 0, \tag{77}$$

$$\sigma_{pq}(t)(D_{pp}D_{qq}-D_{pq}^2)-\frac{\hbar^2\lambda}{4}D_{pq}=0.$$
 (78)

From relations (74) and (76)–(78) it follows that the pure states remain pure for all times only if the variances have the form

$$\sigma_{qq}(t) = \frac{D_{qq}}{\lambda}, \quad \sigma_{pp}(t) = \frac{D_{pp}}{\lambda}, \quad \sigma_{pq}(t) = \frac{D_{pq}}{\lambda}, \quad (79)$$

i.e., they do not depend on time. If these relations are fulfilled, then the equalities (72), (74), and (76) are equivalent. Using the asymptotic values of variances for an underdamped oscillator [given by Eqs. (3.53) in Ref. [9]] and relations (79), we obtain the following expressions of the diffusion coefficients which assure that the initial pure states remain pure for any $t(\Omega^2 = \omega^2 - \mu^2)$:

$$D_{qq} = \frac{\hbar \lambda}{2m\Omega}, \quad D_{pp} = \frac{\hbar \lambda m \omega^2}{2\Omega}, \quad D_{pq} = -\frac{\hbar \lambda \mu}{2\Omega}. \quad (80)$$

Formulas (80) are generalized Einstein relations and represent typical examples of quantum fluctuation-dissipation relations, connecting the diffusion with both Planck's constant and damping constant [4,46]. With Eqs. (80), variances (79) become

$$\sigma_{qq} = \frac{\hbar}{2m\Omega}, \quad \sigma_{pp} = \frac{\hbar m\omega^2}{2\Omega}, \quad \sigma_{pq} = -\frac{\hbar \mu}{2\Omega}.$$
 (81)

Then the corresponding state described by a Gaussian Wigner function is a pure quantum state, namely, a correlated coherent state [18] (squeezed coherent state), with the correlation coefficient (4) $r = -\mu/\omega$. Given σ_{qq} , σ_{pp} , and σ_{pq} , there exists one and only one such a state minimizing the uncertainty σ [Eq. (2)] [47]. A particular case of Lindblad model (corresponding to $\lambda = \mu$ and $D_{pq} = 0$) was considered by Halliwell and Zoupas by using the quantum state diffusion method [22]. We have considered general coefficients λ and μ , and in this respect our expressions for the diffusion coefficients and variances also generalize the ones obtained by Dekker and Valsakumar [45] and Dodonov and Man'ko [48], who used models where $\lambda = \mu$ was chosen. If $\mu = 0$, we obtain $D_{pq} = 0$ from Eq. (80). This case, which was considered in Ref. [10], where we obtained a density operator describing a pure state for any t, is also a particular case of our present results. For $\mu = 0$, expressions (81) become

$$\sigma_{qq} = \frac{\hbar}{2m\omega}, \quad \sigma_{pp} = \frac{\hbar m\omega}{2}, \quad \sigma_{pq} = 0,$$
 (82)

which are the variances of the ground state of the harmonic oscillator; the correlation coefficient is r=0, corresponding to the usual coherent state.

The fluctuation energy of the open harmonic oscillator is

$$E(t) = \frac{1}{2m} \sigma_{pp}(t) + \frac{1}{2} m \omega^2 \sigma_{qq}(t) + \mu \sigma_{pq}(t).$$
 (83)

If the state remains pure in time, then the variances are given by Eqs. (79) and the fluctuation energy is also constant in time:

$$E = \frac{1}{\lambda} \left(\frac{1}{2m} D_{pp} + \frac{1}{2} m \omega^2 D_{qq} + \mu D_{pq} \right). \tag{84}$$

Minimizing this expression with the condition (76), we obtain just the diffusion coefficients (80) and $E_{\rm min}=\hbar\Omega/2$. Therefore, the conservation of purity of state implies that the fluctuation energy of the system has all the time the minimum possible value $E_{\rm min}$. The total energy of the open system is given by the mean value of Hamiltonian (67):

$$\langle \hat{H} \rangle = \frac{1}{2m} \langle \hat{p}^2 \rangle + \frac{m \omega^2}{2} \langle \hat{q}^2 \rangle + \frac{\mu}{2} \langle \hat{q} \hat{p} + \hat{p} \hat{q} \rangle = \frac{1}{2m} \sigma_{pp}(t)$$

$$+ \frac{1}{2} m \omega^2 \sigma_{qq}(t) + \mu \sigma_{pq}(t) + \frac{1}{2m} \sigma_p^2(t) + \frac{1}{2} m \omega^2 \sigma_q^2(t)$$

$$+ \mu \sigma_p(t) \sigma_q(t), \tag{85}$$

and, since the expectation values of coordinate and momentum decay exponentially in time [6,9], the energy is dissipated and reaches its minimum value E_{\min} .

If the asymptotic state is a Gibbs state [6,9], then condition (76) on the diffusion coefficients is satisfied only if $\mu = 0$ and the temperature of the thermal bath is T = 0. As in the Agarwal and Weidlich-Haake models, discussed in Sec.

III, in this limiting case the influence on the oscillator is minimal and $E_{\rm min}=\hbar\omega/2$, which is the oscillator ground state energy; the correlation coefficient (4) vanishes, and therefore the correlated coherent state (squeezed coherent state) becomes the usual coherent (ground) state.

The Lindblad equation with the diffusion coefficients (80) can be used only in the underdamped case, when $\omega > \mu$. Indeed, for the coefficients (80) the fundamental constraint (69) implies that $m^2(\omega^2 - \mu^2)D_{qq}^2 \ge \hbar^2 \lambda^2/4$, which is satisfied only if $\omega > \mu$. It can be shown [48] that there exist diffusion coefficients which satisfy condition (76) and make sense for $\omega < \mu$, but in this overdamped case we have always $\sigma > \hbar^2/4$ and the state of the oscillator cannot be pure for any diffusion coefficients.

If we choose the coefficients of the form of Eq. (80), then the equation for the density operator can be represented in the form of Eq. (66) with only one operator \hat{V} , which up to a phase factor can be written in the form

$$\hat{V} = \left(\frac{2}{\hbar D_{qq}}\right)^{1/2} \left[\left(\frac{\lambda \hbar}{2} - i D_{pq}\right) \hat{q} + i D_{qq} \hat{p} \right], \quad [\hat{V}, \hat{V}^{\dagger}] = 2 \hbar \lambda. \tag{86}$$

The correlated coherent states [Eq. (6)] with nonvanishing momentum average can also be written in the form

$$\Psi(x) = \left(\frac{1}{2\pi\sigma_{qq}}\right)^{1/4} \exp\left[-\frac{1}{4\sigma_{qq}}\left(1 - \frac{2i}{\hbar}\sigma_{pq}\right)\right] \times (x - \sigma_q)^2 + \frac{i}{\hbar}\sigma_p x, \qquad (87)$$

and the most general form of Gaussian density matrix compatible with the generalized uncertainty relation (2) is

$$\langle x|\hat{\rho}|y\rangle = \left(\frac{1}{2\pi\sigma_{qq}}\right)^{1/2} \exp\left[-\frac{1}{2\sigma_{qq}}\left(\frac{x+y}{2} - \sigma_{q}\right)^{2} + \frac{i\sigma_{pq}}{\hbar\sigma_{qq}}\left(\frac{x+y}{2} - \sigma_{q}\right)(x-y) - \frac{1}{2\hbar^{2}}\left(\sigma_{pp} - \frac{\sigma_{pq}^{2}}{\sigma_{qq}}\right) \times (x-y)^{2} + \frac{i}{\hbar}\sigma_{p}(x-y)\right]. \tag{88}$$

These matrices correspond to the correlated coherent state (87) if σ_{qq} , σ_{pp} , and σ_{pq} in Eq. (88) satisfy equality (2), in particular if the variances are taken of the form (81). Consider now the harmonic oscillator initially in a correlated coherent state of the form of Eq. (87), with the corresponding Wigner function (7). For an environment described by the diffusion coefficients (80), the Wigner function at time t is given by

$$W(p,q,t) = \frac{1}{\pi\hbar}$$

$$\times \exp\left\{-\frac{2}{\hbar^2} \left[\sigma_{pp}(q - \sigma_q(t))^2 + \sigma_{qq}(p - \sigma_p(t))^2 - 2\sigma_{pq}(q - \sigma_q(t))(p - \sigma_p(t))\right]\right\}, \tag{89}$$

with the constant variances (81). The correlated coherent state (squeezed coherent state) remains a correlated coherent state with variances constant in time and with $\sigma_q(t)$ and $\sigma_p(t)$ giving the average time-dependent location of the system along its trajectory in phase space. In the long-time limit $\sigma_q(t) = 0$, $\sigma_p(t) = 0$, and then we have

$$\langle x | \hat{\rho}(\infty) | y \rangle = \left(\frac{m\Omega}{\pi \hbar} \right)^{1/2}$$

$$\times \exp \left\{ -\frac{m}{2\hbar} \left[\Omega(x^2 + y^2) + i\mu(x^2 - y^2) \right] \right\}.$$
(90)

The corresponding Wigner function has the form

$$W_{\infty}(p,q) = \frac{1}{\pi\hbar} \exp\left[-\frac{2}{\hbar\Omega} \left(\frac{p^2}{2m} + \frac{m}{2}\omega^2 q^2 + \mu pq\right)\right]. \tag{91}$$

V. ENTROPY AND DECOHERENCE

Besides the von Neumann entropy S [Eqs. (13) and (14)], there is another quantity which can measure the degree of mixing or purity of quantum states. It is the linear entropy S_I , defined as

$$S_l = \text{Tr}(\hat{\rho} - \hat{\rho}^2) = 1 - \text{Tr}\,\hat{\rho}^2.$$
 (92)

For pure states S_l =0 and for a statistical mixture S_l >0. As is well known, the increasing of the linear entropy S_l (and of the von Neumann entropy S_l) due to the interaction with the environment is associated with the decoherence phenomenon (loss of quantum coherence) given by the diffusion process [23,24]. Dissipation increases the entropy, and the pure states are converted into mixed states. The rate of entropy production is given by

$$\dot{S}_{I}(t) = -2 \operatorname{Tr}(\hat{\rho}\dot{\hat{\rho}}) = -2 \operatorname{Tr}(\hat{\rho}\mathcal{L}(\hat{\rho})), \tag{93}$$

where \mathcal{L} is the evolution operator. According to the theory of Refs. [23,24], the maximally predictive states are the pure states which minimize the entropy production in time. These states remain least affected by the openness of the system, and form a "preferred set of states" in the Hilbert space of the system, known as the "pointer basis." Decoherence is the mechanism which selects these preferred states—the most stable ones under the evolution in the presence of the environment.

For the models of the damped harmonic oscillator considered in this paper, we can obtain expressions for the rate of entropy production given by Eq. (93). For Gaussian states the linear entropy (92) becomes

$$S_l(t) = 1 - \frac{1}{\nu}, \quad \nu = \frac{2}{\hbar} \sqrt{\sigma}, \tag{94}$$

and then the time derivative of the linear entropy is given by

$$\dot{S}_{l}(t) = \frac{1}{\nu^{2}} \frac{d\nu}{dt} = \frac{\hbar}{4\sigma\sqrt{\sigma}} \left[\frac{d\sigma_{qq}(t)}{dt} \,\sigma_{pp}(t) + \frac{d\sigma_{pp}(t)}{dt} \,\sigma_{qq}(t) - 2\frac{\sigma_{pq}(t)}{dt} \,\sigma_{pq}(t) \right]. \tag{95}$$

From the system of equations (41)–(43) for the Karrlein-Grabert model, we obtain

$$\dot{S}_{l}(t) = \frac{\hbar}{2\sigma\sqrt{\sigma}} [M^{2}D_{p}(t)\sigma_{qq}(t) - MD_{q}(t)\sigma_{pq}(t) - \gamma_{p}(t)\sigma]. \tag{96}$$

Suppose at the initial moment of time t=0 the state is pure. When conditions (19) and (20) for purity of states are fulfilled for all t, the expression of the rate of linear entropy becomes

$$\begin{split} \dot{S}_l(t) &= \frac{4}{\hbar^2} \left[M^2 D_p(t) \sigma_{qq}(t) - M D_q(t) \sigma_{pq}(t) - \frac{\hbar^2}{4} \gamma_p(t) \right] \\ &= 0, \end{split} \tag{97}$$

and then the entropy production has its minimum value S_l = 0. For the thermal initial condition with coefficients (18), the rate of entropy production is given by

$$\begin{split} \dot{S}_{l}(t) &= \frac{\hbar}{2\,\sigma\sqrt{\sigma}} \bigg[\, \gamma_{p}(t) \langle p^{2} \rangle \sigma_{qq}(t) \\ &- \bigg(M \, \gamma_{q}(t) \langle q^{2} \rangle - \frac{\langle p^{2} \rangle}{M} \bigg) \sigma_{pq}(t) - \gamma_{p}(t) \, \sigma \bigg]; \end{split} \tag{98}$$

for strictly Ohmic damping it is

$$\dot{S}_{l}(t) = \frac{\hbar}{2\sigma\sqrt{\sigma}} \left[\gamma \langle p^{2} \rangle \sigma_{qq}(t) - \left(M \omega_{0}^{2} \langle q^{2} \rangle - \frac{\langle p^{2} \rangle}{M} \right) \right] \times \sigma_{pq}(t) - \gamma \sigma .$$
(99)

For Drude damping the rate of entropy production is also given by an expression like Eq. (98), where now $\gamma_p = 2\alpha$ and $\gamma_q = \alpha^2 + \eta^2$. When the condition for purity is fulfilled for any t, the values of the rate of linear entropy given by Eqs. (98) and (99) also become 0. According to the results of Sec. III, if the condition for purity of states is fulfilled for any t in the Karrlein-Grabert model, then the Gaussian state will be a pure squeezed state, with variances that are constant in time. At the same time the rate of linear entropy production vanishes and, therefore, according to Zurek and co-workers' theory of decoherence, the most stable states are the pure squeezed states, with constant variances. The same conclusion is valid for the weak damping model, given by the master equation (27), for which the rate of entropy production has the expression

$$\dot{S}_{l}(t) = \frac{\hbar^{2}}{2\sigma\sqrt{\sigma}} \left[K_{c}\sigma_{qq}(t) + \frac{K_{s}}{M\omega_{0}}\sigma_{pq}(t) - \gamma_{c}\frac{\sigma}{\hbar} \right], \tag{100}$$

while for the Agarwal model, given by the master equation (28), we obtain

$$\dot{S}_{l}(t) = \frac{\hbar^{2} \kappa}{2\sigma\sqrt{\sigma}} \left[M \omega_{0} \coth\left(\frac{\hbar \omega_{0}}{2k_{B}T}\right) \sigma_{qq}(t) - \frac{2\sigma}{\hbar} \right]. \tag{101}$$

Analogously, for Eq. (33) of Weidlich and Haake, the rate of entropy production is given by

$$\dot{S}_{l}(t) = \frac{\hbar^{2} \gamma_{c}}{8 \sigma \sqrt{\sigma}} \left[\left(M \omega_{0} \sigma_{qq}(t) + \frac{\sigma_{pp}(t)}{M \omega_{0}} \right) \coth \left(\frac{\hbar \omega_{0}}{2k_{B}T} \right) - \frac{4 \sigma}{\hbar} \right], \tag{102}$$

and, according to the results of Sec. III, for Agarwal and Weidlich-Haake models, the usual coherent states are the most stable ones under evolution in the presence of the environment. Using Eq. (93) for the Lindblad equation (68), we obtain the following rate of entropy production:

$$\dot{S}_{l}(t) = \frac{4}{\hbar^{2}} \left[D_{pp} \operatorname{Tr}(\hat{\rho}^{2} \hat{q}^{2} - \hat{\rho} \hat{q} \hat{\rho} \hat{q}) + D_{qq} \operatorname{Tr}(\hat{\rho}^{2} \hat{p}^{2} - \hat{\rho} \hat{p} \hat{\rho} \hat{p}) \right.$$

$$\left. - D_{pq} \operatorname{Tr}(\hat{\rho}^{2} (\hat{q} \hat{p} + \hat{p} \hat{q}) - 2 \hat{\rho} \hat{q} \hat{\rho} \hat{p}) - \frac{\hbar^{2} \lambda}{2} \operatorname{Tr}(\hat{\rho}^{2}) \right]$$

$$(103)$$

or, using Eq. (94) for Gaussian states,

$$\dot{S}_{l}(t) = \frac{\hbar}{2\sigma\sqrt{\sigma}} \times [D_{pp}\sigma_{qq}(t) + D_{qq}\sigma_{pp}(t) - 2D_{pq}\sigma_{pq}(t) - 2\lambda\sigma]. \tag{104}$$

If the initial state is pure, then according to the complete positivity property of the Lindblad model, we have

$$\dot{S}_{l}(0) = \frac{4}{\hbar^{2}} \left[D_{pp} \sigma_{qq}(0) + D_{qq} \sigma_{pp}(0) - 2D_{pq} \sigma_{pq}(0) - \frac{\hbar^{2} \lambda}{2} \right]$$

$$\geqslant 0, \tag{105}$$

which means that the linear entropy can only increase, so that the initial pure state becomes mixed. When the state remains pure, Eq. (104) becomes [cf. Eq. (72)]

$$\dot{S}_{l}(t) = \frac{4}{\hbar^{2}} \left[D_{pp} \sigma_{qq}(t) + D_{qq} \sigma_{pp}(t) - 2D_{pq} \sigma_{pq}(t) - \frac{\hbar^{2} \lambda}{2} \right]$$

$$= 0, \qquad (106)$$

and, therefore, the entropy production will be S_l =0. Since the only initial states which remain pure for any t are the correlated coherent states, we can state that in the Lindblad theory these states are the maximally predictive states. The present results, obtained in the framework of Karrlein-

Grabert and Lindblad models, generalize previous results which asserted that for many models of quantum Brownian motion in the high temperature limit typical coherent states correspond to minimal entropy production and, therefore, are the maximally predictive states. As we have seen, such coherent states can be obtained in the Lindblad model as a particular case of the correlated coherent states by taking μ = 0, so that the correlation coefficient (4) is r = 0. Zurek and co-workers [23,24] considered a harmonic oscillator undergoing quantum Brownian motion in the Caldeira-Leggett model, and concluded that minimizing states, which are initial states generating the least amount of von Neumann or linear entropy (and, therefore, the most predictable or stable states under evolution in the presence of an environment) are the ordinary coherent states. Using an information-theoretic measure of uncertainty for quantum systems, Anderson and Halliwell showed in Ref. [25] that minimizing states are certain general Gaussian states. Anastopoulos and Halliwell [26] offered an alternative characterization of these states by noting that they minimize the generalized uncertainty relation. According to this assertion, we can say that in the Lindblad model the correlated coherent states are the most stable ones which minimize the generalized uncertainty relation (2). Our result confirms that of Ref. [26], where the model for the open quantum system consists of a particle moving in a harmonic oscillator potential and linearly coupled to an environment consisting of a bath of harmonic oscillators in a thermal state. We remind the reader that the Caldeira-Leggett model considered in Refs. [23,24] violates the positivity of the density operator at short time scales [49,50], whereas in the Lindblad model the property of positivity is always fulfilled.

The rate of predictability loss, measured by the rate of linear entropy increase, was also calculated in the framework of Lindblad theory for the damped harmonic oscillator by Paraoanu and Scutaru [27], who have showed that, in general, the pure or mixed state which produces the minimum rate of increase in the area occupied by the system in the phase space is a quasifree state which has the same symmetry as that induced by the diffusion coefficients. For isotropic phase space diffusion, coherent states (or mixture of coherent states) are selected as the most stable ones. In order to generalize the results of Zurek and co-workers, the entropy production was also considered by Gallis [28] within the Lindblad theory of open quantum systems, treating environment effects perturbatively. Gallis considered the particular case with $D_{pq} = 0$, and found that the squeezed states emerge as the most stable states for intermediate times compared to the dynamical time scales. The amount of squeezing decreases with time, so that the coherent states are most stable for large time scales. For $D_{pq} \neq 0$ our results generalize the result of Gallis, and establish that the correlated coherent states are the most stable ones under the evolution in the presence of the environment.

VI. SUMMARY

In the present paper we have considered the generalized quantum master equations derived by Karrlein and Grabert [17] for the microscopic model of a harmonic oscillator coupled to a harmonic bath. We have obtained conditions for purity of states for different initial conditions and different types of damping, including strictly Ohmic, Drude, and weak coupling cases, and the Agarwal and Weidlich-Haake models. We have shown that the states which remain pure all the time are the pure squeezed states with well-determined variances that are constant in time. For pure states, we have also derived corresponding generalized Schrödinger-type nonlinear equations. We have also studied a one-dimensional harmonic oscillator with dissipation within the framework of Lindblad theory, and have shown that the only states which stay pure during the evolution of the system are the correlated coherent states, under the condition of a special choice of environmental coefficients, so that the variances and covariance are constant in time. We have also obtained expressions for the rate of entropy production in the considered models, and have shown that states which preserve their purity in time are also states which minimize the entropy production and, therefore, are connected with the decoherence phenomenon. According to the theory of decoherence of Zurek and co-workers, in Karrlein-Grabert and Lindblad models, as well as in the particular models considered, these states are the most stable ones under the evolution of the system in the presence of the environment. In a future work in the framework of these theories we plan to discuss in greater detail the connection between uncertainty, decoherence and correlations of open quantum systems with their environment.

ACKNOWLEDGMENTS

Two of us (A.I. and A.S.) are pleased to express their sincere gratitude for the hospitality at the Institut für Theoretische Physik in Giessen and to Professor H. Scutaru for enlightening discussions and reading the manuscript. A.I. and A.S. also gratefully acknowledge financial support by the Deutsche Forschungsgemeinschaft (Germany).

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