acta phys. slov. 42 (1992), No. 6, 324—337

# SECOND ORDER APPROXIMATION TO THE MEAN DISPLACEMENT OF A PARTICLE COUPLED WITH A HEAT BATH AND DRIVEN BY AN EXTERNAL FORCE.

KOSTAKIS, G. C.[1], Kifissia, KOSTAKIS, C. G.[2], Pireaus

The interaction of a quantum particle with a heat bath of quantum oscillators under the influence of an external force has been studied and the mean displacement of this particle has been computed up to second order approximation in the propagator. The heat bath has been considered as Brownian and the characteristic frequencies are close to the characteristic frequency of the particle. The mean displacement of the particle has been found to oscillate with time. The temperature dependence of the mean displacement follows an exponential function.

## I. INTRODUCTION

The behaviour of a quantum particle coupled with a heat bath has been studied by many authors. Iche and Nozieres [1] have considered a heavy particle in a thermal bath. The statistical properties of a quantum mechanical system of quantum oscillators have been found to be of the generalized Langevin form (Lindenberg and West [2]). Caldeira and Leggett have studied this model with regard to the influence of an external force, having used a path integral approach [3], [4]. The correlation functions of such a model have been calculated by Astangul, Pottier and Saint James [5].

In this work we study the problem of a quantum particle in a thermal bath under the influence of an external force.

The Hamiltonian of the system is

$$H = \sum_k \hbar\omega_k a_k^+ a_k + \hbar\omega a^+ a + \sum_k C_k (a^+ + a)(a_k^+ + a_k) - F(a^+ + a),$$

where $C_k$ are the coupling constants, which are considered to be small.

The heat bath is initially in thermal equilibrium and the density operator obeys a Boltzmann distribution. The perturbed part of the Hamiltonian has been

1) Hellenic Air Force Academy, Rodon 27, KIFISSIA 14564, Greece
2) Technological Institute of Pireaus, PIREAUS, Greece



treated with the aid of Feynmann's perturbation formula for the propagator. The propagator has been calculated up to second order approximation.

In the calculation of the second order approximation to the propagator we considered another approximation involving the dependence on $\Delta\omega_l$, where $\Delta\omega_l = \omega_l - \omega$ is the difference between the eigenfrequencies of the particle and the oscillators of the heat bath.

In many case one frequency is close to the frequency of the particle and the others do not contribute to the final result.

## II. FORMULATION OF THE PROBLEM

### a) Coherent states

For the harmonic oscillator problem, we use the creation and annihilation operators, $a^+$ and $a$, respectively, and a complete set of basis vectors.

Glauber [2] defined the eigenvector of the non Hermitian operator by

$$a|\alpha\rangle = \alpha|\alpha\rangle. \tag{1}$$

The coherent states $|\alpha\rangle$ can be shown to obey the following relation

$$|\alpha\rangle = e^{-\frac{|\alpha|^2}{2}} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle \tag{2}$$

and they form a complete set of states, i.e.

$$\int \frac{d^2\alpha}{\pi} |\alpha\rangle\langle\alpha| = 1, \tag{3}$$

where

$$d^2\alpha = d(\mathrm{Re}\alpha)d(\mathrm{Im}\alpha). \tag{4}$$

Coherent states were extensively used, see for example Ref. [3].

The operation of $a^+$ upon the eigenstates $|\alpha\rangle$ leads to the formula

$$a^+|\alpha\rangle = \left(\frac{\partial}{\partial\alpha} + \frac{\bar{\alpha}}{2}\right)|\alpha\rangle, \tag{5}$$

where the bar over $\alpha$ means complex conjugation.

Another useful relation of the coherent states is

$$\langle\alpha|\alpha'\rangle = e^{-\frac{|\alpha|^2}{2}} e^{-\frac{|\alpha'|^2}{2}} e^{\bar{\alpha}\alpha'}. \tag{6}$$

For more details on coherent states see Refs. [2], [4], [6].

## b) The propagator

For a time independent Hamiltonian the evolution operator $U(t|t')$ is given by

$$U(t|t') = \exp\left[-\frac{\mathrm{i}}{\hbar}H(t-t')\right] \tag{7}$$

and the propagator associated with two different states is given by

$$K(\alpha t|\alpha' 0) = \langle\alpha|\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Ht}|\alpha'\rangle. \tag{8}$$

The difficulty arises when the terms forming the Hamiltonian operator do not commute with each other, and so they cannot be separated. For more details on non commuting operators see Ref. [10] and on Baker-Hausdorff's theorem of group theory see Ref. [11].

When the Hamiltonian consists of two parts

$$H = H_0 + H' \tag{9}$$

not commuting with each other, we use Feynman's perturbation theory [12] to compute the propagator $k(\alpha t|\alpha' 0)$. In Eq. (9) $H'$ is the perturbed part of the Hamiltonian. In what follows we are going to use the symbol $K(t)$ for the propagator $K(\alpha t|\alpha' 0)$, which is the amplitude of probability for a system being in state $\alpha'$ at time $t_0 = 0$, to go to the state $\alpha$ at time $t$.

The solution of the Schrödinger equation

$$\mathrm{i}\hbar\frac{\partial}{\partial t}K_0(t) = H_0 K_0(t) \tag{10}$$

is the zero-order approximation of the propagator of the system and is given by

$$K_0(\alpha t|\alpha' 0) = \langle\alpha|\mathrm{e}^{-\frac{iH_0 t}{\hbar}}|\alpha'\rangle. \tag{11}$$

In order to find the first order approximation we use the well-know iteration:

$$K_1(t) = K_0(t) - \frac{\mathrm{i}}{\hbar}\int_0^t K_0(t|\tau)H'(\tau)K_0(\tau)\mathrm{d}\tau, \tag{12}$$

where $K_0(t|\tau)$ means $K_0(t-\tau)$.

In our work, we go up to the second order approximation for the propagator, which is given by

$$K_2(t) = K_0(t) - \frac{i}{\hbar}\int_0^t K_0(t|\tau)H'(\tau)K_1(\tau)\mathrm{d}\tau. \tag{13}$$

The propagator associated with the Hamiltonian of the system can be used in calculating the "interaction picture" of any operator describing a variable of the system. If $A(t_0)$ is an operator at time $t = t_0$, the same operator at time $t$ is

$$A(t) = U^+(t|t_0)A(t_0)U(t|t_0), \tag{14}$$

where $U^+(t|t_0)$ is the Hermitian adjoint of $U(t|t_0)$.



## c) The density matrix

In order to compute mean values associated with our system we use a procedure based on the density operator, which at time $t = 0$ is given by

$$R(a, a^+) = \frac{\mathrm{e}^{-\beta\hbar\omega a^+ a}}{Z_0}, \quad \left(\beta = \frac{1}{kT}\right) \tag{15}$$

where $Z_0$ is the normalizing factor given by the trace of the matrix

$$Z_0 = \mathrm{Tr}\,\mathrm{e}^{-\beta\hbar\omega a^+ a} = \int\langle\alpha|\mathrm{e}^{-\beta\hbar\omega a^+ a}|\alpha\rangle\frac{\mathrm{d}^2\alpha}{\pi}. \tag{16}$$

The density operator at time $t$ is given by

$$R(t) = U(t|0)R_0U^+(t|0). \tag{17}$$

We evaluate thermal averages using the generalized Wick theorem [13].

The Hamiltonian of our problem is such that

$$U^+(t) = U(-t), \tag{18}$$

because the annihilation and creation operators obey the following property

$$((a^+a)^n)^+ = (a^+a)^n, \tag{19}$$

the density operator (17) is given by

$$R(t) = U(t)R_0U(-t). \tag{20}$$

To find the matrix elements of our operators we make use of the well-known (see for example Ref. [11]) formula

$$\langle\alpha|\mathrm{e}^{\kappa a^+ a}|\alpha'\rangle = \exp\left[\mathrm{e}^{-\kappa}\bar{\alpha}\alpha' - \frac{|\alpha|^2}{2} - \frac{|\alpha'|^2}{2}\right]. \tag{21}$$

The matrix elements of the equilibrium density operator are given by

$$\rho_0(\alpha, \alpha') = \frac{\langle\alpha|\mathrm{e}^{-\beta\hbar\omega a^+ a}|\alpha'\rangle}{Z_0}. \tag{22}$$

From Eq. (16) we can find $Z_0$

$$Z_0 = \int\langle\alpha|\mathrm{e}^{-\beta\hbar\omega a^+ a}|\alpha\rangle\frac{\mathrm{d}^2\alpha}{\pi} = \sum_n \mathrm{e}^{-\beta\hbar\omega n} = \frac{1}{1-\mathrm{e}^{-\beta\hbar\omega}} \tag{23}$$

and from Eq. (21) we can find

$$\langle\alpha|\mathrm{e}^{-\beta\hbar\omega a^+ a}|\alpha'\rangle = \exp\left(\mathrm{e}^{-\beta\hbar\omega}\bar{\alpha}\alpha' - \frac{|\alpha|^2}{2} - \frac{|\alpha'|^2}{2}\right) \tag{24}$$

The equilibrium density matrix elements in (22) are given by

$$\rho_0(\alpha, \alpha') = \left(1 - \mathrm{e}^{-\beta\hbar\omega}\right)\exp(\mathrm{e}^{-\beta\hbar\omega}\bar{\alpha}\alpha')\mathrm{e}^{\frac{-|\alpha|^2}{2}}\mathrm{e}^{\frac{-|\alpha'|^2}{2}}. \tag{25}$$

If we know the density matrix $R$, we can compute the mean value of any operator $M$, from the trace of the matrix $MR$

$$\langle M\rangle = \mathrm{Tr}(MR). \tag{26}$$

## III. THE DENSITY MATRIX FOR A PARTICLE IN A THERMAL BATH

The Hamiltonian of a quantum particle coupled to a thermal bath and driven by an external force $F$ is given by

$$H = \sum_k \hbar\omega_k a_k^+ a_k + \hbar\omega a^+ a + \sum_k C_k (a^+ + a)(a_k^+ + a_k) - F(a^+ + a). \tag{27}$$

In the third term in the Hamiltonian representing the interaction of the particle with the bath, the coupling constants $C_k$ are small.

The Hamiltonian (27) can be separated into two parts, $H_0$ and $H'$, where

$$H_0 = \sum_k \hbar\omega_k a_k^+ a_k + \hbar\omega a^+ a \tag{28}$$

is the Hamiltonian that corresponds to the particle and to the system of oscillators, and

$$H' = (a^+ + a)\sum_k C_k (a_k^+ + a_k) - F(a^+ + a) \tag{29}$$

is the perturbed part of the Hamiltonian associated with a weak interaction of the particle with the oscillators and with the external force exerted on the particle.

The system is initially in thermal equilibrium and its density operator is given by the following Boltzmann distribution

$$R_0(a_k, a_k^+, a, a^+) = \frac{e^{-\beta h(\sum_k \omega_k a_k^+ a_k + \omega a^+ a)}}{\mathrm{Tr}\left(e^{-\beta h(\sum_k \omega_k a_k^+ a_k + \omega a^+ a)}\right)}. \tag{30}$$

The matrix elements of the density operator are

$$\begin{aligned}\langle \alpha_k \alpha | R_0(a_k, a_k^+, a, a^+) | \alpha_k' \alpha' \rangle &= \prod_k \left(1 - e^{-\beta\hbar\omega_k}\right)\left(1 - e^{-\beta\hbar\omega}\right) \times \\ &\times \exp\left(\sum_k \bar{\alpha}_k \alpha_k' e^{-\beta\hbar\omega_k} + \bar{\alpha}\alpha' e^{-\beta\hbar\omega}\right) \times \\ &\times \exp\left(-\sum_k \frac{|\alpha_k|^2}{2} - \sum_k \frac{|\alpha_k'|^2}{2} - \frac{|\alpha|^2}{2} - \frac{|\alpha'|^2}{2}\right).\end{aligned} \tag{31}$$



## IV. FIRST ORDER APPROXIMATION OF THE MEAN DISPLACEMENT OF THE PARTICLE

We start our evaluations from the propagator $K_0(t|\tau)$ corresponding to the Hamiltonian $H_0$.

Form Eq. (11) we can see that the matrix elements of the zero order propagator are

$$\begin{aligned}K_0(t|0) &= \exp\left(\sum_k \bar{\alpha}_k \alpha_k' e^{-i\omega_k t} + \bar{\alpha}\alpha' e^{-i\omega t}\right) \times \\ &\times \exp\left(-\sum_k \frac{|\alpha_k|^2}{2} - \sum_k \frac{|\alpha_k'|^2}{2} - \frac{|\alpha|^2}{2} - \frac{|\alpha'|^2}{2}\right).\end{aligned} \tag{32}$$

We proceed via Feynman's perturbation theory [12] and with the aid of Eq. (12) we evaluate the first order approximation of the propagator.

The matrix element

$$\langle \alpha_k \alpha | U(t|\tau) H'(\tau) U_0(\tau|0) | \alpha_k' \alpha' \rangle$$

($U_0(t)$ is the evolution operator associated with the zero order propagator $K_0(t)$) can by evaluated from the following integral

$$\int \langle \alpha_k \alpha | U_0(t|\tau) | \alpha_k'' \alpha'' \rangle \langle \alpha_k'' \alpha'' | H'(\tau) U_0(\tau|0) | \alpha_k' \alpha' \rangle \alpha^2 \alpha'' \prod_k d^2 \alpha_k''. \tag{33}$$

For the second factor of this product we use the relation (A12) given in Appendix II

$$\begin{aligned}\langle \alpha_k'' \alpha'' | H'(\tau) U_0(\tau|0) | \alpha_k' \alpha' \rangle &= \exp\left(\sum_k \bar{\alpha}_k'' \alpha_k' e^{-i\omega_k \tau} + \bar{\alpha}'' \alpha' e^{i\omega\tau}\right) \times \\ &\times \left[\left(\bar{\alpha}'' + \alpha' e^{-i\omega\tau}\right)\sum_k C_k\left(\bar{\alpha}'' + \alpha' e^{-i\omega\tau}\right) - F\left(\bar{\alpha}'' + \alpha' e^{-i\omega\tau}\right)\right] \times \\ &\times \exp\left(-\sum_k \frac{|\alpha_k''|^2}{2} - \frac{|\alpha''|^2}{2} - \sum_k \frac{|\alpha_k'|^2}{2} - \frac{|\alpha'|^2}{2}\right).\end{aligned} \tag{34}$$

The first factor of Eq. (33) is the zero order propagator $K_0(t/\tau)$ given by (32) at time $t = -\tau$.

The integral (33) can be written as follows

$$\int \exp\left(\sum_k \bar{\alpha}_k \alpha_k'' e^{-i\omega_k(t-\tau)} + \bar{\alpha}\alpha'' e^{-i\omega(t-\tau)}\right) \times$$
$$\times \exp\left(-\sum_k \frac{|\alpha_k|^2}{2} - \frac{|\alpha|^2}{2} - \sum_k \frac{|\alpha_k''|^2}{2} - \frac{|\alpha''|^2}{2}\right) \times$$
$$\times \left[\left(\alpha'' + \alpha' e^{-i\omega\tau}\right) \sum_k C_k \left(\bar{\alpha}_k'' + \alpha_k' e^{-i\omega_k\tau}\right) - F\left(\bar{\alpha}'' + \alpha' e^{-i\omega\tau}\right)\right] \times \tag{35}$$
$$\times \exp\left(\sum_k \bar{\alpha}_k'' \alpha_k' e^{-i\omega_k\tau} + \bar{\alpha}''\alpha' e^{-i\omega\tau}\right) \times$$
$$\times \exp\left(-\sum_k \frac{|\alpha_k'|^2}{2} - \frac{|\alpha'|^2}{2} - \sum_k \frac{|\alpha_k''|^2}{2} - \frac{|\alpha''|^2}{2}\right) d^2\alpha'' \prod_k d^2\alpha_k''.$$

The integrations over $\alpha_k''$ and $\alpha''$ will be performed with the aid of the generating function given in Appendix I. The corresponding formulae from Appendix I are (A4) and (A5) and the matrix element $\langle \alpha_k \alpha | U_0(t|\tau) H'(\tau) U_0(\tau|0) | \alpha_k' \alpha' \rangle$ is

$$K_0(t|\tau)H'(\tau)K_0(\tau|0) = \left[\left(\bar{\alpha} e^{-i\omega(t-\tau)} + \alpha' e^{-i\omega\tau}\right) \times\right.$$
$$\left.\times \sum_k C_k \left(\bar{\alpha}_k e^{-i\omega_k(t-\tau)} + \alpha_k' e^{-i\omega_k\tau}\right) - F\left(\bar{\alpha} e^{-i\omega(t-\tau)} + \alpha' e^{-i\omega\tau}\right)\right] \times$$
$$\times \exp\left(\sum_k \bar{\alpha}_k \alpha_k' e^{-i\omega_k t} + \bar{\alpha}\alpha' e^{-i\omega t}\right) \times \tag{36}$$
$$\times \exp\left(-\sum_k \frac{|\alpha_k|^2}{2} - \frac{|\alpha|^2}{2} - \sum_k \frac{|\alpha_k'|^2}{2} - \frac{|\alpha'|^2}{2}\right).$$

Feynman's formula (12) requires an integration of (36) over $\tau$, that can easily be performed.

The final result for the first approximation of the propagator $K_1(t)$ is

$$K_1(\alpha\alpha_k t|\alpha_k'\alpha' 0) = \exp\left(\sum_k \bar{\alpha}_k \alpha_k' e^{-i\omega_k t} + \bar{\alpha}\alpha' e^{-i\omega t}\right) \times$$
$$\times \left[1 + \sum_k D_k(t)(\bar{\alpha}_k \bar{\alpha} + \alpha_k' \alpha') + \sum_k E_k(t)(\bar{\alpha}_k \alpha' + \alpha_k' \bar{\alpha}) + A(t)(\bar{\alpha} + \alpha')\right] \times$$
$$\times \exp\left(-\sum_k \frac{|\alpha_k|^2}{2} - \frac{|\alpha|^2}{2} - \sum_k \frac{|\alpha_k'|^2}{2} - \frac{|\alpha'|^2}{2}\right). \tag{37}$$

where

$$D_k(t) = C_k \frac{\left(e^{-i(\omega_k+\omega)t} - 1\right)}{\hbar(\omega_k + \omega)} \tag{38}$$

$$E_k(t) = C_k \frac{\left(e^{-i\omega_k t} - e^{-i\omega t}\right)}{\hbar(\omega_k - \omega)} \tag{39}$$

$$A(t) = \frac{F}{\hbar\omega}\left(1 - e^{-i\omega t}\right). \tag{40}$$

This is the first approximation to the propagator of our system and we use this propagator to compute the first approximation to the density matrix of our system, which was initially in thermodynamical equilibrium. The first order approximation of the density matrix is given by

$$R_1(t) = U_1(t) R_0 U_1(-t), \tag{41}$$

where $R_0$ is given by (30).

To compute the matrix elements of $R_1(t)$, we use the same method as before, i.e.we insert a complete set of states between the operators

$$\rho_1(\alpha_k, \alpha, \alpha_k', \alpha', t) = \langle \alpha_k \alpha | R_1(t) | \alpha_k' \alpha' \rangle =$$
$$= \iint \langle \alpha_k \alpha | U_1(t) | \alpha_k'' \alpha' \rangle \langle \alpha_k'' \alpha'' | R_0 | \alpha_k''' \alpha''' \rangle \times \tag{42}$$
$$\times \langle \alpha_k''' \alpha''' | U_1(-t) | \alpha_k' \alpha' \rangle \alpha^2 \alpha'' \prod_k d^2\alpha_k'' d^2\alpha''' \prod_k d^2\alpha_k'''.$$

The mathematical details are in Appendix III (calculations up to first order approximation to the density matrix and the result given by (A20)).

Now the question is: What is the behaviour of a quantum particle coupled to a thermal bath and under the influence of an external force? Or in other words, what is the average displacement of such a particle? This question can be answered, as soon as we know the density matrix. In terms of the creation and annihilation operators, the operator associated with the position of a particle is $a^+ + a$. So the mean value of the displacement of the particle according to Eq. (26) is given by:

$$\langle a^+ + a \rangle = \mathrm{Tr}\left((a^+ + a) R_1(t)\right). \tag{43}$$

We use again the substitution $a^+ \to \bar{\alpha}$, $a \to \frac{\partial}{\partial \bar{\alpha}}$, mentioned in Appendix II, to evaluate the matrix elements of (43). To find the trace required in (43) of all these states we choose only the diagonal elements, and we integrate over all these states.

$$\langle a^+ + a \rangle = \int \left[\left(\bar{\alpha} + \frac{\partial}{\partial \bar{\alpha}}\right) \rho_1(\bar{\alpha}, \bar{\alpha}_k, \alpha', \alpha_k', t)\right]_{\substack{\alpha_k' = \alpha_k \\ \alpha' = \alpha}} \mathcal{D}^2\alpha \prod_k \mathcal{D}^2\alpha_k \tag{44}$$

where

$$\mathcal{D}^2\alpha = \frac{1}{\pi} e^{-\frac{|\alpha|^2}{2}} d^2\alpha, \qquad \mathcal{D}^2\alpha_k = \frac{1}{\pi} e^{-\frac{|\alpha_k|^2}{2}} d^2\alpha_k. \tag{45}$$

There are only two kinds of non-vanishing integrals that will appear in (44). These integrals are the following

$$\int_{-\infty}^{\infty} \exp(|\alpha|^2 e^{-\beta\hbar\omega}) \mathcal{D}^2\alpha = \frac{1}{\pi} \int_{-\infty}^{\infty} \exp\left[-|\alpha|^2 \left(1 - e^{-\beta\hbar\omega}\right)\right] d^2\alpha = \frac{1}{1 - e^{-\beta\hbar\omega}} \tag{46}$$

$$\int_{-\infty}^{\infty} |\alpha|^2 \exp(|\alpha|^2 e^{-\beta\hbar\omega}) \mathcal{D}^2\alpha = \frac{1}{\pi}\int_{-\infty}^{\infty} |\alpha|^2 \exp\left[-|\alpha|^2\left(1-e^{-\beta\hbar\omega}\right)\right] d^2\alpha = = \left(\frac{1}{1-e^{-\beta\hbar\omega}}\right)^2. \tag{47}$$

The general formula for computing these integrals is given by (A9).

Using (46) and (47) in (44) we find that the average displacement of the particle is

$$\langle a^+ + a\rangle = \frac{F}{\hbar\omega}\left(e^{i\omega t} + e^{-i\omega t} - 2\right). \tag{48}$$

This is a result already known from Ref. [5] but we take procedure followed here as very interesting because we can proceed to the next higher order approximation.

## V. SECOND ORDER APPROXIMATION

The first order approximation of the quantum particle in a system of other quantum particles does not show any dependence on the motion of the other particles and the coupling of the test particle with them. The displacement of the particle is sinusoidal as we can see from (48) and depends only on the external force acting on it, a result in agreement with previous ones. We use the same method as in the previous paragraph for the second order approximation of the propagator. This can be evaluated with the aid of Feynman's formula (13).

The propagator $K_1(\tau|0)$ from (37) will be used in (13) and the matrix element

$$\langle \alpha_k\alpha|K_0(t|\tau)H'(\tau)K_1(\tau|0)|\alpha'_k\alpha'\rangle$$

will be evaluated according to the following integration

$$\int \langle \alpha_k\alpha|K_0(t|\tau)|\alpha''_k\alpha''\rangle\langle\alpha''_k\alpha''|H'(\tau)K_1(\tau|0)|\alpha'_k\alpha'\rangle \cdot \mathcal{D}^2\alpha''\prod_k \mathcal{D}^2\alpha''_k. \tag{49}$$

The first factor of (49) is given by (32) with the following substitution

$$t\to t-\tau,\quad \alpha'\to\alpha'',\quad \alpha'_k\to\alpha''_k.$$

The second factor of (49) can be evaluated with the aid of (A12) of Appendix II.

In our problem we consider a set of particles with frequencies close to the frequency of the particle. Then the thermal bath will affect the motion of the particle although the coupling is weak. The differences $\omega_k-\omega$ are small and in our result we keep only the terms involving $1/(\omega_k-\omega)$ and higher order terms. All other terms are neglected because they are small in comparison to these. In order to find the propagator $K_2(\bar\alpha_k,\bar\alpha,\alpha'_k,\alpha',t)$ we perform the integration over $\tau$ in Eq. (13).

The second order approximation to the density matrix is given by

$$R_2(t) = U_2(t)R_0U_2(-t) \tag{50}$$



where $U_2(t)$ is the evolution operator associated to the propagator with the following formula

$$K_2(\bar\alpha_k,\bar\alpha,\alpha'_k,\alpha',t) = \langle\bar\alpha_k\bar\alpha|U_2(t)|\alpha'_k\alpha'\rangle. \tag{51}$$

The matrix elements of (50) can by evaluated as before, i.e. by inserting a complete set of states between the operators and then by integrating over these states. So the matrix elements of (50) are

$$\rho_2(\bar\alpha_k,\bar\alpha,\alpha'_k,\alpha',t) = \iint K_2(\bar\alpha_k,\bar\alpha,\alpha'''_k,\alpha''',t)\cdot R_0(\bar\alpha'''_k,\bar\alpha''',\alpha''_k,\alpha'',t)\times \times K_2(\bar\alpha''_k,\bar\alpha'',\alpha'_k,\alpha',-t)\mathcal{D}^2\alpha'''\mathcal{D}^2\alpha''\prod_k \mathcal{D}^2\alpha'''_k\mathcal{D}^2\alpha''_k. \tag{52}$$

The integrations involving the coherent states can be performed with the aid of (A4) – (A8).

Finally, the displacement of the particle up to second order approximation will be given by

$$\langle a^+ + a\rangle = \int\left[\left(\bar\alpha + \frac{\partial}{\partial\bar\alpha}\right)\rho_2\left(\bar\alpha\bar\alpha_k,\alpha',\alpha'_k,t\right)\right]_{\substack{\alpha'_k=\alpha_k\\ \alpha'=\alpha}}\mathcal{D}^2\alpha\prod_k\mathcal{D}^2\alpha_k. \tag{53}$$

According to Eq. (51) the propagator $K_2(\bar\alpha_k,\bar\alpha,\alpha'_k,\alpha',t)$ will be given by

$$K_2(\bar\alpha_k,\bar\alpha,\alpha'_k,\alpha',t) = \exp\left(\sum_k \bar\alpha_k\alpha'_k e^{-i\omega_k t} + \bar\alpha\alpha' e^{-i\omega t}\right)\times \times\left[1 - f_l(t)\bar\alpha_l\alpha' - f_l(t)\alpha'_l\bar\alpha - g_l(t)\alpha'_l\bar\alpha^2 + g_l(t)\bar\alpha_l\alpha_l'^2\right]\times \times\exp\left(-\frac{|\alpha|^2}{2} - \frac{|\alpha'|^2}{2} - \frac{|\alpha_l|^2}{2} - \frac{|\alpha'_l|^2}{2}\right), \tag{54}$$

where

$$f_l(t) = \sum_l C_l\frac{e^{-i\omega t} - e^{-i\omega_l t}}{h(\omega_l-\omega)} \tag{55}$$

$$g_l(t) = F\sum_l C_l\frac{e^{-i\omega_l t} - e^{-i\omega t}}{h^2(\omega_l-\omega)(\omega_l-2\omega)}. \tag{56}$$

We perform the integrations in (52), then the integrations in (53) and we keep only the real part for the mean displacement $\langle a^+ + a\rangle$.

The final result is

$$\langle a^+ + a\rangle = 2\sum_l\frac{FC_l^2}{1-e^{-\beta\hbar\omega_l}}\cdot\frac{1}{(1-e^{-\beta\hbar\omega})^2}\cdot\frac{1}{\hbar^3(\omega_l-\omega)^2(\omega_l-2\omega)}\times \times\Big\{\left[-\cos(\omega_l-2\omega)t + 1 + \cos\omega t - \cos(\omega_l-\omega)t\right]e^{-4\beta\hbar\omega} + + \left[\cos(\omega_l-2\omega)t + 1 + \cos\omega t - \cos(\omega_l-\omega)t\right]e^{-2\beta\hbar\omega_l}e^{-\beta\hbar\omega} + + 2\left[\cos(\omega_l-2\omega)t - \cos\omega t - 1 + \cos(\omega_l-\omega)t\right]e^{-2\beta\hbar\omega_l}\Big\}. \tag{57}$$

This is the approximation involving the third order dependence of the mean displacement of the particle in the inverse values of $\Delta\omega$.

The result involves a summation over all frequencies that are close to the eigenfrequency of the particle. Usually only one frequency, say $\omega_k$, is close to that of the particle and only one term remains in (57), the term involving $\omega_k$.

The result (57) shows an oscillation of the mean displacement of the particle and is positive.

## VI. SUMMARY

The problem of interaction of a quantum particle with a thermal bath has been studied up to second order in coupling and up to third order in the difference between eigenfrequency of the particle and frequencies of the quantum oscillators of the bath.

The procedure which was followed involved a perturbation method for the propagators of the problem and the use of the density matrix for the evaluation of the averages.

The results, up to first order approximation in the propagator, are in agreement with previous ones (see for example Ref. [5]), but with our method, we can easily proceed to higher order approximations in the propagator.

We have computed the mean displacement of the particle in the presence of an external force and the results show an oscillation of the particle as expected.

## VII. APPENDIX I

In order to perform some integrations, that otherwise would require a lot of work, we use a generating function defined as follows

$$F(\lambda,\mu)=\frac{1}{\pi}\int_{-\infty}^{\infty} e^{-\gamma|\alpha|^2+\lambda\alpha+\mu\bar{\alpha}}d^2\alpha, \tag{A1}$$

where $\alpha = x + iy$ is a complex variable and

$$d^2\alpha = d(\mathrm{Re}\alpha)d(\mathrm{Im}\alpha) = dxdy. \tag{A2}$$

The integration of (A1) gives the generating function

$$F(\lambda,\mu)=\frac{1}{\gamma}e^{\frac{\lambda\mu}{\gamma}}. \tag{A3}$$

Using this formula we can compute the following integrals used in our work:

$$\frac{1}{\pi}\int \alpha e^{-|\alpha|^2+\lambda\alpha+\mu\bar{\alpha}}d^2\alpha=\frac{\partial}{\partial\lambda}F(\lambda,\mu)=\mu e^{\lambda\mu} \tag{A4}$$



$$\frac{1}{\pi}\int \bar{\alpha} e^{-|\alpha|^2+\lambda\alpha+\mu\bar{\alpha}}d^2\alpha=\frac{\partial}{\partial\mu}F(\lambda,\mu)=\lambda e^{\lambda\mu} \tag{A5}$$

$$\frac{1}{\pi}\int |\alpha^2| e^{-|\alpha|^2+\lambda\alpha+\mu\bar{\alpha}}d^2\alpha=(1+\lambda\mu)e^{\lambda\mu} \tag{A6}$$

$$\frac{1}{\pi}\int \alpha e^{-|\alpha|^2}d^2\alpha=0 \tag{A7}$$

$$\frac{1}{\pi}\int \bar{\alpha} e^{-|\alpha|^2}d^2\alpha=0 \tag{A8}$$

$$\frac{1}{\pi}\int |\alpha|^{2n} e^{-\lambda|\alpha|^2}d^2\alpha=\frac{n!}{\lambda^{n+1}}. \tag{A9}$$

Some other useful relations are:

$$\frac{1}{\pi}\int \alpha\bar{\alpha}^2 e^{-\gamma|\alpha|^2+\lambda\alpha+\mu\bar{\alpha}}d^2\alpha=\left(\frac{2\lambda}{\gamma^3}+\frac{\lambda^2\mu}{\gamma^4}\right)e^{\frac{\lambda\mu}{\gamma}} \tag{A10}$$

$$\frac{1}{\pi}\int \bar{\alpha}\alpha^2 e^{-\gamma|\alpha|^2+\lambda\alpha+\mu\bar{\alpha}}d^2\alpha=\left(\frac{2\mu}{\gamma^3}+\frac{\mu^2\lambda}{\gamma^4}\right)e^{\frac{\lambda\mu}{\gamma}}. \tag{A11}$$

## VIII. APPENDIX II

We are going to show that

$$\langle\alpha|H(a,a^+)U(a,a^+)|\bar{\alpha}\rangle = H\left(\frac{\partial}{\partial\bar{\alpha}},\bar{\alpha}\right)K(\bar{\alpha},\alpha'), \tag{A12}$$

where $H(a,a^+)$ is a Hamiltonian of the form

$$H(a^+,a)=A_1a+B_1a^++C_1a^+a+D_1 \tag{A13}$$

and $U(a,a^+)$ is the evolution operator with the matrix elements:

$$\langle\alpha|U(a,a^+)|\alpha'\rangle = K(\bar{\alpha},\alpha') = e^{A\bar{\alpha}+B\alpha'+C\bar{\alpha}\alpha'+D}e^{-\frac{|\alpha|^2}{2}}e^{-\frac{|\alpha'|^2}{2}}. \tag{A14}$$

In (A11) we have used $K(\bar{\alpha},\alpha')$ instead of $K(\alpha t/|\alpha' 0)$ or $K(t)$ in order to indicate that the propagator is a function of $\bar{\alpha}$ and $\alpha'$.

The operator $a^+$ is the Hermitian adjoint to the operator $a$ and operates only on the bra form ($\langle\alpha|$) of the state vector $|\alpha\rangle$. We start from the left hand side of (A12) and we proceed by using the complex integrations of Appendix I.

$$\begin{aligned}&\langle\alpha|H(a,a^+)U(a,a^+)|\alpha'\rangle = \\ &= [A_1(A+C\alpha')+B_1\bar{\alpha}+C_1\bar{\alpha}(A+C\alpha')+D_1]e^{A\bar{\alpha}+B\alpha'+C\bar{\alpha}\alpha'+D}e^{-\frac{|\alpha|^2}{2}}e^{-\frac{|\alpha'|^2}{2}} = \\ &= \left[A_1\frac{\partial}{\partial\bar{\alpha}}+B_1\bar{\alpha}+C_1\bar{\alpha}\frac{\partial}{\partial\bar{\alpha}}+D_1\right]e^{A\bar{\alpha}+B\alpha'+C\bar{\alpha}\alpha'+D}e^{-\frac{|\alpha|^2}{2}}e^{-\frac{|\alpha'|^2}{2}} = \\ &= H(\frac{\partial}{\partial\bar{\alpha}},\bar{\alpha})K(\bar{\alpha},\alpha').\end{aligned} \tag{A15}$$

Note that according to our notation in the differentiation of $K(\bar{\alpha},\alpha')$ we do not include the factor $e^{-|\alpha|^2/2}\,e^{-|\alpha'|^2/2}$ which remains unchanged.

## IX. APPENDIX III

Evaluation of the matrix elements of the first order approximation of the density matrix

$$\langle\alpha_k\alpha|R_1(t)|\alpha_k'\alpha'\rangle = \langle\alpha_k\alpha|U_1(t)R_0U_1(-t)|\alpha_k'\alpha'\rangle. \quad (A16)$$

We start by computing the following integral

$$\int\langle\alpha_k''\alpha''|R_0|\alpha_k'''\alpha'''\rangle\langle\alpha_k'''\alpha'''|U_1(-t)|\alpha_k'\alpha'\rangle \mathrm{d}^2\alpha'''\prod_k \mathrm{d}^2\alpha_k'''. \quad (A17)$$

The second matrix element of (A17) is given by (37), if we substitute $t$ by $-t$ and $\alpha_k, \alpha$ by $\alpha_k''', \alpha'''$. The integral (A17) can by written as follows:

$$\int(1-\mathrm{e}^{-\beta\hbar\omega})\prod_k(1-\mathrm{e}^{-\beta\hbar\omega_k})\exp\left(\sum_k\bar{\alpha}_k''\alpha_k'''\mathrm{e}^{-\beta\hbar\omega_k}+\bar{\alpha}''\alpha'''\mathrm{e}^{-\beta\hbar\omega}\right)\times$$
$$\times\exp\left(-\sum_k\frac{|\alpha_k''|^2}{2}-\frac{|\alpha''|^2}{2}-\sum_k\frac{|\alpha_k'''|^2}{2}-\frac{|\alpha'''|^2}{2}\right)\times$$
$$\times\exp\left(\sum_k\bar{\alpha}_k'''\alpha_k'\mathrm{e}^{\mathrm{i}\omega_k t}+\bar{\alpha}'''\alpha'\mathrm{e}^{\mathrm{i}\omega t}\right)\times$$
$$\times\left[1+\sum_k D_k(-t)(\bar{\alpha}_k'''\bar{\alpha}'''+\alpha_k'\alpha')+\sum_k E_k(-t)(\bar{\alpha}_k'''\alpha'+\alpha_k'\bar{\alpha}''')+A(-t)(\bar{\alpha}'''+\alpha')\right]$$
$$\times\exp\left(-\sum_k\frac{|\alpha_k'''|^2}{2}-\frac{|\alpha'''|^2}{2}-\sum_k\frac{|\alpha_k'|^2}{2}-\frac{|\alpha'|^2}{2}\right)\mathrm{d}^2\alpha'''\prod_k\mathrm{d}^2\alpha_k'''. \quad (A18)$$

The integrations can be performed with the aid of (A4) and (A5).

In order to find the matrix elements given in (A17) we multiply $K_1(\alpha\alpha_k t|\alpha_k''\alpha''.0)$ given by (37) by the result of the integration (A18).

The final result for the first order approximation to the density matrix is:

$$\rho_1(\alpha,\alpha_k,\alpha',\alpha_k',t)=(1-\mathrm{e}^{-\beta\hbar\omega})\prod_k(1-\mathrm{e}^{-\beta\hbar\omega})\exp\left(\sum_k\bar{\alpha}_k\alpha_k'\mathrm{e}^{-\beta\hbar\omega_k}+\bar{\alpha}\alpha'\mathrm{e}^{-\beta\hbar\omega}\right)\times$$
$$\times\left[1+D_k(t)\left(\bar{\alpha}_k\bar{\alpha}+\alpha_k'\mathrm{e}^{-\beta\hbar\omega_k}\mathrm{e}^{\mathrm{i}\omega_k t}\alpha'\mathrm{e}^{-\beta\hbar\omega}\mathrm{e}^{\mathrm{i}\omega t}\right)+\right.$$
$$\left.+\sum_k E_k(t)\left(\bar{\alpha}_k\alpha'\mathrm{e}^{-\beta\hbar\omega}\mathrm{e}^{\mathrm{i}\omega t}+\alpha_k'\mathrm{e}^{-\beta\hbar\omega_k}\mathrm{e}^{\mathrm{i}\omega_k t}\bar{\alpha}\right)+A(t)\left(\bar{\alpha}+\alpha'\mathrm{e}^{-\beta\hbar\omega}\mathrm{e}^{\mathrm{i}\omega t}\right)\right]\times$$
$$\times\left[1+\sum_k D_k(-t)\left(\bar{\alpha}_k\mathrm{e}^{-\mathrm{i}\omega_k t}\mathrm{e}^{-\beta t\omega_k}\bar{\alpha}\mathrm{e}^{-\mathrm{i}\omega t}\mathrm{e}^{-\beta\hbar\omega}+\alpha_k'\alpha'\right)+\right. \quad (A19)$$
$$+\sum_k E_k(-t)\left(\bar{\alpha}_k\mathrm{e}^{-\mathrm{i}\omega_k t}\mathrm{e}^{-\beta\hbar\omega_k}\alpha'+\alpha_k'\bar{\alpha}\mathrm{e}^{-\mathrm{i}\omega t}\mathrm{e}^{-\beta\hbar\omega}\right)+$$
$$\left.+A(-t)\left(\bar{\alpha}\mathrm{e}^{-\mathrm{i}\omega t}\mathrm{e}^{-\beta\hbar\omega}+\alpha'\right)\right]\cdot\exp\left(-\sum_k\frac{|\alpha_k|^2}{2}-\frac{|\alpha|^2}{2}-\sum_k\frac{|\alpha_k'|^2}{2}-\frac{|\alpha'|^2}{2}\right).$$



## REFERENCES


[1] Iche, G. Nozieres, P.: Physica *91A* (1978) 485.
[2] Lindenberg, K. West, B. J.: Phys. Rev. *A30* (1984) 568.
[3] Caldeira, A. Legget, A.: Physica *121A* (1983) 587.
[4] Caldeira, A. Legget, A.: Phys. Rev. Lett. *46* (1981) 211.
[5] Astangul, C., Pottier, N., Saint James, D.: J. of Stat. Phys. *40* (1985) 167.
[6] Glauber, R. J.: Phys. Rev. *131* (1963) 2766.
[7] Horak, R., Mista, L., Perina, J.: Phys. Lett. A (Netherlands), *35A* (1971) 400.
[8] Kubo, R.: J. Phys. Soc. Japan *7* (1962) 100.
[9] Kay, Maitland: *Quantum Optics.* Academic Press 1970.
[10] Wichman, E.: J. Math. Phys. *2* (1961) 876.
[11] Louisall, W.: *Quantum Statistical Properties of Radiation.* John Willey and Sons, 1973.
[12] Feynman, Hibbs: *Quantum Mechanics and Path Integrals.* Mc Graw Hill, N. Y. 1965.
[13] Wick, G. C.: Phys. Rev. *80* (1950) 268.



Received March 11th, 1992
Accepted for publication June 22nd, 1992


### ПРИБЛИЖЕНИЕ ВТОРОГО ПОРЯДКА СРЕДНЕГО РАССТОЯНИЯ ЧАСТИЦ В ТЕПЛОВОМ БАССЕЙНЕ С ДВИЖЕНИЕМ ВНЕШНЕЙ СИЛОЙ


**В работе изученно взаимодействие квантовой частицы с тепловым бассейном квантовых осцилляторов при действии внешней силы. Расчитанно в приближении до второго порядка пропагатора среднее расстояние частиц. Тепловой бассейн предполагается Бравновским с характеристическими частотами близкими частотам частиц. Установлено, что среднее расстояние частиц осциллирует во времени. Температурная зависимость среднего расстояния частиц подчиняется экспоненциальной зависимости.**