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

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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 of $e^{-1/T}$.

1. Introduction

The behaviour of a quantum particle coupled with a heat bath has been studied by many authors. Iche and Nozieres[1] have been 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 been studied this model under the influence of an external force using 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 heat bath is initially in thermal equilibrium and the density operator obeys a Bolzmann distribution. The perturbed part of the Hamiltonian has been treated with the aid of Feynman'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 cases one frequency is close to the frequency of the particle and the others do not contribute to the final result.

2. 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[6] 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:

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

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

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

where

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

Coherent states have been 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 a means complex conjugation. Another useful relation of the coherent states is:

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

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

b) *The propagator*

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

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

and the propagator associated with two different states is given by:

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

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

When the Hamiltonian consists of two parts

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

that don't commute with each other, we use Feynman's perturbation theory[12] to compute the propagator $K(a\, t \mid a'\, 0)$. 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 $K(a\, t \mid a'\, 0)$, which is the probability for a system being in state a' at time $t = 0$, to go to the state a at time $t = t$.

The solution of the Schrödinger equation

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

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

$$K_0(a\, t|a'\, 0) = \langle a|\, e^{-iH_0 t}\, |a'\rangle. \tag{11}$$

In order to find the first order approximation we use the known Feynman's formula:

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

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

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

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

The propagator associated with the Hamiltonian of the system can be used to propagate in time 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:

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

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

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

The density operator at time t is given by:

$$R(t) = U(t|0) R_0 U^+(t|0). \tag{17}$$

We evaluate thermal averages using the generalized Wick's 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:

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

so the density operator (17) is given by:

$$R(t) = U(t) R_0 U^+(-t). \tag{20}$$

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

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

The matrix elements of the equilibrium density operator are given by:

$$\varrho_0 (\alpha, \alpha') = \frac{\langle \alpha | \, e^{-\beta \hbar \omega a^+ a} \, | \alpha' \rangle}{Z_0}. \tag{22}$$

From Eq. (16) we can find Z_0

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

and from Eq. (21) we obtain

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

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

$$\varrho_0 (\alpha, \alpha') = (1 - e^{-\beta \hbar \omega}) \exp (e^{-\beta \hbar \omega} \bar{\alpha} \alpha') \, e^{-\frac{|\alpha|^2}{2}} \, e^{-\frac{|\alpha'|^2}{2}}. \tag{25}$$

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

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

3. *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:

$$H = \sum_K \hbar \omega_K a_K a_K + \hbar \omega a^+ a + \sum_K C_K (a^+ + a)(a_K^+ + a_K) - F (a^+ + a). \tag{27}$$

The third term in the Hamiltonian represents the interaction of the particle with the bath and the coupling constants C_K are small.

The Hamiltonian (27) can be separated in 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

$$H' = (a^+ + a) \sum_K C_K (a_K^+ + a_K) - F(a^+ + a) \tag{29}$$

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

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

$$R_0 (a_K, a_K^+, a, a^+) = \frac{e^{-\beta\hbar (\sum_K \omega_K a_K^+ a_K + \omega a^+ a)}}{\mathrm{Tr}\,(e^{-\beta\hbar (\sum_K \omega_K a_K^+ a_K + \omega a^+ a)})}. \tag{30}$$

The matrix elements of the density operator are:

$$\langle a_K a| R_0 (a_K, a_K^+, a, a^+) |a_K' a'\rangle = \prod_K (1 - e^{-\beta\hbar\omega_K}) (1 - e^{-\beta\hbar\omega}) \cdot$$

$$\cdot \exp (\sum_K \overline{a}_K a_K' e^{-\beta\hbar\omega_K} + \overline{a} a' e^{-\beta\hbar\omega})$$

$$\cdot \exp \left(- \sum_K \frac{|a_K|^2}{2} - \sum_K \frac{|a_K'|^2}{2} - \frac{|a|^2}{2} - \frac{|a'|^2}{2}\right). \tag{31}$$

4. 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.

From Eq. (11) we can see that the matrix elements of the zero order propagator is:

$$K_0 (t|0) = \exp (\sum_K \overline{a}_K a_K' e^{-i\omega_K t} + \overline{a} a' e^{-i\omega t}) \cdot$$

$$\cdot \exp \left(- \sum_K \frac{|a_K|^2}{2} - \sum_K \frac{|a_K'|^2}{2} - \frac{|a|^2}{2} - \frac{|a'|^2}{2}\right). \tag{32}$$

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

$$\langle a_K a| U_0 (t|\tau) H'(\tau) U_0 (\tau|0) |a_K' a'\rangle$$

($U_0(t)$ is the evolution operator associated with the zero order propagator $K_0(t)$) will be evaluated from the following integral:

$$\int \langle a_K a| \, U_0(t|\tau) \, |a''_K \, a''\rangle \, \langle a''_K \, a''| \, H'(\tau) \, U_0(\tau|0) \, |a'_K \, a'\rangle \, \mathrm{d}^2 a'' \prod_K \mathrm{d}^2 a''_K. \quad (33)$$

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

$$\langle a''_K \, a''| \, H'(\tau) \, U_0(\tau|0) | \, a'_K \, a'\rangle = \exp\left(\sum_K \bar{a}''_K \, a'_K \, \mathrm{e}^{-\mathrm{i}\omega_K \tau} + \bar{a}'' \, a' \, \mathrm{e}^{-\mathrm{i}\omega\tau}\right) \cdot$$
$$\cdot \left[(\bar{a}'' + a' \, \mathrm{e}^{-\mathrm{i}\omega\tau}) \sum_K C_K (\bar{a}''_K + a'_K \, \mathrm{e}^{-\mathrm{i}\omega_K \tau}) - F(\bar{a}'' + a' \, \mathrm{e}^{-\mathrm{i}\omega\tau})\right] \cdot$$
$$\cdot \exp\left(-\sum_K \frac{|a''_K|^2}{2} - \frac{|a''|^2}{2} - \sum_K \frac{|a'_K|^2}{2} - \frac{|a'|^2}{2}\right). \quad (34)$$

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:

$$\int \exp\left(\sum_K \bar{a}_K \, a''_K \, \mathrm{e}^{-\mathrm{i}\omega_K (t-\tau)} + \bar{a} \, a'' \, \mathrm{e}^{-\mathrm{i}\omega(t-\tau)}\right) \cdot$$
$$\cdot \exp\left(-\sum_K \frac{|a_K|^2}{2} - \frac{|a|^2}{2} - \sum_K \frac{|a''_K|^2}{2} - \frac{|a''|^2}{2}\right) \cdot$$
$$\cdot \left[(a'' + a' \, \mathrm{e}^{-\mathrm{i}\omega\tau}) \sum_K C_K (\bar{a}''_K + a'_K \, \mathrm{e}^{-\mathrm{i}\omega_K \tau}) - F(\bar{a}'' + a' \, \mathrm{e}^{-\mathrm{i}\omega\tau})\right] \cdot$$
$$\cdot \exp\left(\sum_K \bar{a}''_K a'_K \, \mathrm{e}^{-\mathrm{i}\omega_K \tau} + \bar{a}'' \, a' \, \mathrm{e}^{-\mathrm{i}\omega\tau}\right) \cdot$$
$$\cdot \exp\left(-\sum_K \frac{|a'_K|^2}{2} - \frac{|a'|^2}{2} - \sum_K \frac{|a''_K|^2}{2} - \frac{|a''|^2}{2}\right) \mathrm{d}^2 a'' \prod_K \mathrm{d}^2 a''_K. \quad (35)$$

The integrations over a''_K and a' 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 $\langle a_K a| \, U_0(t/\tau) \, H'(\tau) \, U_0(\tau/0) | \, a'_K \, a'\rangle$ is:

$$K_0(t/\tau) \, H'(\tau) \, K_0(\tau/0) = \left[(\bar{a} \, \mathrm{e}^{-\mathrm{i}\omega(t-\tau)}) + a' \, \mathrm{e}^{-\mathrm{i}\omega\tau}\right) \cdot$$
$$\cdot \sum_K C_K (\bar{a}_K \, \mathrm{e}^{-\mathrm{i}\omega_K (t-\tau)} + a'_K \, \mathrm{e}^{-\mathrm{i}\omega_K \tau}) - F(\bar{a} \, \mathrm{e}^{-\mathrm{i}\omega(t-\tau)} + a' \, \mathrm{e}^{-\mathrm{i}\omega\tau})\right] \cdot$$
$$\cdot \exp\left(\sum_K \bar{a}_K \, a'_K \, \mathrm{e}^{-\mathrm{i}\omega_K t} + \bar{a} \, a' \, \mathrm{e}^{-\mathrm{i}\omega t}\right) \cdot$$
$$\cdot \exp\left(-\sum_K \frac{|a_K|^2}{2} - \frac{|a|^2}{2} - \sum_K \frac{|a'_K|^2}{2} - \frac{|a'|^2}{2}\right). \quad (36)$$

Feynman's formula (12) requires an integration of (36) over τ, that can be easily performed

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

$$K_1(a\, a_K\, t \mid a'_K\, a'\, 0) = \exp\left(\sum_K \bar{a}_K\, a'_K\, e^{-i\omega_K t} + \bar{a}\, a'\, e^{-i\omega t}\right) \cdot$$

$$\cdot \left[1 + \sum_K D_K(t)(\bar{a}_K \bar{a} + a'_K a') + \sum_K E_K(t)(\bar{a}_K a' + a'_K \bar{a}) + A(t)(\bar{a} + a')\right] \cdot$$

$$\cdot \exp\left(-\sum_K \frac{|a_K|^2}{2} - \frac{|a|^2}{2} - \sum_K \frac{|a'_K|^2}{2} - \frac{|a'|^2}{2}\right), \tag{37}$$

where

$$D_K(t) = C_K \frac{(e^{-i(\omega_K+\omega)t} - 1)}{\hbar(\omega_K + \omega)}, \tag{38}$$

$$E_K(t) = C_K \frac{(e^{-i\omega_K t} - e^{-i\omega t})}{\hbar(\omega_K - \omega)}, \tag{39}$$

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

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, i. e.

$$\varrho_1(a_K, a, a'_K, a', t) = \langle a_K\, a|\, R_1(t)|\, a'_K\, a'\rangle = \int\int \langle a_K\, a|\, U_1(t)|\, a''_K\, a''\rangle \cdot$$

$$\cdot \langle a''_K\, a''|\, R_0|\, a'''_K\, a'''\rangle \langle a'''_K\, a'''|\, U_1(-t)|\, a'_K\, a'\rangle\, d^2 a'' \prod_K d^2 a''_K d^2 a''' \prod_K d^2 a'''_K. \tag{42}$$

The mathematical work can be seen in Appendix III up to first order approximation to the density matrix and the result is 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 long 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)) will be given by:

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

We use again the substitution $a^+ \to \bar{a}$, $a \to \frac{\partial}{\partial \bar{a}}$ 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 ones, and we integrate over all these states

$$\langle a^+ + a \rangle = \int \left[\left(\bar{a} + \frac{\partial}{\partial \bar{a}} \right) \varrho_1 (\bar{a}, \bar{a}_K, a', a'_K, t) \right]_{\substack{\alpha'_K = \alpha_K \\ \alpha' = \alpha}} \mathscr{D}^2 \, a \prod_K \mathscr{D}^2 \, a_K \quad (44)$$

where

$$\mathscr{D}^2 \, a = \frac{1}{\pi} \mathrm{e}^{-\frac{|\alpha|^2}{2}} \mathrm{d}^2 \, a, \qquad \mathscr{D}^2 \, a_K = \frac{1}{\pi} \mathrm{e}^{-\frac{|\alpha_K|^2}{2}} \mathrm{d}^2 \, a_K. \quad (45)$$

There are only two kinds of integrals that will appear in (44) and that they will not vanish. These integrals are the following:

$$\int_{-\infty}^{\infty} \exp (|a|^2 \, \mathrm{e}^{-\beta \hbar \omega}) \, \mathscr{D}^2 \, a = \frac{1}{\pi} \int_{-\infty}^{\infty} \exp [-|a|^2 (1 - \mathrm{e}^{-\beta \hbar \omega})] \, \mathrm{d}^2 a = \frac{1}{1 - \mathrm{e}^{-\beta \hbar \omega}} \quad (46)$$

$$\int_{-\infty}^{\infty} |a|^2 \exp (|a|^2 \, \mathrm{e}^{-\beta \hbar \omega}) \, \mathscr{D}^2 \, a = \frac{1}{\pi} \int_{-\infty}^{\infty} |a|^2 \exp [-|a|^2 (1 - \mathrm{e}^{-\beta \hbar \omega})] \, \mathrm{d}^2 \, a =$$

$$= \frac{1}{(1 - \mathrm{e}^{-\beta \hbar \omega})^2}. \quad (47)$$

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

Using (46) and (47) in (44) we compute the average displacement of the particle

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

This is a result already known from Ref. 5 but the procedure followed is very interesting because we can go up to higher order approximation, as we are going to do in what follows.

5. *Second order approximation*

The first order approximation to the mean displacement of the quantum particle coupled to a system of other quantum particles does not show 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 elemen

$$\langle a_K\, a|\, K_0(t|\tau)\, H'(\tau)\, K_1(\tau|0)\, |a'_K\, a'\rangle$$

will be evaluated according to the following integrations

$$\int \langle a_K\, a|\, K_0(t/\tau)\, |a''_K\, a''\rangle \langle a''_K\, a''|\, H'(\tau)\, K_1(\tau/0)|\, a'_K a'\rangle\, \mathscr{D}^2\, a'' \prod \mathscr{D}^2\, a''_K. \tag{49}$$

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

$$t \to t - \tau, \qquad a' \to a'', \qquad a'_K \to a''_K.$$

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 $\frac{1}{\omega_K - \omega}$ and higher order terms; all the other terms are neglected because they are small compared to this. In order to find the propagator $K_2(\bar{a}_K, \bar{a}, a'_K, a', t)$ we perform the integration over τ in Eq. (13).

The second order approximation to the density matrix is given by:

$$R_1(t) = U_2(t)\, R_0\, U_2(-t) \tag{50}$$

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

$$K_2(\bar{a}_K, \bar{a}, a'_K, a', t) = \langle \bar{a}_K\, \bar{a}|\, U_2(t)\, |a'_K\, a'\rangle. \tag{51}$$

The matrix elements of (50) can be 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:

$$\varrho_2(\bar{a}_K, \bar{a}, a'_K, a', t) = \int\int K_2(\bar{a}_K, \bar{a}, a'''_K, a''', t)\, R_0(\bar{a}'''_K, \bar{a}''', a''_K, a'', t)\, \cdot$$
$$\cdot\, K_2(\bar{a}''_K, \bar{a}'', a'_K, a', -t)\, \mathscr{D}^2\, a'''\, \mathscr{D}^2\, a'' \prod_K \mathscr{D}^2\, a'''_K\, \mathscr{D}^2\, a''_K. \tag{52}$$

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:

$$\langle a^+ + a\rangle = \int \left[\left(\bar{a} + \frac{\partial}{\partial \bar{a}}\right) \varrho_2 (\bar{a}, \bar{a}_K, a', a'_K, t)\right]_{\substack{a'_K = a_K \\ a' = a}} \mathscr{D}^2\, a \prod_K \mathscr{D}^2\, a_K. \quad (53)$$

According to Eq. (51) the propagator $K_0 (\bar{a}_K, \bar{a}, a'_K, a', t)$ will be given by:

$$K_2 (\bar{a}_K, \bar{a}, a'_K, a', t) = \exp \left(\sum_K \bar{a}_K\, a'_K\, e^{-i\omega_K t} + \bar{a}\, a'\, e^{-i\omega t}\right) \cdot$$
$$\cdot \left[1 - f_l (t)\, \bar{a}_l\, a' - f_l (t)\, a'_l\, \bar{a} - g_l (t)\, a'_l\, \bar{a}^2 + g_l (t)\, \bar{a}_l\, a_l'^2\right] \cdot$$
$$\cdot \exp \left(-\frac{|a|^2}{2} - \frac{|a'|^2}{2} - \frac{|a_l|^2}{2} - \frac{|a'_l|^2}{2}\right), \quad (54)$$

where

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

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

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:

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

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

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

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

6. *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 of the eigenfrequency of the particle with the frequencies of the quantum ocillators of the bath.

The procedure 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 the method used, we can proceed up to higher order approximations in the propagator.

We wave computed the mean displacement of such a particle in the presence of an external force and the results shows an oscillation of the particle as expected.

Appendix I

In order to perform some complex integrations, that otherwise would require a lot of work, we use a generating function.

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

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

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

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, that we are going to use our work:

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

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

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

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

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

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

Some other useful relations are:

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

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

Appendix II

We are going to show that

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

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

$$H(a^+, a) = A_1\, a + B_1\, a^+ + C_1\, a^+\, a + D_1 \tag{A13}$$

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

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

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

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

$$\langle a|\, H(a, a^+)\, U(a, a^+)\, |a'\rangle =$$

$$= [A_1(A + Ca') + B_1\, \bar{a} + C_1\, \bar{a}\,(A + C\, a') + D_1]\, \cdot$$

$$\cdot\, e^{A\bar{\alpha} + B\alpha' + C\bar{\alpha}\alpha' + D}\, e^{-\frac{|\alpha|^2}{2}}\, e^{\frac{|\alpha'|^2}{2}} =$$

$$= \left[A_1 \frac{\partial}{\partial \bar{\alpha}} + B_1\, \bar{\alpha} + C_1\, \bar{\alpha} \frac{\partial}{\partial \bar{\alpha}} + D_1\right] e^{A\bar{\alpha} + B\alpha' + C\bar{\alpha}\alpha' + D}\, \cdot$$

$$\cdot\, e^{-\frac{|\alpha|^2}{2}}\, e^{-\frac{|\alpha'|^2}{2}} = H\left(\frac{\partial}{\partial \bar{\alpha}}, \bar{\alpha}\right) K(\bar{\alpha}, \alpha'). \tag{A15}$$

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

Appendix III

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

$$\langle a_K\, a|\, R_1(t)\, |a_K' a'\rangle = \langle a_K\, a|\, U_1(t)\, R_0\, U_1(-t)\, |a_K'\, a'\rangle. \tag{A16}$$

We start by computing the following integral:

$$\int \langle a_K''\, a''|\, R_0\, |a_K'''\, a'''\rangle \langle a_K'''\, a'''|\, U_1(-t)\, |a_K'\, a'\rangle\, d^2 a''' \prod_K d^2 a_K'''. \tag{A17}$$

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

$$\int (1 - e^{-\beta\hbar\omega}) \prod_K (1 - e^{-\beta\hbar\omega_K}) \exp\left(\sum_K \bar{a}_K''\, a_K'''\, e^{-\beta\hbar\omega_K} + \bar{a}''\, a'''\, e^{-\beta\hbar\omega}\right) \cdot$$

$$\cdot \exp\left(-\sum_K \frac{|a_K''|^2}{2} - \frac{|a''|^2}{2} - \sum_K \frac{|a_K'''|^2}{2} - \frac{|a'''|^2}{2}\right) \cdot$$

$$\cdot\, \exp\left(\sum_K \bar{a}_K'''\, a_K'\, e^{i\omega_K t} + \bar{a}'''\, a'\, e^{i\omega t}\right) \cdot$$

$$\cdot \left[1 + \sum_K D_K(-t)\,(\bar{a}_K'''\, \bar{a}''' + a_K'\, a') + \sum_K E_K(-t)\,(\bar{a}_K'''\, a' + a_K'\, \bar{a}''') +\right.$$

$$\left. + A(-t)\,(\bar{a}''' + a')\right] \cdot \exp\left(-\sum_K \frac{|a_K'''|^2}{2} - \frac{|a'''|^2}{2} -\right.$$

$$\left. - \sum_K \frac{|a_K'|^2}{2} - \frac{|a'|^2}{2}\right) d^2 a''' \prod d^2 a_K'''. \tag{A18}$$

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

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

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

$$\varrho_1 (a, a_K, a', a'_K, t) = (1 - e^{-\beta\hbar\omega}) \prod_K (1 - e^{-\beta\hbar\omega}) \cdot$$

$$\cdot \exp (\sum_K \overline{a}_K\, a'_K\, e^{-\beta\hbar\omega_K} + \overline{a}\, a'\, e^{-\beta\hbar\omega}) [1 + D_K (t) (\overline{a}_K\, \overline{a} +$$

$$+ a'_K\, e^{-\beta\hbar\omega_K}\, e^{i\omega_K t}\, a'\, e^{-\beta\hbar\omega}\, e^{i\omega t}) + \sum_K E_K (t) (\overline{a}_K\, a'\, e^{-\beta\hbar\omega}\, e^{i\omega t} +$$

$$+ a'_K\, e^{-\ \beta\omega_K}\, e^{i\omega_K t}\, \overline{a}) + A (t) (\overline{a} + a'\, e^{-\beta\hbar\omega}\, e^{i\omega t})] \cdot$$

$$\cdot [1 + \sum_K D_K (-t) (\overline{a}_K\, e^{-i\omega_K t}\, e^{-\beta\hbar\omega_K}\, \overline{a}\, e^{-i\omega t}\, e^{-\beta\hbar\omega} - a'_K\, a') +$$

$$+ \sum_K E_K (-t) (\overline{a}_K\, e^{-i\omega_K t}\, e^{-\beta\hbar\omega_K}\, a' + a'_K\, \overline{a}\, e^{-i\omega t}\, e^{-\beta\hbar\omega}) +$$

$$+ A (-t) (\overline{a}\, e^{-i\omega t}\, e^{-\beta\hbar\omega} + a')] \exp \left(- \sum_K \frac{|a_K|^2}{2} - \frac{|a|^2}{2} - \sum_K \frac{|a'_K|^2}{2} - \frac{|a'|^2}{2} \right). \tag{A19}$$

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APROKSIMACIJA DRUGOG REDA ZA SREDNJI POMAK ĆESTICE URONJENE U TOPLINSKU KUPKU UZ PRISUSTVO VANJSKE SILE

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