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Correlation functions of the non-stationary quantum singular oscillator

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Abstract. The exact density matrix elements and the correlation functions of the one-dimensional non-stationary singular oscillator (the potential $U(x, t) = \omega^2(t)x^2/2 + g/x^2$) excited from the thermodynamic equilibrium states are obtained. Generating functions for ρ_{nm} and also for transition probabilities are constructed.

1. Introduction

Investigations of non-stationary quantum systems which possess dynamical symmetry arouse a great deal of interest nowadays because of the remarkable possibility of obtaining exact solutions of quantum mechanical problems. The term 'dynamical symmetry' in this paper means that the Hamiltonian of the system (which is, generally, time dependent) can be considered as an element of some finite-dimensional Lie algebra g and, consequently, a trajectory is a curve in the corresponding Lie group G. Well known examples of such a situation include the motion of a spin in an external magnetic field, or a one-dimensional harmonic oscillator, when the Hamiltonian is the element of su(2) or su(1, 1), respectively. Another example is an n-level quantum system interacting with a classical electromagnetic field ($n \geqslant 3$) (see, e.g., Amirav *et al* (1980), Elgin (1980) and Hioe (1983); the corresponding group is SU(n)). Recently the algebras so(6) and u(8) were used to describe the phenomena of superconductivity and charge-density waves in many-electron systems (Solomon 1981, Solomon and Birman 1982).

In the present paper we consider a quantum system in one dimension described by the Hamiltonian

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{m\omega^2(t)}{2}x^2 + \frac{g}{x^2} \qquad x > 0 \qquad g = \text{constant}. \tag{1}$$

This system is called 'a singular oscillator'; the Hamiltonian (1) is related to the Lie algebra su(1, 1). Therefore the corresponding Schrödinger equation can be solved exactly, as was done for the first time by Camiz *et al* (1971). Later Dodonov *et al* (1974) calculated exactly the propagator and the matrix elements of the evolution operator. Various properties of quantum systems described by the Hamiltonian (1) were also studied, for example, by Hartly and Ray (1981). As for the physical applications, we refer to the paper by Gorokhov (1971) who used the Hamiltonian (1) to study vibrational modes of polyatomic molecules.

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The aim of our paper is to consider the evolution of the density matrix of the singular oscillator which was initially in the equilibrium state corresponding to the initial value ω_{in}. We calculate the exact density matrix elements in the basis of the final Hamiltonian eigenstates and, therefore, the exact expressions for the energy level populations in the final state. The generating function for these matrix elements will also be obtained. We note that, under certain relations between the initial temperature and the form of the excitation $\omega(t)$, it turns out that in the final state the maximum occupation probabilities correspond not to the ground energy level (as it would for the equilibrium distribution) but to the excited levels, i.e. an inversion of populations can be obtained (it is supposed that the relaxation effects can be neglected). We discuss numerical examples of such a situation in appendix 1, where the simple asymptotic formula for the occupation probabilities is also obtained. We also calculate the multi-time correlation functions for the generators of the dynamical symmetry algebra of the problem under study and show that all of them can be expressed in terms of the first- and the second-order correlation functions. In appendix 2 we obtain a generating function for the transition probabilities between the initial and final Hamiltonian eigenstates. As a consequence, a new generating function for the products of the Jacobi polynomials is found.

2. The density matrix

It is well known that the eigenstates of the singular oscillator Hamiltonian (1) form the basis of the infinite-dimensional irreducible representation of the Lie algebra su(1, 1) (see, e.g., Camiz *et al* 1971). The generators of the representation can be chosen as follows:

$$K_0=(p^2+x^2)/4+g/2x^2 \qquad p\equiv -\mathrm{i}\,\partial/\partial x$$
$$K_1=(p^2-x^2)/4+g/2x^2 \qquad K_2=(px+xp)/4 \tag{2}$$
$$K_\pm=K_1\pm \mathrm{i}K_2 \qquad [K_0, K_\pm]=\pm K_\pm \qquad [K_+, K_-]=-2K_0.$$

We suppose that $g>-\hbar^2/8m$. In the opposite case, the Hamiltonian becomes non-Hermitian and a special analysis is required (Case 1950, Alliluyev 1971). The dimensional constants can be restored in the final formulae by means of the substitutions

$$x\to(m\omega_{in}/\hbar)^{1/2}x \qquad t\to\omega_{in}t \qquad g\to mg\hbar^{-2} \qquad \omega(t)\to\omega_{in}\omega(t).$$

Let us introduce a complete orthogonal set of states

$$|n\rangle,\ n=0,1,\ldots,\ 2K_0|n\rangle=(2n+a+1)|n\rangle \qquad a\equiv(1+8g)^{1/2}/2$$
$$K_+|n\rangle=[(n+1)(n+a+1)]^{1/2}|n+1\rangle \qquad K_-|n\rangle=[n(n+a)]^{1/2}|n-1\rangle. \tag{3}$$

The explicit form of $|n\rangle$ in the coordinate representation can be found in the paper by Dodonov *et al* (1974). When $a=\frac{1}{2}$, the vectors $|n\rangle$ become the eigenvectors of the usual oscillator with the infinite wall at the point $x=0$. The Casimir operator $C=K_0^2-K_1^2-K_2^2$ is equal to the number $(a^2-1)/4$ for this representation. In this paper we will use the representation of the group $\overline{\mathrm{SU}(1,1)}$ (the universal covering of the group SU(1, 1)) which corresponds to the representation (2) and (3) of the algebra su(1, 1) (see Barut and Girardello 1971). Let $\hat{T}$ be an arbitrary operator from the representation of the group $\overline{\mathrm{SU}(1,1)}$, for which we suppose that the corresponding element of the

group possesses the Gauss decomposition: $\hat{T}=\exp(AK_+)\exp(BK_0)\exp(CK_-)$ (parameters A, B, C are independent of the choice of the representation). It will be convenient to use the following formula which expresses the matrix elements of the operator $\hat{T}$ in terms of Jacobi polynomials:

$$\langle n|\hat{T}|m\rangle \equiv \langle n|\exp(AK_+)\exp(BK_0)\exp(CK_-)|m\rangle = C^{m-n}\exp[B(a+1)/2] \times (e^B-AC)^n\left(\frac{n!\Gamma(m+a+1)}{m!\Gamma(n+a+1)}\right)^{1/2} P_n^{(m-n,a)}\left(\frac{e^B+AC}{e^B-AC}\right). \tag{4}$$

Equation (4) can be checked by direct calculation in the basis (3) if one uses the definition of Jacobi polynomials $P_n^{(\alpha,\beta)}(x)$ (Erdelyi 1953) and the relation

$$P_n^{(m-n,\beta)}(x)=\left(\frac{x-1}{2}\right)^{n-m}\frac{m!\Gamma(n+\beta+1)}{n!\Gamma(m+\beta+1)}P_m^{(n-m,\beta)}(x). \tag{5}$$

We will also use the overcomplete basis of 'coherent states' (Dodonov *et al* 1974; later the same was done by Gerry 1983):

$$K_-|\alpha\rangle=\frac{\alpha^2}{2}|\alpha\rangle \qquad |\alpha\rangle=\sum_{n=0}^{\infty}\left(\frac{\alpha^2}{2}\right)^n\left(\frac{\Gamma(a+1)}{n!\Gamma(n+a+1)}\right)^{1/2}|n\rangle$$
$$\langle\alpha|\gamma\rangle=\Gamma(a+1)(\bar{\alpha}\gamma/2)^{-a}I_a(\bar{\alpha}\gamma). \tag{6}$$

Here, α is an arbitrary complex number and $I_q(z)$ is a modified Bessel function. We consider a Hamiltonian of a more general form than (1):

$$H=\Omega_0K_0+\Omega_1K_1+\Omega_2K_2\equiv\exp(-i\varphi K_0)\exp(-i\chi K_2)2\omega K_0\exp(i\chi K_2)\exp(i\varphi K_0)$$
$$\Omega_0=2\omega\cosh\chi \qquad \Omega_1=2\omega\sinh\chi\cos\varphi \qquad \Omega_2=2\omega\sinh\chi\sin\varphi \tag{7}$$

where $\Omega_i(t)$ are arbitrary real functions ($i=0,1,2$). We assume that $4\omega^2=\Omega_0^2-\Omega_1^2-\Omega_2^2>0$ for any t. Moreover, we assume that

$$\chi(t)=\varphi(t)=\Omega_1(t)=\Omega_2(t)=0 \qquad \Omega_0(t)=2\omega(t)=2$$

when $t\leqslant 0$. Therefore at any time $t\leqslant 0$ we have a singular oscillator with unit frequency.

The evolution operator which satisfies the Schrödinger equation with the Hamiltonian (7)

$$i\,dU/dt\equiv i\dot{U}=HU \qquad U(0)=\hat{1} \tag{8}$$

belongs to the representation of the group $\overline{SU(1,1)}$. Consequently, it can be determined exactly. It is convenient to use the Gauss decomposition for the evolution operator U:

$$U(t)\equiv\exp(A(t)K_+)\exp(B(t)K_0)\exp(C(t)K_-). \tag{9}$$

The substitution of the form (9) in equation (8) leads to the following system of equations for the parameters A, B and C:

$$\dot{A}-A\dot{B}+A^2\dot{C}\,e^{-B}=-i\Omega_+$$
$$\dot{B}-2A\dot{C}\,e^{-B}=-i\Omega_0 \qquad \dot{C}\,e^{-B}=-i\Omega_- \tag{10}$$
$$\Omega_+=\bar{\Omega}_-\equiv(\Omega_1-i\Omega_2)/2$$

with the initial conditions $A(0)=B(0)=C(0)=0$. (In order to check (10) one has to use the identities

$$\exp(AK_+)K_0\exp(-AK_+)=K_0-AK_+$$
$$\exp(AK_+)K_-\exp(-AK_+)=K_--2AK_0+A^2K_+$$
$$\exp(BK_0)K_0\exp(-BK_0)=\exp(-B)K_-$$

which follow from the commutation relation of the algebra su(1, 1).) It is easy to verify that the solutions of the system (10) which satisfy the required initial conditions can be represented in the following form:

$$A=\frac{\mathrm{i}\dot{\varepsilon}+\sigma\varepsilon}{\mathrm{i}\dot{\varepsilon}-\sigma\varepsilon}\exp(-\mathrm{i}\varphi) \qquad \exp(-B/2)=-\frac{\mathrm{i}\dot{\varepsilon}-\sigma\varepsilon}{2\sigma}\exp(\mathrm{i}\varphi/2)$$
$$C=\frac{\mathrm{i}\dot{\bar{\varepsilon}}-\sigma\bar{\varepsilon}}{\mathrm{i}\dot{\varepsilon}-\sigma\varepsilon} \tag{11}$$

where $\sigma\equiv\omega\,\mathrm{e}^{\chi}-\dot{\varphi}/2$ and the functions $\varepsilon(t)$ and $\bar{\varepsilon}(t)$ are the complex conjugate solutions of the equation

$$\ddot{\varepsilon}-(\dot{\sigma}/\sigma)\dot{\varepsilon}+\tilde{\omega}^2\varepsilon=0 \qquad \varepsilon(t\leqslant 0)=\exp(\mathrm{i}t)$$
$$\tilde{\omega}^2\equiv\omega^2+\dot{\varphi}^2/4-\dot{\varphi}\omega\cosh\chi. \tag{12}$$

Let us suppose that when $t\to\infty$, the parameters $\varphi(t)$, $\chi(t)$, $\omega(t)$ tend sufficiently fast to constant values φ_0, χ_0, ω_0. Consequently, when $t\to\infty$, $\tilde{\omega}^2\to\omega_0^2$, $\sigma\to\omega_0\exp(\chi_0)$, equations (12) are transformed into $\ddot{\varepsilon}+\omega_0^2\varepsilon=0$, $\varepsilon\to\exp(\chi_0/2)[\xi\exp(\mathrm{i}\omega_0 t)-\eta\exp(-\mathrm{i}\omega_0 t)]$ where complex parameters ξ, η satisfy the restriction $|\xi|^2-|\eta|^2=1$. Further, we shall use the notation

$$|\xi|\equiv\cosh\mu/2 \qquad |\eta|\equiv\sinh\mu/2 \qquad 2\eta\bar{\xi}\equiv\exp(\mathrm{i}\psi)\sinh\mu. \tag{13}$$

Let us write down the asymptotic form of the evolution operator when $t\to\infty$. Corresponding values of the parameters A, B, C are given as follows:

$$A_{\mathrm{f}}=\frac{\eta\exp(-\mathrm{i}\omega_0 t)\cosh\chi_0/2-\xi\exp(\mathrm{i}\omega_0 t)\sinh\chi_0/2}{\xi\exp(\mathrm{i}\omega_0 t)\cosh\chi_0/2-\eta\exp(-\mathrm{i}\omega_0 t)\sinh\chi_0/2}\exp(-\mathrm{i}\varphi_0)$$
$$\exp(-B_{\mathrm{f}}/2)=\exp(\mathrm{i}\varphi_0/2)[\xi\exp(\mathrm{i}\omega_0 t)\cosh\chi_0/2-\eta\exp(-\mathrm{i}\omega_0 t)\sinh\chi_0/2]$$
$$C_{\mathrm{f}}=\frac{\bar{\xi}\exp(-\mathrm{i}\omega_0 t)\sinh\chi_0/2-\bar{\eta}\exp(\mathrm{i}\omega_0 t)\cosh\chi_0/2}{\xi\exp(\mathrm{i}\omega_0 t)\cosh\chi_0/2-\eta\exp(-\mathrm{i}\omega_0 t)\sinh\chi_0/2} \tag{14}$$
$$U(t\to\infty)=\exp(A_{\mathrm{f}}K_+)\exp(B_{\mathrm{f}}K_0)\exp(C_{\mathrm{f}}K_-).$$

We consider now the physical situation, when a singular oscillator with unit frequency is excited from the thermodynamic equilibrium state with the temperature T.

The excitation is described by the functions $\Omega_i(t)$ (i.e. $\varphi(t)$, $\omega(t)$, $\chi(t)$). Suppose that at the time $t\to\infty$ the system again becomes a singular oscillator but with a new frequency ω_0. Then it is necessary to put $\varphi_0=0$, $\exp(-\chi_0)=\omega_0$. Let us introduce a new basis $|n,f\rangle$ consisting of the eigenstates of the final Hamiltonian

$$H_{\mathrm{f}}=\lim_{t\to\infty}H\equiv V2\omega_0 K_0 V^{-1}$$
$$|n,f\rangle=V|n\rangle \qquad V\equiv\exp(-\mathrm{i}\chi_0 K_2). \tag{15}$$

One can obtain the matrix elements describing the transitions from the initial states (3) to the final states (15):

$$\langle n,f|U(t\to\infty)|m\rangle=\langle n|V^{-1}U(t\to\infty)|m\rangle.$$

It is convenient again to use the Gauss decomposition for the operator $S\equiv V^{-1}U(t\to\infty)\equiv\exp(\alpha K_+)\exp(\delta K_0)\exp(\gamma K_-)$. We find from (14) the following expressions for the parameters:

$$\alpha=(\eta/\xi)\exp(-2\mathrm{i}\omega_0 t) \qquad \exp(-\delta/2)=\xi\exp(\mathrm{i}\omega_0 t) \qquad \gamma=-\bar{\eta}/\xi. \tag{16}$$

Now, (4) with the specification of the Gauss decomposition parameters (16) leads to the expressions for the transition matrix elements $\langle n, f|U(t\to\infty)|m\rangle$ in terms of Jacobi polynomials which were obtained (using another approach) by Dodonov *et al* (1974). Now let us suppose that the duration of the external influence which caused the change of the parameters $\Omega_i(t)$ of the Hamiltonian is small with respect to the relaxation time. Then the system will be described in the final state by the (unnormalised) density matrix:

$$\rho(t\to\infty) = U(t\to\infty)\rho(0)U^{-1}(t\to\infty)$$
$$\rho(0) = \exp(-2\beta K_0) \qquad \beta = (KT)^{-1}.$$

(We assume that the initial state was at equilibrium.) We calculate the density matrix elements in the final-state basis $|n, f\rangle \equiv V|n\rangle$:

$$\langle n, f|\rho(t)|m, f\rangle = \langle n|S\rho(0)S^{-1}|m\rangle \equiv \langle n|\tilde{\rho}(t)|m\rangle \qquad S = V^{-1}U$$

and we obtain, keeping in mind (13):

$$\lim_{t\to\infty}\tilde{\rho}(t) = S\rho(0)S^{-1} \equiv \exp(A_1K_+)\exp(B_1K_0)\exp(C_1K_-)$$

$$A_1 = \frac{\exp(-2i\omega_0 t + i\psi)\sinh\mu\sinh\beta}{\cosh\beta + \cosh\mu\sinh\beta} = \bar{C}_1 \tag{17}$$

$$\exp(-B_1/2) = \cosh\beta + \cosh\mu\sinh\beta.$$

Now, it follows from (4) that

$$\rho_{nm} = \langle n, f|\rho(t\to\infty)|m, f\rangle = \bar{\rho}_{mn}$$
$$= \left(\frac{e^{-i\psi}\sinh\mu\sinh\beta}{\cosh\beta+\cosh\mu\sinh\beta}\right)^{m-n}\left(\frac{n!\Gamma(m+a+1)}{m!\Gamma(n+a+1)}\right)^{1/2}$$
$$\times(\cosh\beta+\cosh\mu\sinh\beta)^{-(a+1)}\left(\frac{\cosh\beta-\cosh\mu\sinh\beta}{\cosh\beta+\cosh\mu\sinh\beta}\right)^{n}$$
$$\times P_n^{(m-n,a)}\left(\frac{1+\sinh^2\mu\sinh^2\beta}{1-\sinh^2\mu\sinh^2\beta}\right) \tag{18}$$

where, for simplicity, we take $m > n$. (Here and below in the analogous situations we drop the factor of type $\exp[-i\omega_0 t(2n+a+1)]$ which appears due to our choice of time-independent wavefunctions $|n, f\rangle$.)

Using the coherent states basis (6) one can obtain generating functions for the density matrix elements. It follows from (6) that

$$\langle\alpha|\hat{T}|\beta\rangle \equiv \langle\alpha|\exp(AK_+)\exp(BK_0)\exp(CK_-)|\beta\rangle$$
$$= \exp\left(\frac{\bar{\alpha}^2A+\beta^2C+b}{2}\right)\Gamma(a+1)\left(\frac{\bar{\alpha}\beta}{2}\right)^{-a} I_a(\bar{\alpha}\beta\, e^{B/2}). \tag{19}$$

Using the connections of $|\alpha\rangle$ and $|n\rangle$ states we obtain the generating function for the matrix elements

$$\exp(z_1^2A+z_2^2C)v(z_1z_2)^{-a}I_a(2z_1z_2v) = \sum_{n,m=0}^{\infty}\frac{z_1^{2n}z_2^{2m}\langle n|\hat{T}|m\rangle}{(n!m!\Gamma(n+a+1)\Gamma(m+a+1))^{1/2}} \tag{20}$$

where $z_1 \equiv \bar{\alpha}/\sqrt{2}$, $z_2 \equiv \beta/\sqrt{2}$, $v \equiv \exp(B/2)$. Now, (20) with specification (17) of parameters A, B, C gives the generating function for the density matrix elements. In appendix 2 we will obtain the generating function for transition probabilities, which leads to the new generating function for the products of the Jacobi polynomials.

The occupation probabilities of the energy levels are proportional to the diagonal elements ρ_{nn}. The analysis of (18) for ρ_{nn} shows that a population inversion can be obtained for certain values of the parameters β and μ (see appendix 1).

3. Correlation functions

In this section we obtain expressions for the correlation functions which are defined as follows:

$$G_{j_1 j_2 \ldots j_n}(t_1, \ldots, t_n) \equiv \langle K_{j_1}(t_1) K_{j_2}(t_2) \cdot \ldots \cdot K_{j_n}(t_n) \rangle$$
$$= Q^{-1} \operatorname{Tr}(\exp(-2\beta K_0) K_{j_1}(t_1) \cdot \ldots \cdot K_{j_n}(t_n)) \qquad j_k = 0, 1, 2 \tag{21}$$
$$Q \equiv \operatorname{Tr} \rho(0) = \operatorname{Tr}(\exp(-2\beta K_0)) = \exp(-\beta a)/2 \sinh \beta.$$

Here $K_j(t)$ are operators in the Heisenberg representation, and average values are calculated over the initial density matrix $\rho_0 = \exp(-2\beta K_0)$. The values $K_j(t)$ evolve as follows:

$$K_j(t) = U^{-1}(t) K_j U(t) = \Lambda_j^i(t) K_i. \tag{22}$$

Here $\Lambda(t) = \|\Lambda_j^i(t)\|$ is the evolution operator in the adjoint representation (hereafter we mean a summation over repeated indices). The matrix elements $\Lambda_j^i(t)$, $i, j = 1, 2, 3$, are expressed in terms of the parameters $A(t)$, $B(t)$, $C(t)$ (see (9) and (11)):

$$\Lambda = \begin{Vmatrix} 1 - 2AC\,\mathrm{e}^{-B} & A\,\mathrm{e}^{-B} + \bar{A}\,\mathrm{e}^{-\bar{B}} & \mathrm{i}(A\,\mathrm{e}^{-B} - \bar{A}\,\mathrm{e}^{-\bar{B}}) \\ -\mathrm{e}^{-B}C - \mathrm{e}^{-\bar{B}}\bar{C} & \dfrac{\mathrm{e}^{-B}(1+C^2) + \mathrm{e}^{-\bar{B}}(1+\bar{C}^2)}{2} & \dfrac{\mathrm{e}^{-\bar{B}}(1-\bar{C}^2) - \mathrm{e}^{-B}(1-C^2)}{2\mathrm{i}} \\ \mathrm{i}(\mathrm{e}^{-B}C - \mathrm{e}^{-\bar{B}}\bar{C}) & \dfrac{\mathrm{e}^{-B}(1+C^2) - \mathrm{e}^{-\bar{B}}(1+\bar{C}^2)}{2\mathrm{i}} & \dfrac{\mathrm{e}^{-B}(1-C^2) + \mathrm{e}^{-\bar{B}}(1-\bar{C}^2)}{2} \end{Vmatrix}. \tag{23}$$

We get directly from the definition (22)

$$G_{j_1 \ldots j_n}(t_1, \ldots, t_n) = \Lambda_{j_1}^{k_1}(t_1) \cdot \ldots \cdot \Lambda_{j_n}^{k_n} \langle K_{k_1} \cdot \ldots \cdot K_{k_n} \rangle. \tag{24}$$

For the average values of generators we have

$$\langle K_0 \rangle = Q^{-1} \operatorname{Tr}(\exp(-2\beta K_0) K_0) = -\tfrac{1}{2} Q^{-1} \frac{\partial}{\partial \beta} Q$$
$$= (a + \coth \beta)/2$$
$$\langle K_1 \rangle = \langle K_2 \rangle = 0.$$

For the non-vanishing average products of the generators we obtain

$$\langle K_0^2 \rangle = [(a + \coth \beta)^2 + \sinh^{-2} \beta]/4$$
$$\langle K_1^2 \rangle = \langle K_2^2 \rangle = (\coth \beta + a) \coth \beta / 4$$
$$\langle K_2 K_1 \rangle = -\langle K_1 K_2 \rangle = \tfrac{1}{4}\mathrm{i}(\coth \beta + a).$$

We write down the expressions for the first- and second-order correlation functions

$$G_j(t) = \Lambda_j^0(t) \langle K_0 \rangle$$
$$G_{ij}(t_1, t_2) = \Lambda_i^0(t_1) \Lambda_j^0(t_2) \langle K_0^2 \rangle + [\Lambda_i^2(t_1) \Lambda_j^1(t_2) - \Lambda_i^1(t_1) \Lambda_j^2(t_2)] \langle K_2 K_1 \rangle \tag{25}$$
$$+ [\Lambda_i^1(t_1) \Lambda_j^1(t_2) + \Lambda_i^2(t_1) \Lambda_j^2(t_2)] \langle K_1^2 \rangle.$$

One can note that for the system under consideration all the correlation functions are expressed in terms of the first- and the second-order ones, because all the matrix elements of the evolution operator $\Lambda_l^j(t)$ are determined by the functions $G_i(t)$ and $G_{ij}(0, t)$. In order to see this we derive from equation (25)

$$\Lambda_l^0(t) = G_l(t)\langle K_0\rangle^{-1}$$

$$\Lambda_l^1(t)\langle K_1^2\rangle - \Lambda_l^2(t)\langle K_2K_1\rangle = G_{1l}(0, t)$$

$$\Lambda_l^1(t)\langle K_2K_1\rangle + \Lambda_l^2(t)\langle K_1^2\rangle = G_{2l}(0, t) \qquad l = 0, 1, 2.$$

We may consider the last two equations as a system which uniquely determines the elements $\Lambda_l^{1,2}(t)$ $(l = 1, 2, 0)$ since its determinant equals $[(a + \coth\beta)/(4\sinh\beta)]^2 \neq 0$. So, all the information about the evolution of the system is contained in the first- and second-order correlation functions. This fact is the consequence of the dynamical symmetry of the system under consideration.

The correlation functions defined by the formulae (21) are the averages of the non-Hermitian operators. One can define 'symmetrical correlation functions' which take the real values

$$G_{\{i_1,\ldots,i_n\}} = (n!)^{-1}\langle\{K_{i_1}(t_1)K_{i_2}(t_2)\cdot\ldots\cdot K_{i_n}(t_n)\}\rangle \equiv (n!)^{-1}\sum\langle K_{i_1}(t_1)\cdot\ldots\cdot K_{i_n}(t_n)\rangle \qquad (26)$$

(the sum is taken over all the permutations of the numbers $i_1, i_2, \ldots, i_n$). We are able to obtain the simple generating functional for the symmetrical correlation functions. For this goal let us consider an element of the representation of SU(1, 1) (which is locally coincident with the representation of $\overline{\mathrm{SU}(1,1)}$):

$$T = \exp(\rho^j K_j) \qquad \rho^j \equiv \int_{-\infty}^{\infty} \varphi^i(t)\Lambda_i^j(t)\,\mathrm{d}t \qquad j = 0, 1, 2 \qquad (27)$$

where $\varphi^i(t)$ are arbitrary functions. We get for the functional derivatives of the element T at the point $\varphi^0 = \varphi^1 = \varphi^2 = 0$:

$$\left.\frac{\delta^n T}{\delta\varphi^{j_1}(t_1)\cdot\ldots\cdot\delta\varphi^{j_n}(t_n)}\right|_{\varphi=0} = \frac{1}{n!}\{K_{j_1}(t_1)\cdot\ldots\cdot K_{j_n}(t_n)\}.$$

Taking the mean value with respect to the initial density matrix we obtain $Z \equiv \langle T\rangle = Q^{-1}\,\mathrm{Tr}(\rho(0)T)$. The functional derivatives of Z will be the symmetrical correlation functions

$$\left.\frac{\delta^n Z}{\delta\varphi^{j_1}(t_1)\cdot\ldots\cdot\delta\varphi^{j_n}(t_n)}\right|_{\varphi=0} = G_{\{j_1\ldots j_n\}}(t_1, \ldots, t_n). \qquad (28)$$

The value Z can be calculated simply. To do this we can represent the element $\exp(-2\beta K_0)T$ in the form

$$\exp(-2\beta K_0)\exp(\rho^i K_i) = \exp(\tilde\rho^i K_i)$$

$$= \exp(V^{-1}2\tilde\omega K_0 V) = V^{-1}\exp(2\tilde\omega K_0)V$$

(here $\tilde\rho^i$ are new parameters dependent on β and ρ^i, $2\tilde\omega = ((\tilde\rho^0)^2 - (\tilde\rho^1)^2 - (\tilde\rho^2)^2)^{1/2}$). Then we obtain

$$Z = Q^{-1}\,\mathrm{Tr}(V^{-1}\exp(2\tilde\omega K_0)V) = -\frac{\exp[a(\tilde\omega+\beta)]\sinh\beta}{\sinh\tilde\omega}. \qquad (29)$$

The value $\tilde{\omega}(\beta, \rho^0, \rho^1, \rho^2)$ is independent of the choice of representation, and it is convenient to use for its calculation the two-dimensional fundamental representation of $\overline{SU(1,1)}$ (in fact, SL(2, C)). Finally we obtain

$$-\tilde{\omega} = \cosh^{-1}[\cosh\beta \cosh\Delta - \rho^0 \sinh\beta \sinh\Delta/(2\Delta)]$$
$$4\Delta^2 \equiv (\rho^0)^2 - (\rho^1)^2 - (\rho^2)^2 \qquad \rho^l \equiv \int_{-\infty}^{\infty} \varphi^j(\tau)\Lambda_j^l(\tau)\,\mathrm{d}\tau. \tag{30}$$

Equations (28)-(30) give the generating functional for symmetrical correlation functions.

Appendix 1

It is interesting to consider the dependence (18) of the occupation probabilities $P_n \sim \rho_{nn}$ on the initial-state temperature $\sim\beta^{-1}$ and the parameter μ, which characterises the form of excitation (see (12) and (13)). Let us remember that to return to the physical (dimensional) values of the parameters one should put $\beta = \hbar\omega_{\text{in}}/kT$, $a = \frac{1}{2}(1+8mg\hbar^{-2})^{1/2}$. For the fixed temperature and small values of μ the value of ρ_{nn} decreases monotonously with the increasing n, as in the case of the initial exponential distribution with $\mu = 0$. However, for the large enough values of μ, it turns out that excitation levels are more occupied than the ground one. We give two typical figures (figures 1 and 2) for the value P_n, which correspond to the choice $a = 1$, $\beta = 0.1$, $\mu = 3.5$, 4, 4.5 and the choice $a = 100$, $\beta = 1$, $\mu = 0.2$, 0.25, 0.3, 0.35 (if the spectroscopic frequency is $\bar{\nu}(\text{cm}^{-1})$, then $\beta \simeq 0.7\bar{\nu}/T$).

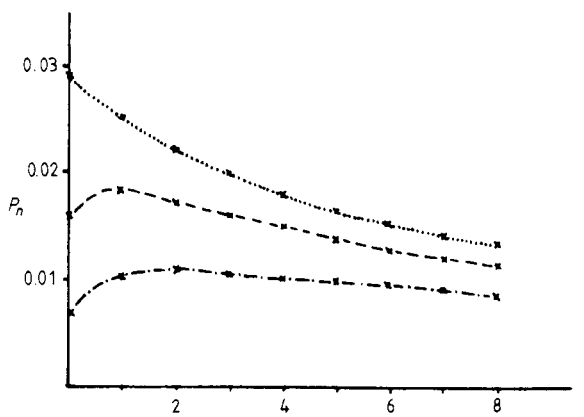

Figure 1. The occupation probabilities in the final state, $a = 1$; $\beta = 0.1$; $\mu = 3.5$ (·····), 4.0 (---), 4.5 (—·—).

Let us now suppose that the Hamiltonian (1) serves to describe (qualitatively, of course) the vibrations of a diatomic molecule. Then the equilibrium distance between the nuclei equals $r_0 = (2g/M\omega^2)^{1/4}$, where M is the reduced mass of two nuclei. However, it is well known that in real molecules the energy of vibrations is of the order of $\hbar\omega \sim E_e(m/M)^{1/2}$, where m is the electron mass, and E_e is the characteristic electron energy which is, in turn, of the order of $E_e \sim \hbar^2/(mr_0)^2$ (because r_0 is the

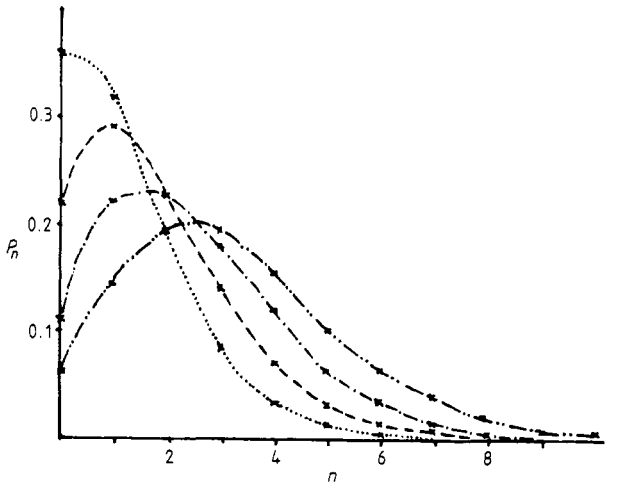

Figure 2. The occupation probabilities in the final state; $a = 100$; $\beta = 1$; $\mu = 0.2$ (·····), 0.25 (---), 0.3 (—·—), 0.35 (—··—).

characteristic length of the region which electrons move in). Consequently, the parameter g must be of the order of $g \sim \hbar^2/m$. Therefore the parameter a in such a situation must be of the order of $a \sim (Mg\hbar^{-2})^{1/2} \sim (M/m)^{1/2} \gg 1$. If one wants to apply this model to real molecules, then the following relation should be used:

$$a = \frac{M}{m}\frac{\pi\bar{\nu}r_0}{\Lambda}$$

where Λ is the electron Compton wavelength, and $\bar{\nu}$ is the frequency of vibrations in spectroscopic units (cm^{-1}). (Note that the frequency of vibrations $2\pi c\bar{\nu}$ is equal to 2ω.) In particular, the parameter a is equal to 18 for the H_2 molecule, $a = 300$ for N_2 and $a = 1450$ for I_2. Calculations according to (18) for the values $a = 100$ and $a = 200$ demonstrate the existence of population inversion (for appropriate choices of the parameters β and μ). On the other hand, one can obtain from (18) a simple asymptotic expression for the occupation probabilities P_n, which is valid for $a \gg n \geqslant 0$ and $\sinh\beta \sinh\mu > 1$. Simple manipulations with the use of an asymptotical formula for Jacobi polynomials (Erdelyi 1953, equations I.2.3.2(14), II.10.8(16)) lead to the following expression:

$$p_n = Q^{-1}(\cosh\beta + \cosh\mu \sinh\beta)^{-(a+1)}\frac{1}{n!}\left(\frac{a\sinh^2\mu\sinh^2\beta}{(\cosh\beta+\sinh\mu\sinh\beta)^2}\right)^n$$

$$Q = \exp(-\beta a)/(2\sinh\beta)$$

which coincides with Poisson distribution and also demonstrates 'population inversion'.

Appendix 2

Here we obtain both generating functions for the transition probabilities $W_{nm} = |\langle n, f|U(t\to\infty)|m\rangle|^2$ and the corresponding generating function for the products of the

Jacobi polynomials. For this goal one has to calculate the integral

$$I(r,y)=\int_0^{2\pi}\frac{d\varphi}{2\pi}\int d\mu(\beta)\langle\alpha|T_1|y\beta\rangle\langle\beta|T_2|\alpha\rangle \tag{A1}$$

where $\alpha\equiv r\exp(i\varphi)$, y is a real parameter, $\int|\beta\rangle\,d\mu(\beta)\langle\beta|=1$, coherent states $|\alpha\rangle$ are defined by formula (6), and

$$T_l\equiv\exp(A_lK_+)\exp(B_lK_0)\exp(C_lK_-)\qquad(l=1,2)$$

are the arbitrary elements of the representation. The relation (19) implies that $\langle\alpha|T_l|\beta y\rangle=y_l^{-(a+1)}\langle\alpha|\tilde T_l|\beta\rangle$, where $\tilde T\equiv\exp(A_lK_+)\exp((B_l+2\ln y_l)K_0)\exp(y_l^2C_lK_-)$.

Now we can calculate the integral (A1):

$$I(r,y)=\int_0^{2\pi}\frac{d\varphi}{2\pi}\langle\alpha|\tilde T_1T_2|\alpha\rangle y^{-(a+1)}$$

$$=y^{-(a+1)}\Gamma(a+1)\exp(B_0/2)x^{-a}I_a(2x\exp(B_0/2))I_0(2x(A_0C_0)^{1/2}) \tag{A2}$$

where we have used (4) and introduced the notation

$$x\equiv r^2/2=|\alpha|^2/2\qquad T_0\equiv\tilde T_1T_2=\exp(A_0K_+)\exp(B_0K_0)\exp(C_0K_-).$$

Furthermore (4) implies $\langle n|\tilde T|m\rangle=y^{2m+a+1}\langle n|T|m\rangle$ so that we can rewrite the integral (A1) using the definition (6) of the states $|\alpha\rangle$:

$$I(r,y)=\int_0^{2\pi}\frac{d\varphi}{2\pi}\sum_{m,k,l=0}^{\infty}\frac{\langle k|\tilde T_1|m\rangle\langle m|T_2|l\rangle(\bar\alpha^2/2)^k(\alpha^2/2)^l\Gamma(a+1)}{(l!\,k!\,\Gamma(l+a+1)\Gamma(k+a+1))^{1/2}y^{a+1}}$$

$$=\Gamma(a+1)\sum_{k,m}^{\infty}\frac{x^{2k}y^{2m}\langle k|T_1|m\rangle\langle m|T_2|k\rangle}{k!\,\Gamma(k+a+1)}. \tag{A3}$$

Comparing (A2) and (A3) we obtain

$$\exp(B_0/2)y^{-(a+1)}x^{-a}I_a(2x\exp(B_0/2))I_0(2x(A_0C_0)^{1/2})$$

$$=\sum_{k,m=0}^{\infty}\frac{x^{2k}y^{2m}\langle k|T_1|m\rangle\langle m|T_2|k\rangle}{k!\,\Gamma(k+a+1)}. \tag{A4}$$

To calculate the parameters A_0, B_0, C_0 in the Gauss decomposition of operator $T_0=T_1T_2$, one can use the (non-unitary) (2×2) matrix representation of the group SU(1, 1):

$$T=\exp(AK_+)\exp(BK_0)\exp(CK_-)=\begin{Vmatrix}e^{-B/2} & iC\,e^{-B/2}\\ iA\,e^{-B/2} & e^{B/2}-AC\,e^{-B/2}\end{Vmatrix}. \tag{A5}$$

Let us take, first $T_1=T_2^{-1}=V^{-1}U(t\to\infty)\equiv S$ (the operator S corresponds to the transitions between the initial and final states (15)). Equations (A4) and (A5) in this case lead to the generating function for the transition probabilities

$W_{nm}\equiv|\langle n,f|U(t\to\infty)|m\rangle|^2=|\langle n|S|m\rangle|^2$:

$$\frac{(xy)^{-a}}{|\xi|^2-y^2|\eta|^2}I_a\left(\frac{2xy}{|\xi|^2-y^2|\eta|^2}\right)I_0\left(\frac{2x|\eta\xi|(1-y^2)}{|\xi|^2-y^2|\eta|^2}\right) \tag{A6}$$

$$=\sum_{n,m=0}^{\infty}\frac{x^{2n}y^{2m}W_{nm}}{n!\,\Gamma(n+a+1)}.$$

Finally, using formula (4) which expresses the matrix elements of an operator T (in the representation (1)) in terms of the Jacobi polynomials we get the generating function for the products of the Jacobi polynomials

$$\frac{(xyt_1t_2)^{-a}}{1-y^2C_1A_2}I_a\left(\frac{2xyt_1t_2}{1-y^2C_1A_2}\right)I_0(2x(A_0C_0)^{1/2})$$
$$= \sum_{k,m=0}^{\infty} \frac{x^{2k}y^{2m}}{k!\Gamma(k+a+1)} C_1^{m-k}C_2^{k-m}(t_1^2-A_1C_1)^k(t_2^2-A_2C_2)^m$$
$$\times P_k^{(m-k,a)}\left(\frac{t_1^2+A_1C_1}{t_1^2-A_1C_1}\right)P_m^{(k-m,a)}\left(\frac{t_2^2+A_2C_2}{t_2^2-A_2C_2}\right) \tag{A7}$$

$$A_0 \equiv \frac{A_1+y^2A_2(t_1^2-A_1C_1)}{1-y^2C_1A_2} \qquad C_0 \equiv \frac{C_2+y^2C_1(t_2^2-A_2C_2)}{1-y^2C_1A_2}.$$

Here $A_{k_1}C_{k_1}t_k \equiv \exp(B_k/2)$, $(k=1,2)$ are arbitrary parameters. Note that the function $P_k^{(m-k,a)}(x)$ with $k>m$ is defined by (5). We do not discuss here the convergence of the series in the right-hand part of equation (A7), e.g. it evidently converges if $A_1C_1<0$, $A_2C_2<0$, $t_{1,2}$ real, and $|y^2C_1A_2|<1$, $|x^2C_2A_1|<1$.

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