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LETTER TO THE EDITOR

The Green function and thermodynamical properties of quadratic systems

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Abstract. The explicit expression for the Green function of the quantum system with the Hamiltonian which is the most general quadratic form of coordinates and momenta with time-dependent coefficients is obtained. The thermodynamical properties of systems with quadratic Hamiltonians are briefly discussed.

During recent years many interesting papers concerning different properties of quantum systems with Hamiltonians which are quadratic forms of coordinates and momenta have appeared (see eg Moshinsky and Quesne 1971, Boon and Seligman 1973, Papadopoulos 1974a,b, Titulaer 1973). However, up to now the explicit expression for the Green function (GF) of the most general quadratic system (including linear terms) has not been written anywhere, though the Green functions of different special examples of such systems were obtained in many papers. In this letter we want to remove this gap. Knowledge of the GF allows us to give exact solutions to many interesting physical problems which can be reduced to studying the systems with quadratic Hamiltonians, among these problems are those connected with the thermodynamical properties of quadratic systems. The detailed investigation of these problems will form the substance of following publications, so that here we shall only briefly discuss them, from the viewpoint of possible applications of the exact GF obtained.

For the first time the GF of the general non-stationary quadratic system was obtained by Malkin *et al* (1971, 1973) with the aid of the coherent states method. However, the result was not given in a form suitable for applications. Here we shall obtain the GF using the connection between the Green function and the integrals of the motion. We call the integral of the motion an operator \hat{I} which transforms every solution of the Schrödinger equation again into a solution of the same equation. Consequently, \hat{I} must satisfy in the space of the solutions of the Schrödinger equation ψ , the equation $[i\hbar(\partial/\partial t) - \hat{H}, \hat{I}]\psi = 0$. Note that the Hamiltonian \hat{H} need not be Hermitian. One can easily verify that the operators $\hat{X} = \hat{U}\hat{x}\hat{U}^{-1}$ and $\hat{P} = \hat{U}\hat{p}\hat{U}^{-1}$, where \hat{U} is the evolution operator (the kernel of this operator is the Green function), are integrals of the motion. The physical meaning of these operators is quite lucid: they determine the initial points of the trajectory in the phase space of the system. Let us note now that at the initial moment $t = 0$ the GF (in the coordinate representation) coincides with the eigenfunction of the operator $\hat{x}: G(\mathbf{x}_2, \mathbf{x}_1; 0) = \delta(\mathbf{x}_2 - \mathbf{x}_1)$, so that $G(\mathbf{x}_2, \mathbf{x}_1; t) = \hat{U}G(\mathbf{x}_2, \mathbf{x}_1; 0)$. At the same time $\hat{x} = \hat{X}(t = 0)$. Consequently, the GF is the eigenfunction of the integral of the motion \hat{X} :

$$\hat{X}G(\mathbf{x}_2, \mathbf{x}_1; t) = \mathbf{x}_1 G(\mathbf{x}_2, \mathbf{x}_1; t) \tag{1a}$$

(the operator \hat{X} in this equation acts only on the variable x_2 , while the variable x_1 should be considered as a parameter).

Using similar reasonings one can derive the second equation for the GF:

$$\hat{P}G(x_2, x_1; t) = i\hbar \frac{\partial}{\partial x_1} G(x_2, x_1; t). \quad (1b)$$

Equations (1a)–(1b) determine the GF up to a phase factor depending on time. To calculate this factor one should substitute the GF into the Schrödinger equation and take into account the initial condition.

The most general quadratic Hamiltonian with N degrees of freedom has the following form:

$$\hat{H} = \frac{1}{2}\hat{q}B(t)\hat{q} + C(t)\hat{q} + \phi(t);$$

$$q = \begin{pmatrix} p \\ x \end{pmatrix}; \quad C = \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}; \quad B = \begin{vmatrix} B_1 & B_2 \\ B_3 & B_4 \end{vmatrix}; \quad \begin{matrix} x = (x_1, \dots, x_N) \\ p = (p_1, \dots, p_N) \end{matrix} \quad (2)$$

One can always assume that the $2N \times 2N$ matrix B is symmetrical. However, it is not necessarily real, nor is the $2N$ -dimensional vector C , since the Hamiltonian may be a non-Hermitian operator. One can easily verify that the integrals of the motion \hat{X} and \hat{P} are linear functions of the operators \hat{x} and \hat{p} :

$$\begin{pmatrix} \hat{P} \\ \hat{X} \end{pmatrix} = \Lambda(t) \begin{pmatrix} \hat{p} \\ \hat{x} \end{pmatrix} + \Delta(t); \quad \Lambda = \begin{vmatrix} \lambda_1 & \lambda_2 \\ \lambda_3 & \lambda_4 \end{vmatrix}; \quad \Delta = \begin{pmatrix} \delta_1 \\ \delta_2 \end{pmatrix}$$

$$\dot{\Lambda} = \Lambda \Sigma B; \quad \Lambda(t) = \tilde{T} \exp \left(\int_0^t \Sigma B d\tau \right); \quad \Sigma = \begin{vmatrix} 0 & E_N \\ -E_N & 0 \end{vmatrix};$$

$$\Delta(t) = \int_0^t \Lambda \Sigma C d\tau \quad (3)$$

(E_N is the N -dimensional unity matrix). It can be shown that Λ is a symplectic matrix: $\Lambda \tilde{\Sigma} \Lambda = \Sigma$. Equations (1a–b) together with the Schrödinger equation lead to the following expression for the GF of the general quadratic system (for details of calculations see Dodonov *et al* 1974b; we confine ourselves here to the simplest case $\det \lambda_3 \neq 0$):

$$G(x_2, x_1; t) = (-2\pi i \hbar)^{-N/2} (\det \lambda_3)^{-1/2} \exp \left[-\frac{i}{2\hbar} \left(x_2 \lambda_3^{-1} \lambda_4 x_2 - 2x_2 \lambda_3^{-1} x_1 \right. \right.$$

$$\left. \left. + x_1 \lambda_1 \lambda_3^{-1} x_1 + 2x_2 \lambda_3^{-1} \delta_2 + 2x_1 (\delta_1 - \lambda_1 \lambda_3^{-1} \delta_2) + \delta_2 \lambda_1 \lambda_3^{-1} \delta_2 \right. \right.$$

$$\left. \left. - 2 \int_0^t (\delta_1 \delta_2 - \phi) d\tau \right) \right]. \quad (4)$$

A similar expression but without the important phase factor was given by Boon and Seligman (1973). Therefore, the study of an arbitrary quadratic system is reduced to the calculation of the matrix $\Lambda(t)$ and vector $\Delta(t)$.

The equilibrium density matrix $\rho(x_2, x_1; T)$ of an arbitrary quadratic system with a stationary Hermitian Hamiltonian can be obtained from equation (4) by the substitution $t = -i\hbar T^{-1}$, T being the absolute temperature. To obtain the thermodynamical characteristics of the system one has to know the partition function, ie the trace of the density matrix (ter Haar 1961). In the case of Maxwell–Boltzmann statistics the partition function can be calculated without difficulty, since the trace of the density

matrix (4) is a Gaussian integral. If the system considered is an ideal gas in uniform external electric and magnetic fields and the internal degrees of freedom of a particle can be described by a quadratic Hamiltonian, then the thermodynamical characteristics of the system can be calculated in the case of Fermi–Dirac and Bose–Einstein statistics too.

Indeed, the one-particle density matrix in this case has the form (4), so that the one-particle partition function $Z(\beta)$ can be easily obtained ($\beta = (kT)^{-1}$). After this the Ω potential of the system ($\Omega = -PV$, P is the pressure, V is the volume of the container) can be calculated with the aid of the following relation (Rumer 1948, Dodonov *et al* 1974b):

$$\Omega(\beta, \eta) = (-2i\beta)^{-1} \int_{\sigma-i\infty}^{\sigma+i\infty} e^{i\eta} \frac{[-\cos(\pi\lambda/\beta)]^\gamma}{\lambda \sin(\pi\lambda/\beta)} Z(\lambda) d\lambda \quad 0 < \text{Re } \lambda < \beta. \quad (5)$$

Here η is the chemical potential, and the parameter γ equals zero for fermions and unity for bosons.

Let us consider the special case of the general quadratic system, when the matrix B is positive definite. In this case the quadratic form in the argument of the exponent in equation (4) is non-degenerate. Therefore the characteristic function (Louisell 1964) of any operator \hat{A} which is an arbitrary linear combination of the operators \hat{x} and \hat{p} has the form of an exponential of a quadratic form:

$$\begin{aligned} \chi(\xi; \hat{A}) &= \langle \exp(i\xi\hat{A}) \rangle = [\text{sp } \hat{\rho}(\beta)]^{-1} \text{sp}[\hat{\rho} \exp(i\xi\hat{A})] = \exp(-\xi h \xi + i\xi l); \\ l &= \langle \hat{A} \rangle; \quad h = \|h_{ik}\|; \\ h_{ik} &= \frac{1}{2}[\langle \hat{A}_i \hat{A}_k \rangle - \langle \hat{A}_i \rangle \langle \hat{A}_k \rangle] \end{aligned} \quad (6)$$

where the coefficients h_{ik} and l_k , $i, k = 1, 2, \dots, N$, can be easily expressed in terms of the elements of the matrix Λ and the vector Δ .

Since the characteristic function is the generating function for the moments of the operators \hat{A}_j , $j = 1, 2, \dots, N$, equation (5) shows that all these moments can be expressed in terms of Hermite polynomials of many variables:

$$\langle \hat{A}_1^{n_1} \hat{A}_2^{n_2} \dots \hat{A}_N^{n_N} \rangle = H_{n_1, n_2, \dots, n_N}(-\frac{1}{2}h^{-1}\Delta) \quad (7)$$

where the matrix C defining these polynomials (Bateman Manuscript Project 1953) is equal to $-2h$ (for simplicity we assume here that all operators \hat{A}_j commute with each other). Evidently, the Fourier transform of the function $\chi(\xi; \hat{A})$ is again an exponential of a quadratic form. But this transformation yields the probability distribution of the eigenvalues of the operators \hat{A}_j (provided $[\hat{A}_j, \hat{A}_k] = 0$, $j, k = 1, 2, \dots, N$) (Louisell 1964), so that we have proved the following theorem (for the first time it was proved by Bloch 1932 for the one-dimensional oscillator).

The generalized Bloch theorem. If a system has an arbitrary quadratic positive definite Hamiltonian, then in the thermal equilibrium state the probability distribution of the eigenvalues of any real linear combination of coordinates and momenta has the Gaussian form.

To consider a non-equilibrium quadratic system one should suppose this system to interact with a large reservoir (both reservoir and interaction Hamiltonians must be quadratic too). At the initial moment let the extended system be in the equilibrium state. Then one can switch on a time-dependent external field and calculate the density

matrix of the extended system at an arbitrary moment $t > 0$ with the aid of the exact GF (4). After this one has only to integrate the complete density matrix over the variables of the reservoir, and the non-equilibrium density matrix of the system under study will be obtained in a closed form, since all integrals will be Gaussian. The method described has been already applied to a quadratic system of a special kind by Papadopoulos (1974b).

As to non-quadratic systems, we can note that using the Baker–Hausdorff formula

$$\hat{X} = \exp(-\beta\hat{H})\hat{x}\exp(\beta\hat{H}) = \hat{x} - \beta[\hat{H}, \hat{x}] + \frac{1}{2!}(-\beta)^2[\hat{H}, [\hat{H}, \hat{x}]] + \dots \quad (8)$$

one can obtain approximate expressions for the integrals of the motion \hat{X} and \hat{P} and consequently for the density matrix of any system. In the special case

$$\hat{H} = \hat{p}^2/2m + \frac{1}{2}m\omega^2(t)x^2 + gx^{-2}$$

the Green function can be calculated exactly (Dodonov *et al* 1974a).

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