International Journal of Theoretical Physics, Vol. 37, No. 1, 1998

The Entropy of Open Finite-Level Systems

S. M. Chumakov,[1] K.-E. Hellwig,[2] and A. B. Klimov[3]

Received July 4, 1997

1. INTRODUCTION

In the dynamics of open quantum systems the development of the entropy and other properties of the state are of great interest, e.g., with respect to thermodynamics, measuring processes, and quantum optics. Clearly, any state property is expressed by the set of eigenvalues of the density operator. But in the case of an open system these eigenvalues depend on time and their explicit computation is tedious. One may ask whether the state properties can be described by other parameters which are functions of the eigenvalues, but are more accessible. This is possible when the open system in consideration is a finite-level system. In this case the eigenvalues are the roots of the characteristic equation which is of finite degree. Closed algebraic expressions for the roots do not exist in general, but symmetric functions of them may be expressed algebraically in terms of the elements of the density matrix. To exploit this fact is the main idea of this paper.

We derive an explicit analytical expression for the von Neumann entropy in terms of density matrix elements which does not involve the diagonalization of the density matrix. More precisely, the entropy is obtained as a single integral of a rational function on the real line which is determined by the density matrix elements; see equation (5) below. Clearly, the computation of the rational function involves a finite recursion. It can be easily solved because it is a linear algebraic problem in n dimensions, where n is the number of levels.

First we will demonstrate the method for two- and three-level systems (Section 2), which also can be treated directly. Then we will consider the

[1] IIMAS, UNAM, 62191 Cuernavaca, Mor., México.
[2] Institut für Theoretische Physik, Technische Universität Berlin, D-10623 Berlin, Germany.
[3] Departamento de Física, Universidad de Guadalajara, 44410, Guadalajara, Jal., México.

0020-7748/98/0100-0471$15.00/0

general n-level case (Section 3), where our procedure seems to be profitable for explicit numerical or analytical calculations.

2. THE CASES OF TWO OR THREE LEVELS

In the *two-level case* let the density matrix be given by

$$\rho = \begin{vmatrix} p_1 & \rho_{12} \\ \overline{\rho}_{12} & p_2 \end{vmatrix}$$

which obviously fulfills

$$\rho^2 = \rho - \mu \mathbf{1}, \qquad \mu := p_1 p_2 - |\rho_{12}|^2$$

w.r.t. an orthonormal basis of eigenvectors and hence in any basis of $\mathbf{c}^2$, since μ is a unitary invariant. Since this identity is tightly connected to the characteristic equation for the eigenvalues, we will call it the *characteristic identity.* Note that the eigenvalues λ_1, λ_2 are positive or zero, fulfilling $\lambda_1 + \lambda_2 = 1$, $\lambda_1\lambda_2 = \mu$, and, hence, $0 \leq \mu \leq 1/4$. By definition the entropy is

$$S = -\mathrm{Tr}[\rho \log(1 + \rho - 1)] = \mathrm{Tr}\left[\sum_{k=1}^{\infty} \frac{\pi_k}{k}\right]$$

where

$$\rho_k := \rho(1 - \rho)^k = \alpha_1^{(k)}\rho + \alpha_0^{(k)}$$

The latter equality is a consequence of the characteristic identity; the numbers $\alpha_0^{(k)}$ and $\alpha_1^{(k)}$ are determined by the recursion relations

$$\alpha_1^{(1)} = 0, \qquad \alpha_0^{(1)} = \mu$$

$$\alpha_1^{(k+1)} - \alpha_1^{(k)} + \mu\alpha_1^{(k-1)} = 0,$$

$$\alpha_0^{(k)} = -\alpha_1^{(k+1)}$$

Forming the generating functions for these recursion relations,

$$f_0 := \sum_{k=1}^{\infty} z^{k-1}\alpha_0^{(k)}, = \frac{\mu}{1 - z + \mu z^2}$$

$$f_1 := \sum_{k=1}^{\infty} z^{k-1}\alpha_1^{(k)}, = \frac{-\mu z}{1 - z + \mu z^2}$$

we get for the entropy

$$S = \mathrm{Tr} \int_0^1 dz \sum_{k=1}^{\infty} z^{k-1} [\alpha_1^{(k)}\rho + \alpha_0^{(k)}] = \int_0^1 dz (f_1 \, \mathrm{Tr}\, \rho + f_0 \, \mathrm{Tr}\, \mathbf{1})$$

Inserting $\mathrm{Tr}\,\rho = 1$, $\mathrm{Tr}\,\mathbf{1} = 2$, we have

$$S = \int_0^1 dz \, \frac{(2 - z)\mu}{1 - z + \mu z^2}$$

Elementary integration using $\lambda_{1,2} = \frac{1}{2}(1 \pm \sqrt{1 - 4\mu})$ shows that the integral indeed has the correct value

$$S = -\lambda_1 \log \lambda_1 - \lambda_2 \log \lambda_2$$

The advantage of our procedure arizes for higher level systems when there is no formula for the roots of the characteristic equation.

Similarly the *three-level case* can be treated. We will only repeat the main steps. The density matrix

$$\rho = \begin{vmatrix} p_1 & \rho_{12} & \rho_{13} \\ \rho_{21} & p_2 & \rho_{23} \\ \rho_{31} & \rho_{32} & p_3 \end{vmatrix}$$

fulfills the characteristic identity

$$\rho^3 = \rho^2 - \mu\rho + \delta$$

where

$$\mu = p_1 p_2 + p_2 p_3 + p_1 p_3 - |\rho_{12}|^2 - |\rho_{13}|^2 - |\rho_{23}|^2, \qquad \delta = \det\rho$$

Here two parameters μ and δ are necessary. We write again the entropy as

$$S = -\mathrm{Tr}[\rho \log(1 + \rho - 1)] = \mathrm{Tr}\left[\sum_{k=1}^{\infty} \frac{\rho_k}{k}\right]$$

where the ρ_k are now defined by

$$\rho_k := \rho(1 - \rho)^k = \alpha_2^{(k)}\rho^2 + \alpha_1^{(k)}\rho + \alpha_0^{(k)}$$

The coefficients are to be determined by the characteristic identity. Again one may write down the recursion relations for them and form the generating functions. The result is

$$S = \int_0^1 dz \, \frac{(\mu - \delta)z^2 - 3(\mu - \delta)z + 2\mu}{1 - 2z + (\mu + 1)z^2 - (\mu - \delta)z^3} \tag{1}$$

By elementary integration one can check that

$$S = -\lambda_1 \log \lambda_1 - \lambda_2 \log \lambda_2 - \lambda_3 \log \lambda_3$$

In the next section we will derive the integral formula in case of an arbitrary finite number of levels.

3. THE CASE OF *n* LEVELS

The characteristic identity is

$$\rho^n - \mu_{n-1}\rho^{n-1} + \cdots + (-1)^{n-1}\mu_1\rho + (-1)^n\mu_0 = 0$$

and the coefficients μ_k are symmetric functions of the roots of the characteristic equation, namely

$$\mu_1 = \sum_j \lambda_j, \qquad \mu_2 = \sum_{j<k} \lambda_j\lambda_k, \ldots, \qquad \mu_n = \prod_j \lambda_j$$

As already stated in the introduction, it is the main idea of the present paper to use symmetric functions of the roots rather than the roots themselves as natural parameters to describe the properties of the density matrix. Instead of the μ_k one may also use the symmetric functions

$$\mathcal{P}_k = \mathrm{Tr}\, \rho^k = \sum_{j=1}^{n} \lambda_j^k, \qquad 0 \leq k \leq n$$

Moreover, for the present task it is convenient to rewrite the characteristic identity as a polynomial in $x = 1 - \rho$,

$$x^n + A_{n-1}x^{n-1} + \cdots + A_1x + A_0 = 0 \tag{2}$$

where the symmetric functions A_k arise as coefficients. These three sets μ_k, $\mathcal{P}_k$, and A_k are equivalent in that each one can be expressed in terms of another. The A_k and μ_k are connected by the linear transformation

$$A_k = \sum_{j=k}^{n} (-1)^{j-k} \frac{j!}{k!(j-k)!} \mu_{n-j}$$

The relation between the μ_k and the $\mathcal{P}_k$ is given by the following determinants.

$$\mu_k = \frac{1}{k}\begin{vmatrix} 1 & \mathcal{P}_2 & \mathcal{P}_3 & \dots & \mathcal{P}_{k-1} & \mathcal{P}_k \\ 1 & 1 & \mathcal{P}_2 & \dots & \mathcal{P}_{k-2} & \mathcal{P}_{k-1} \\ 0 & 1 & 1 & \dots & \mathcal{P}_{k-3} & \mathcal{P}_{k-2} \\ \dots & \dots & \dots & \dots & \dots & \dots \\ & & & \dots & 1 & \mathcal{P}_2 \\ & & & \dots & 1 & 1 \end{vmatrix}$$

$$\mathcal{P}_k = \begin{vmatrix} 1 & 2\mu_2 & 3\mu_3 & \dots & (k-1)\mu_{k-1} & k\mu_k \\ 1 & 1 & \mu_2 & \dots & \mu_{k-2} & \mu_{k-1} \\ 0 & 1 & 1 & \dots & \mu_{k-3} & \mu_{k-2} \\ \dots & \dots & \dots & \dots & \dots & \dots \\ & & & \dots & 1 & \mu_2 \\ & & & \dots & 1 & 1 \end{vmatrix}$$

In the formula

$$S = -\mathrm{Tr}[\rho \log(1 + \rho - 1)] = \mathrm{Tr}\left[\sum_{k=1}^{\infty} \frac{\rho_k}{k}\right]$$

the ρ_k are defined by

$$\rho_k = \rho(1-\rho)^k = \sum_{j=0}^{n-1} \alpha_j^{(k)} x^k$$

and the coefficients $\alpha_j^{(k)}$ can be determined with help of the characteristic identity, eliminating the powers higher than $n-1$ of x. The recursion relations for the coefficients $\alpha_j^{(k)}$ can be written in matrix notation,

$$\overline{\alpha}^{(k+1)} = \mathcal{A}\overline{\alpha}^{(k)}$$

where the matrix $\mathcal{A}$ is given by

$$\mathcal{A} = \begin{pmatrix} -A_{n-1} & 1 & 0 & \dots & 0 & 0 \\ -A_{n-2} & 0 & 1 & \dots & 0 & 0 \\ -A_{n-3} & 0 & 0 & \dots & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ -A_1 & 0 & 0 & \dots & 0 & 1 \\ -A_0 & 0 & 0 & \dots & 0 & 0 \end{pmatrix}$$

and

$$\bar{\alpha}^k = \begin{pmatrix} \alpha^k_{n-1} \\ \alpha^k_{n-2} \\ \cdots \\ \alpha^k_2 \\ \alpha^k_1 \\ \alpha^k_0 \end{pmatrix}, \qquad \bar{\alpha}^{(1)} = \begin{pmatrix} 0 \\ \cdots \\ 0 \\ -1 \\ 1 \\ 0 \end{pmatrix}$$

Forming another column vector from the n generation functions

$$\bar{f} \begin{pmatrix} f_{n-1} \\ f_{n-2} \\ f_{n-3} \\ \cdots \\ f_2 \\ f_1 \\ f_0 \end{pmatrix}, \qquad f_m = \sum_{k=1}^{\infty} z^{k-1} \alpha_m^{(k)}$$

we may write

$$\bar{f} = \sum_{k=1}^{\infty} (z\mathcal{A})^{k-1} \bar{\alpha}^{(1)} = (1 - z\mathcal{A})^{-1} \bar{\alpha}^{(1)}$$

The resolvent of the matrix $\mathcal{A}$ is easily computed. The principal minors of $1 - z\mathcal{A}$ are

$$\begin{aligned} D_1 &= 1 + zA_{n-1} \\ D_2 &= \begin{vmatrix} 1 + zA_{n-1} & -z \\ zA_{n-2} & 1 \end{vmatrix} = 1 + zA_{n-1} + z^2 A_{n-2} \\ &\vdots \\ D_k &= 1 + zA_{n-1} + z^2 A_{n-2} + \cdots + z^k A_{n-k} \\ D_k &= D_{k-1} + z^k A_{n-k}, \qquad 1 \leq k \leq n \\ D_n &= \det(1 - z\mathcal{A}) \end{aligned} \tag{3}$$

Hence we obtain the generating functions for the n-level case

$$\bar{\bar{f}} \equiv \begin{pmatrix} f_{n-1} \\ f_{n-2} \\ f_{n-3} \\ \cdots \\ f_2 \\ f_1 \\ f_0 \end{pmatrix} = \frac{1}{D_n} \begin{pmatrix} z^{n-3}(z-1) \\ D_1 z^{n-4}(z-1) \\ D_2 z^{n-5}(z-1) \\ \cdots \\ D_{n-3}(z-1) \\ z^{n-2}A_1 + z^{n-1}A_0 + D_{n-2} \\ A_0 z^{n-2}(1-z) \end{pmatrix} \tag{4}$$

Since

$$S = \mathrm{Tr}\left[\sum_{k=1}^{\infty} \frac{\rho_k}{k}\right] = \mathrm{Tr}\left[\int_0^1 dz \sum_{k=1}^{\infty} \sum_{m=0}^{n-1} \alpha_m^{(k)} z^{k-1} x^m\right]$$

the final expression for the entropy is

$$S = \int_0^1 dz \sum_{m=0}^{n-1} f_m(z)\, \mathrm{Tr}\, x^m \tag{5}$$

and

$$\mathrm{Tr}\, x^k = \sum_{m=0}^{k} (-1)^m \mathcal{P}_k \frac{k!}{m!(k-m)!}, \qquad \mathcal{P}_0 = n, \quad \mathcal{P}_1 = 1$$

The formula for the entropy, equation (5), is the principal result of this paper. It can be easily shown that the integrand is a regular functions on the integration domain. Equation (5) can be used for numerical and analytical calculations.

We will illustrate the use of the method by two examples.

Example. $n = 3$: The coefficients of the characteristic identity (2) are

$$A_0 = \delta - \mu, \qquad A_1 = \mu + 1, \qquad A_2 = -2$$

and from equation (3) we have

$$D_3 = 1 - 2z + (\mu + 1)z^2 - (\mu - \delta)z^3$$

Equation (4) takes the form

$$\bar{\bar{f}}(z) = \frac{1}{D_3} \begin{pmatrix} (z-1) \\ 1 + z(A_1 + A_2) + z^2 A_0 \\ z(1-z)A_0 \end{pmatrix}$$

Calculating the entropy from equation (5) making use of

$$\mathrm{Tr}\,\mathbf{1} = 3, \qquad \mathrm{Tr}\,x = 2, \qquad \mathrm{Tr}\,x^2 = 2 - 2\mu$$

we find the result already stated in equation (1).

Example. $n = 4$: The coefficients in the characteristic equation (2) are

$$A_0 = \mu_4 - \mu_3 + \mu_2,$$

$$A_1 = \mu_3 - 2\mu_2 - 1,$$

$$A_2 = \mu_2 + 3,$$

$$A_3 = -3$$

$$D_3 = 1 - 3z + (\mu_2 + 3)z^2 + (\mu_3 - 2\mu_2 - 1)z^3 + (\mu_4 - \mu_3 + \mu_2)z^4$$

The generating functions are

$$f_3 = z^2 - z$$

$$f_2 = -1 + 4z - 3z^2$$

$$f_1 = z^3(\mu_4 - \mu_3 + \mu_2) + z^2(\mu_3 - \mu_2 + 2) - 3z + 1$$

$$f_0 = (\mu_4 - \mu_3 + \mu_2)(z^2 - z^3)$$

We calculate the entropy from equation (5), making use of

$$\mathrm{Tr}\,x^3 = 3 - 3\mu_2 - - 3\mu_3,$$

$$\mathrm{Tr}\,x^2 = 3 - 2\mu_2,$$

$$\mathrm{Tr}\,x = 3,$$

$$\mathrm{Tr}\,\mathbf{1} = 4$$

and we have

$$S = \int_0^1 dz\, \frac{-(\mu_4 - \mu_3 + \mu_2)z^3 + 4(\mu_4 - \mu_3 + \mu_2)z^2 + (3\mu_3 - 5\mu_2)z + 2\mu_2}{1 - 3z + (\mu_2 + 3)z^2 + (\mu_3 - 2\mu_2 - 1)z^3 + (\mu_4 - \mu_3 + \mu_2)z^4}$$

$$= \int_0^1 dz\, \frac{-A_0z^3 + 4A_0z^2 + (3A_3 + A_2)z - 2A_2 - 6}{1 - 3z + A_2z^2 + A_3z_z{}^3 + A_4z^4}$$

The case $n = 3$ arises when $\mu_4 = 0$; then the denominator and nominator have a common factor $z - 1$.

4. CONCLUSIONS

We have proposed an analytical expression for the von Neumann entropy for n-level quantum systems which does not involve the diagonalization of the density matrix. The expression determines the entropy in form of an integral of a rational function over $(0,1) \subseteq \mathbf{R}$. The coefficients in the rational function are symmetric functions of the eigenvalues of the density matrix. Our numerical tests show that this formula can be efficiently used for computer simulations. We also believe that it can be useful for analytical work.

REFERENCES

Araki, H., and Lieb, E. (1970). *Communications in Mathematical Physics,* **18**, 160.

Chumakov, S. M., and Kozierowski, M. (1996). *Quantum and Semiclassical Optics,* **8**, 775.

Chumakov, S. M., Klimov, A. B., and Sanchez-Mondragon, J. J. (1994). *Physical Review A,* **49**, 4972.

Dicke, R. H. (1954). *Physical Review,* **93**, 99.

Gea-Banacloche, J. (1990). *Physical Review Letters,* **65**, 3385.

Giulini, D., Joos, E., Kiefer, C., *et al.* (1996). *Decoherence and the Appearance of a Classical World in Quantum Theory*, Springer, Berlin.

Jaynes, E. T., and Cummings, F. W. (1963). *Proceedings IEEE,* **51**, 89.

Knight, P. L., and Shore, B. W. (1993). *Physical Review A,* **48**, 642.

Kozierowski, M., Mamedov, A. A., and Chumakov, S. M. (1990). *Physical Review A,* **42**, 1762.

Paul, H. (1963). *Annalen der Physik,* **11**, 411.

Phoenix, S. J. D., and Knight, P. L. (1988). *Annals of Physics,* **186**, 381.

Phoenix, S. J. D., and Knight, P. L. (1991). *Physical Review A,* **44**, 6023.

Von Neumann, J. (1932). *Mathematische Grundlagen der Quantenmechanik*, Springer, Berlin.

Wehrl, A. (1978). *Reviews of Modern Physics,* **50**, 221.