On the BCH formula of Rezek and Kosloff

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Abstract

The BCH formula of Rezek and Kosloff is a convenient tool to handle a family of density matrices, which occurs in the study of quantum heat engines. We prove the formula using a known argument from Lie theory.

1 Introduction

The Hamiltonian

$$H = \frac{1}{2}\hbar\omega(a^\dagger a + aa^\dagger) \tag{1}$$

of the quantum harmonic oscillator belongs to the Lie algebra $\mathfrak{su}(1,1)$ with generators

$$\begin{aligned} S_1 &= \frac{1}{4}((a^\dagger)^2 + a^2), \\ S_2 &= \frac{i}{4}((a^\dagger)^2 - a^2), \\ S_3 &= \frac{1}{4}(a^\dagger a + aa^\dagger). \end{aligned} \tag{2}$$

As a consequence, it is possible to write down simplified Baker-Campbell-Haussdorf (BCH) relations [1, 2]. These have been used to study the quantum harmonic oscillator in a time-dependent external field [3, 4, 5, 6, 7, 8, 9]. The topic of the present paper is a new BCH relation, introduced recently by Rezek and Kosloff [10]. They consider the family of density matrices

$$\rho = \frac{1}{Z(\beta,\gamma)} e^{\gamma a^2} e^{-\beta H} e^{\overline{\gamma}(a^\dagger)^2} \tag{3}$$

with real β and complex γ, and with

$$Z(\beta,\gamma) = \operatorname{Tr} e^{\gamma a^2} e^{-\beta H} e^{\overline{\gamma}(a^\dagger)^2}. \tag{4}$$

Because all operators appearing in (3) belong to the Lie algebra it is clear from the general Baker-Campbell-Haussdorf relation that it must be possible to write

$$e^{\gamma a^2} e^{-\beta H} e^{\overline{\gamma}(a^\dagger)^2} = e^{\chi a^2 - \xi H + \overline{\chi}(a^\dagger)^2} \tag{5}$$

The explicit expression of the coefficients χ and ξ as a function of β and γ is found in the Appendix of [10]. The functions were derived [11] using the algebraic manipulation software Mathematica.

Note that the special case of (5) with $\xi = 0$ appeared in the physics literature before (see Example I of Section II of [12]; see also [13, 14]). In the present paper the relation (5) is derived using the argument of [12].

The relation (5) is of interest in its own. But it is also very useful in the study of quasi-stationary processes [10, 15]. Indeed, from (5) it is clear that the density matrix ρ describes a system in thermal equilibrium at inverse temperature ξ. On the other hand, the expression (3) is more convenient for practical calculations.

We derive the BCH formula in the next section. In Section 3 follows a similar BCH formula valid for $\mathfrak{su}(2)$. In the final section follows a short discussion.

2 The identity

The the l.h.s. of (5) can be written in terms of the generators of the Lie algebra $\mathfrak{su}(1,1)$ as

$$e^{2\gamma(S_1+iS_2)} e^{-2\beta\hbar\omega S_3} e^{2\overline{\gamma}(S_1-iS_2)}. \tag{6}$$

These generators satisfy the commutation relations

$$\begin{aligned} [S_1,S_2] &= iS_3, \\ [S_2,S_3] &= -iS_1, \\ [S_3,S_1] &= -iS_2. \end{aligned} \tag{7}$$

Introduce $\mathfrak{su}(2)$ generators $T_1 = -iS_1$, $T_2 = iS_2$, and $T_3 = S_3$. Then (6) becomes

$$X \equiv e^{2\gamma(iT_1+T_2)} e^{-2\beta\hbar\omega T_3} e^{2\overline{\gamma}(iT_1-T_2)}. \tag{8}$$

The relation (5) does not depend on the choice of the representation of the $\mathfrak{su}(2)$ algebra. Therefore, we may change it. A favourable choice is that of the Pauli spin matrices $\sigma_\alpha = 2T_\alpha$. Using that $(\sigma_1 \pm i\sigma_2)^2 = 0$ and $\sigma_\alpha^2 = \mathbb{I}$ the calculation becomes very easy. One obtains

$$\begin{aligned} X &= e^{i\gamma(\sigma_1 - i\sigma_2)} e^{-\beta\hbar\omega\sigma_3} e^{i\overline{\gamma}(\sigma_1 + i\sigma_2)} \\ &= (\mathbb{I} + i\gamma(\sigma_1 - i\sigma_2))(\cosh(\hbar\omega) - \sigma_3 \sinh(\hbar\omega))(\mathbb{I} + i\overline{\gamma}(\sigma_1 + i\sigma_2)) \\ &= e^{-\beta\hbar\omega\sigma_3} - 2\kappa|\gamma|^2 + i\kappa(\gamma + \overline{\gamma})\sigma_1 + \kappa(\gamma - \overline{\gamma})\sigma_2 + 2\kappa|\gamma|^2\sigma_3, \end{aligned} \tag{9}$$

with $\kappa = e^{-\beta\hbar\omega}$ as before. On the other hand is

$$\begin{aligned} \exp\left(\chi a^2 - \xi H + \overline{\chi}(a^\dagger)^2\right) &= \exp\left(2\chi(S_1 + iS_2) - 2\xi\hbar\omega S_3 + 2\overline{\chi}(S_1 - iS_2)\right) \\ &= \exp\left(2\chi(iT_1 + T_2) - 2\xi\hbar\omega T_3 + 2\overline{\chi}(iT_1 - T_2)\right). \end{aligned} \tag{10}$$

In the Pauli spin representation this becomes e^Y with

$$Y = i(\chi + \overline{\chi})\sigma_1 + (\chi - \overline{\chi})\sigma_2 - \xi\hbar\omega\sigma_3. \tag{11}$$

Because the Pauli matrices anti-commute and their squares equal $\mathbb{I}$ there follows that

$$Y^2 = \lambda^2\mathbb{I} \quad \text{with} \quad \lambda = \sqrt{\xi^2(\hbar\omega)^2 - 4|\chi|^2}. \tag{12}$$

Hence one obtains

$$e^Y = \cosh(\lambda) + \frac{1}{\lambda}\sinh(\lambda)Y. \tag{13}$$

Comparison with (9) gives the 4 conditions

$$\cosh(\lambda) = \alpha + \kappa, \tag{14}$$

$$\frac{1}{\lambda}\sinh(\lambda)(\chi + \overline{\chi}) = \kappa(\gamma + \overline{\gamma}), \tag{15}$$

$$\frac{1}{\lambda}\sinh(\lambda)(\chi - \overline{\chi}) = \kappa(\gamma - \overline{\gamma}), \tag{16}$$

$$\frac{1}{\lambda}\sinh(\lambda)\xi\hbar\omega = \alpha, \tag{17}$$

with

$$\begin{aligned} \alpha &= \sinh(\beta\hbar\omega) - 2\kappa|\gamma|^2 \\ &= \frac{1}{2\kappa}\left[1 - \kappa^2 - 4\kappa|\gamma|^2\right]. \end{aligned} \tag{18}$$

The solution of these equations is

$$\xi = \frac{\alpha}{\hbar\omega}\frac{\lambda}{\sinh(\lambda)}, \tag{19}$$

$$\chi = \kappa\frac{\lambda}{\sinh(\lambda)}\gamma. \tag{20}$$

with

$$\sinh(\lambda) = \sqrt{\alpha^2 - 4\kappa^2|\gamma|^2} \tag{21}$$

These results coincide with those found in the Appendix of [10].

Note that the expressions for ξ and χ can be inverted easily. Given ξ and χ one obtains λ from (12). Then α follows by inverting (19). This gives

$$\alpha = \hbar\omega\xi\frac{\sinh(\lambda)}{\lambda}. \tag{22}$$

Next β is obtained from (14)

$$\kappa = \cosh(\lambda) - \alpha. \tag{23}$$

Finally, γ follows from (20)

$$\gamma = \frac{\sinh(\lambda)}{\kappa\lambda}\chi. \tag{24}$$

3 An example with SU(2) symmetry

Formulas similar to (5) can be derived for other symmetry groups than SU(1,1). For instance, in the case of SU(2) one has

$$e^{\gamma\sigma_+}e^{-\beta\sigma_z}e^{\overline{\gamma}\sigma_-} = \exp\left(\chi\sigma_+ - \xi\sigma_z + \overline{\chi}\sigma_-\right) \tag{25}$$

with $\sigma_\pm = \frac{1}{2}(\sigma_x \pm i\sigma_y)$. Using $\sigma_\pm^2 = 0$, $\sigma_z^2 = \mathbb{I}$, $\sigma_\pm\sigma_z = \mp\sigma_\pm$, and $\sigma_+\sigma_- = \frac{1}{2}(1+\sigma_z)$ the l.h.s. becomes

$$\begin{aligned} \text{l.h.s.} &= (1+\gamma\sigma_+)\left(\cosh(\beta) - \sinh(\beta)\sigma_z\right)(1+\overline{\gamma}\sigma_-) \\ &= \cosh(\beta) + \frac{1}{2}|\gamma|^2 e^\beta + e^\beta(\gamma\sigma_+ + \overline{\gamma}\sigma_-) - (\sinh(\beta) - \frac{1}{2}e^\beta|\gamma|^2)\sigma_z. \end{aligned} \tag{26}$$

The r.h.s. of (25) is evaluated using

$$\left(\chi\sigma_+ - \xi\sigma_z + \overline{\chi}\sigma_-\right)^2 = \lambda^2\mathbb{I}, \tag{27}$$

with $\lambda = \sqrt{\xi^2 + |\chi|^2}$. One finds

$$\text{r.h.s.} \quad = \quad \cosh(\lambda) + \frac{1}{\lambda}\sinh(\lambda)\left(\chi\sigma_+ - \xi\sigma_z + \overline{\chi}\sigma_-\right). \tag{28}$$

Equating both expressions yields the set of equations

$$\cosh(\beta) + \frac{1}{2}e^\beta|\gamma|^2 \quad = \quad \cosh(\lambda), \tag{29}$$

$$-\sinh(\beta) + \frac{1}{2}e^\beta|\gamma|^2 \quad = \quad -\frac{1}{\lambda}\sinh(\lambda)\xi, \tag{30}$$

$$\gamma e^\beta \quad = \quad \frac{1}{\lambda}\sinh(\lambda)\chi. \tag{31}$$

Given ξ and χ, the value of λ can be obtained from its definition. The solution then reads

$$\begin{aligned} e^\beta &= \cosh(\lambda) + \frac{1}{\lambda}\sinh(\lambda)\xi \\ \gamma &= \frac{\frac{1}{\lambda}\sinh(\lambda)}{\cosh(\lambda) + \frac{1}{\lambda}\sinh(\lambda)\xi}\chi. \end{aligned} \tag{32}$$

Conversely, given β and γ one obtains λ from (29). Then ξ and χ follow from (30) and (31), respectively.

4 Discussion

The BCH relation of Rezek and Kosloff is somewhat special because it is written in a form suited for application to density matrices. Similar results found in the literature [1, 2, 3, 4, 5, 6, 7, 8, 9] aim at the calculation of time evolution operators and refer to similarity transformations, this is, to expressions of the form $e^A B e^{-A}$. But the l.h.s. of (5) is not a similarity transformation. This is precisely the reason why this BCH relation is of interest! The change of the spectrum implies that the average energy $\langle H \rangle = \mathrm{Tr}\,\rho H$ will depend on the value of the parameter γ. This dependence is essential in the context of heat engines.

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