On the BCH formula of Rezek and Kosloff

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ABSTRACT

The BCH formula of Rezek and Kosloff (2006) [10] 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.

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1. Introduction

The Hamiltonian

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

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

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

As a consequence, it is possible to write down simplified Baker–Campbell–Hausdorff (BCH) relations [1,2]. These are used to study the quantum harmonic oscillator in a time-dependent external field [3–9]. 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

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

with real β and complex γ , and with

$$Z(\beta, \gamma) = \text{Tr} e^{\gamma a^2} e^{-\beta H} e^{\bar{\gamma} (a^\dagger)^2}. \quad (4)$$

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

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

The explicit expression of the coefficients χ and ξ as a function of β and γ is found in the Appendix of Ref. [10]. The functions were derived [11] using the algebraic manipulation software Mathematica. Here, the same relations are derived by a simple analytic argument.

Note that the special case of (5) with $\xi = 0$ appeared in the physics literature before (see Example I of Section II of Ref. [12]; see also Refs. [13,14]). In the present paper, relation (5) is derived using the argument of Ref. [12]. This relation is of interest in its own. But it is also very useful in the study of quasi-stationary processes [10,15].

We derive the BCH formula in the next section. In the final section follows a short discussion.

2. The identity

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

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

These generators satisfy the commutation relations

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

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

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

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

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

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

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

In the Pauli spin representation this becomes e^Y with

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

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

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

Hence one obtains

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

Comparison with (9) gives the 4 conditions

$$\cosh(\lambda) = \alpha + \kappa, \quad (14)$$

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

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

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

with

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

The solution of these equations is

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

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

with

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

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

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

Next β is obtained from (14)

$$\kappa = \cosh(\lambda) - \alpha. \quad (23)$$

Finally, γ follows from (20)

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

3. 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 [1–9] aim at the calculation of time evolution operators and refer to similarity transformations, that 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 $\langle H \rangle = \text{Tr } \rho H$ will depend on the value of the parameter γ . This dependence is essential in the context of heat engines.

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