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Exponential Operators and Parameter Differentiation in Quantum Physics

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Elementary parameter-differentiation techniques are developed to systematically derive a wide variety of operator identities, expansions, and solutions to differential equations of interest to quantum physics. The treatment is largely centered around a general closed formula for the derivative of an exponential operator with respect to a parameter. Derivations are given of the Baker–Campbell–Hausdorff formula and its dual, the Zassenhaus formula. The continuous analogs of these formulas which solve the differential equation $dY(t)/dt = A(t)Y(t)$, the solutions of Magnus and Fer, respectively, are similarly derived in a recursive manner which manifestly displays the general repeated-commutator nature of these expansions and which is quite suitable for computer programming. An expansion recently obtained by Kumar and another new expansion are shown to be derivable from the Fer and Magnus solutions, respectively, in the same way. Useful similarity transformations involving linear combinations of elements of a Lie algebra are obtained. Some cases where the product $e^A e^B$ can be written as a closed-form single exponential are considered which generalize results of Sack and of Weiss and Maradudin. Closed-form single-exponential solutions to the differential equation $dY(t)/dt = A(t)Y(t)$ are obtained for two cases and compared with the corresponding multiple-exponential solutions of Wei and Norman. Normal ordering of operators is also treated and derivations, corollaries, or generalization of a number of known results are efficiently obtained. Higher derivatives of exponential and general operators are discussed by means of a formula due to Poincaré which is the operator analog of the Cauchy integral formula of complex variable theory. It is shown how results obtained by Aizu for matrix elements and traces of derivatives may be readily derived from the Poincaré formula. Some applications of the results of this paper to quantum statistics and to the Weyl prescription for converting a classical function to a quantum operator are given. A corollary to a theorem of Bloch is obtained which permits one to obtain harmonic-oscillator canonical-ensemble averages of general operators defined by the Weyl prescription. Solutions of the density-matrix equation are also discussed. It is shown that an initially canonical ensemble behaves as though its temperature remains constant with a "canonical distribution" determined by a certain fictitious Hamiltonian.

1. INTRODUCTION

OPERATOR identities, expansions, and solutions to differential equations occur widely in quantum physics and have been derived with the aid of a variety of abstract or complicated methods. These include functional analysis, Lie algebra theory, the Feynman ordering-operator calculus,[1] the commutator superoperator, special function theory, and special methods which appear to be of limited use. Although we do not doubt the power and usefulness of some of these methods, it is interesting to see what may be accomplished with a few simple but versatile tools. One of these tools, the parameter differentiation of quantum-mechanical linear operators, has been instructively discussed by Aizu.[2] However, that treatment is confined to obtaining matrix elements and traces involving derivatives. We are here particularly interested in identities involving operators themselves, especially exponential operators. A device which we make extensive use of in establishing identities involving exponential operators is to require that both sides of an equation satisfy the same first-order differential equation and the same initial condition. We refer to this tool as *the differential equation method.*

Another device, used to obtain results for general operator functions from those involving exponential operators, is to assume that the general functions can be expressed as linear combinations of exponential operators. We refer to this tool as *the method of linear superposition.* Special cases of it are Fourier and Laplace series or integrals. This procedure is often easier to apply than the often-used method which constructs general functions from linear combinations of powers of operators,[3] but the set of functions which may be represented by either method appears to be the same. Using mainly these tools, we intend to derive a variety of scattered results in a concise systematic and elementary manner which many physicists may find easier to understand. Nevertheless, we believe that we have occasionally obtained a new application or generalization of a known result.

[1] R. P. Feynman, Phys. Rev. 84, 108 (1951).
[2] K. Aizu, J. Math. Phys. 4, 762 (1963).
[3] W. H. Louisell, *Radiation and Noise in Quantum Electronics* (McGraw-Hill Book Company, Inc., New York, 1964), Chap. 3, p. 98.

Although everyone knows how to differentiate an ordinary exponential function, it is not widely realized that a general closed formula exists for the derivative of an exponential operator with respect to a parameter. [See Eq. (2.1) of Sec. 2.] We believe that this formula is sufficiently simple and useful that many physicists and applied mathematicians can profitably commit it to memory. In Sec. 2, this formula is verified by the differential equation method and compared with formulas of Feynman[1] and Kubo.[4] A basic lemma is derived which displays the formal correspondence between parameter differentiation and commutation. The concept of differentiation with respect to an operator is also discussed. In Sec. 3, Eq. (2.1) is shown to be of use for problems in equilibrium quantum statistics. In Sec. 4, Eq. (2.1) and the differential equation method are used to easily derive the Baker–Campbell–Hausdorff (BCH) formula.[5] This important formula determines Z such that $e^Ae^{\tilde{B}} = e^Z$ is identically satisfied. A good review of the history of this formula is given by Weiss and Maradudin.[6] A formula of Zassenhaus,[7] said to be the dual of the BCH formula, is also derived in Sec. 4 in a similar manner. This formula expresses e^{A+B} as an infinite product of exponential operators. A number of examples of the type of problem which exploits the BCH formula occur in connection with the Weyl prescription for converting a classical function to a quantum operator. This is described in Sec. 5. A more direct derivation of a useful formula recently obtained by Daughaday and Nigam[8] is given there, while interesting theorems of McCoy,[9] Moyal, and Wigner[10] are stated without proof.

In Sec. 6, a definition of a Lie algebra is given and examples of various Lie algebras which occur in quantum mechanics are given. Similarity transformations involving operators which are linear combinations of Lie elements (denoted LCLE) are readily obtained by the differential equation method. The results may be used to "change the representation" in quantum-mechanical problems, and are also used in Secs. 7, 8, and 10. In Sec. 7, Eq. (2.1) and the differential equation method are used to obtain closed-form expressions for $Z = \ln (e^Ae^B)$ for certain cases where A and B are LCLE's. Generalizations of formulas obtained by Sack[11] and by Weiss and Maradudin[6] are obtained. A corollary to a theorem of Bloch[12] is also derived which is useful for obtaining harmonic-oscillator thermal averages of general operator functions.

In Sec. 8, we obtain solutions to the important operator differential equation, $dY(t)/dt = A(t)Y(t)$. In Sec. 8.1, we obtain the Magnus[7] and Fer[13] solutions in a manner similar to that used to derive the BCH and Zassenhaus formulas, respectively. It should be noted that all four of these formulas are derived by a recursion procedure which manifestly displays the repeated-commutator nature of these expansions and which is quite suitable for computer programming. An expansion recently obtained by Kumar[14] and another new expansion are shown to be derivable from the Fer and Magnus solutions, respectively, in the same way. Both of these expansions may be more suitable than the Zassenhaus expansion for certain purposes. In Sec. 8.2, Lie algebraic solutions in terms of a single exponential are obtained and compared with corresponding multiple-exponential solutions of Wei and Norman.[15] In Sec. 9, solutions of the density matrix equation, Eq. (9.1), are discussed. It is shown that an initially canonical ensemble behaves as though its temperature remains constant with a "canonical distribution" determined by a certain fictitious Hamiltonian.

In Sec. 10, a collection of old and recent results involving normal ordering of operators are efficiently derived with the aid of the results and methods of previous sections. Derivations, corollaries, or generalizations of formulas obtained by Louisell,[3] Heffner and Louisell,[16] Schwinger,[17] McCoy,[18] Kermack and McCrea,[19] and Cohen[20] are given. In Sec. 11, higher derivatives of exponential operators are treated with a formula due to Poincaré.[21] [See Eq. (10.1).] Although

[4] *Lectures in Theoretical Physics* R. Kubo, W. E. Brittin, and L. G. Dunham, Eds. (Interscience Publishers, Inc., New York, 1959), Vol. I, p. 139, Eq. (2.17).

[5] J. E. Campbell, Proc. London Math. Soc. **29**, 14 (1898); H. F. Baker, *ibid.* **34**, 347 (1902); **35**, 333 (1903); **2**, 293 (1904); **3**, 24 (1904); F. Hausdorff, Ber. Verhandl. Saechs. Akad. Wiss. Leipzig, Math.-Naturw. Kl. **58**, 19 (1906); N. Jacobson, *Lie Algebras* (Interscience Publishers, Inc., New York, 1962), Chap. 5, p. 170.

[6] G. H. Weiss and A. A. Maradudin, J. Math. Phys. **3**, 771 (1962).

[7] W. Magnus, Commun. Pure Appl. Math. **7**, 649 (1954).

[8] H. Daughaday and B. P. Nigam, Phys. Rev. **139**, B1436 (1965).

[9] N. H. McCoy, Proc. Math. Acad. Sci. U.S. **18**, 674 (1932).

[10] J. E. Moyal, Proc. Cambridge Phil. Soc. **45**, 99 (1949); E. P. Wigner, Phys. Rev. **40**, 749 (1932); C. L. Mehta, J. Math. Phys. **5**, 677 (1964).

[11] R. A. Sack, Phil. Mag. **3**, 497 (1958).

[12] F. Bloch, Z. Physik **74**, 295 (1932).

[13] F. Fer, Bull. Classe Sci. Acad. Roy. Belg. **44**, 818 (1958).

[14] K. Kumar, J. Math. Phys. **6**, 1928 (1965).

[15] J. Wei and E. Norman, J. Math. Phys. **4**, 575 (1963).

[16] H. Heffner and W. H. Louisell, J. Math. Phys. **6**, 474 (1965).

[17] *Quantum Theory of Angular Momentum*, J. Schwinger, L. C. Biedenharn, and H. van Dam, Eds. (Academic Press Inc., New York, 1965), pp. 274–276.

[18] N. H. McCoy, Proc. Edinburgh Math. Soc. **3**, 118 (1932).

[19] W. O. Kermack and W. H. McCrea, Proc. Edinburgh Math. Soc. **2**, 220 (1931).

[20] L. Cohen, J. Math. Phys. **7**, 244 (1966).

[21] H. Poincaré, Trans. Cambridge Phil. Soc. **18**, 220 (1899); see also R. Bellman, *Introduction to Matrix Analysis* (McGraw-Hill Book Company, Inc., New York, 1960), p. 103, Ex. 43. This formula is the basis of resolvent theory. See, e.g., Messiah, Ref. 48, Chap. 16, Sec. 3, p. 712.

even greater formal efficiency may be obtained with the Feynman ordering-operator calculus,[1] we have preferred to use the Poincaré formula since it is more firmly rooted in classical analysis and since it readily permits one to differentiate *general* operator functions in a concise manner. It is shown to provide a compact alternative for the derivation of formulas of the type derived by Aizu.[2] We note that such formulas may be used to derive all of the interesting sum rules and hypervirial theorems treated in a recent paper by Morgan and Landsberg.[22]

2. DERIVATIVE OF EXPONENTIAL OPERATOR

If the operator H is a function of a parameter λ, $H \equiv H(\lambda)$, then

$$\frac{\partial}{\partial\lambda} e^{-\beta H} = -\int_0^\beta e^{-(\beta-u)H} \frac{\partial H}{\partial \lambda} e^{-uH}\, du. \quad (2.1)$$

This identity (aside from notation) has been derived and used by Snider in treating a quantum Boltzmann equation.[23] Snider's derivation was based upon the commutator superoperator and an integral representation for the beta function. The present author found Eq. (2.1) independently by employing the parameter-differentiation technique explained by Aizu,[2] together with the well-known expansion[24]

$$e^A B e^{-A} = B + [A, B] + (1/2!)[A, [A, B]] + \cdots. \quad (2.2)$$

The author has applied Eq. (1) to the calculation of the polarizability of a one-dimensional NaCl lattice.[25] Equation (2.1) has also been obtained recently by Kumar,[26] but the full generality of the result is not obvious in that treatment.

Like any operator identity, Eq. (2.1) may be verified by showing that the matrix elements of both sides of the equation are the same in some suitable representation. This may be done, using Aizu's techniques,[2] by choosing a representation in which $H(\lambda)$ is diagonal. However, an easier method is to show that both sides of the equation satisfy the first-order differential equation

$$[\partial F(\beta)/\partial\beta] + HF(\beta) = -(\partial H/\partial\lambda)e^{-\beta H}, \quad (2.3)$$

with the initial condition $F(0) = 0$.

[22] D. J. Morgan and P. T. Landsberg, Proc. Phys. Soc. (London) **86**, 261 (1965).
[23] R. F. Snider, J. Math. Phys. **5**, 1586 (1964), Appendix B.
[24] See, e.g., Louisell, Ref. 3, p. 101, Eq. (3. 14).
[25] R. M. Wilcox, National Bureau of Standards Report (1964).
[26] Reference 14, Eqs. (46) and (A1).

A special case of Eq. (2.1) is an identity of Feynman,[27]

$$\left[\frac{d}{d\epsilon} e^{\alpha+\epsilon\beta}\right]_{\epsilon=0} = \int_0^1 e^{(1-s)\alpha}\beta e^{s\alpha}\, ds, \quad (2.4)$$

where α and β are independent of ϵ. Equation (2.4) has been obtained by Feynman by means of his ordering-operator calculus, and this method may also be used to derive Eq. (2.1).[28] Also, Eq. (2.1) may be obtained from Eq. (4) by considering the Taylor expansion

$$H(\lambda + \epsilon) = H(\lambda) + \epsilon(\partial H/\partial\lambda) + O(\epsilon^2).$$

However, Eq. (2.1) is a more convenient form to use than Eq. (2.4), particularly for differential equations.

An identity of Kubo is a corollary of Eq. (2.1).[4]

$$[A, e^{-\beta\mathcal{H}}] = -\int_0^\beta du e^{-(\beta-u)\mathcal{H}}[A, \mathcal{H}]e^{-u\mathcal{H}}. \quad (2.5)$$

In Eq. (2.5), A and $\mathcal{H}$ are arbitrary operators. This identity has had much use in the theory of irreversible processes. Like Eq. (2.1), it is easily established by the differential equation method, as Montroll has noted.[29] It may also be derived from Eq. (2.1) by making the similarity transformation

$$\begin{aligned} H(\lambda) &= e^{\lambda A}\mathcal{H}e^{-\lambda A}, \\ e^{-\beta H} &= e^{\lambda A}e^{-\beta\mathcal{H}}e^{-\lambda A}. \end{aligned} \quad (2.6)$$

Conversely, Eq. (2.1) follows from Eq. (2.5) by setting $\mathcal{H} = H(\lambda)$ and $A = \partial/\partial\lambda$. Another form of Eq. (2.5), obtained by setting $\beta = -it/\hbar$, occurs as the solution to the Heisenberg equation of motion, $\dot{A}(t) = i\hbar^{-1}[\mathcal{H}, A(t)]$, for $\mathcal{H}$ independent of t. A generalization to the case where $\mathcal{H}$ is time dependent may also be readily established by the differential equation method.[30]

Equations (2.1) and (2.5) may be used to derive a useful basic lemma.

Lemma: If $[A, H(\lambda)] = \partial H/\partial\lambda$, then $[A, f(H)] = \partial f(H)/\partial\lambda$. (Note: in the language of Lie algebra, A is said to be the generator of an infinitesimal transformation due to a change in the parameter λ.)

Proof: Equations (2.1) and (2.5) imply this result for the special case where $f(H) = e^{-\beta H}$, while the general case easily follows by the method of linear superposition.

[27] Reference 1, Eq. (6). A related identity occurs in R. Karplus and J. Schwinger, Phys. Rev. **73**, 1025 (1948), Eq. (I. 8).
[28] The author is indebted to Dr. J. H. Shirley for pointing this out to him.
[29] E. Montroll, in *Lectures in Theoretical Physics*, W. E. Brittin, B. W. Downs, and J. Downs, Eds. (Interscience Publishers, Inc., New York, 1961), Vol. III, p. 259, Eq. (XI.6).
[30] See, e.g., R. L. Peterson, Rev. Mod. Phys. **39**, 69 (1967), Eq. (23).

Another kind of differentiation which frequently occurs in quantum physics is the differentiation of an operator by an operator. This may be defined by means of parameter differentiation as follows.[31] Let $H \equiv H(Q_1, Q_2, \cdots, Q_n)$ be a function of the operators $Q_1, Q_2, \cdots, Q_n$ which need not commute with each other. Then the operator derivative with respect to Q_j is defined by

$$\frac{\partial H}{\partial Q_j} \equiv \lim_{\lambda \to 0} \frac{\partial H}{\partial \lambda}(Q_1, \cdots, Q_j + \lambda, \cdots, Q_n). \quad (2.7)$$

From Eqs. (2.1) and (2.7), it follows that

$$\frac{\partial e^{-\beta H}}{\partial Q_j} = -\int_0^\beta du e^{-(\beta-u)H} \frac{\partial H}{\partial Q_j} e^{-uH}. \quad (2.8)$$

The above basic lemma is also clearly valid with λ replaced by Q_j. To obtain a familiar result which we make use of later, let $A = q$, $H = p$, $\lambda = p/i\hbar$, so that $[q, p] = i\hbar = i\hbar\partial p/\partial p$. Then by the lemma,

$$[q, f(p)] = i\hbar \partial f(p)/\partial p. \quad (2.9)$$

Letting $f(p) = e^{-i\mu p/\hbar}$, Eq. (2.9) becomes

$$[q, e^{-i\mu p/\hbar}] = \mu e^{-i\mu p/\hbar}. \quad (2.10)$$

From Eq. (2.10), it follows by a simple standard argument that if $|q'\rangle$ is an eigenstate of q so that $q\,|q'\rangle = q'\,|q'\rangle$, then $e^{-i\mu p/\hbar}$ acts as a displacement operator,[32]

$$e^{-i\mu p/\hbar}\,|q'\rangle = |q' + \mu\rangle. \quad (2.11)$$

3. APPLICATION OF EQ. (2.1) TO EQUILIBRIUM QUANTUM STATISTICS

Equation (2.1) is well suited for applications to equilibrium quantum statistics, where the thermal average of any operator Q is given by

$$\langle Q\rangle = \mathrm{Tr}\,[e^{-\beta\mathcal{H}}Q]/\mathrm{Tr}\,e^{-\beta\mathcal{H}}. \quad (3.1)$$

In Eq. (1), β denotes $(KT)^{-1}$, where K is Boltzmann's constant and T is the absolute temperature. We assume that $\mathcal{H}$ depends upon n parameters λ_i, $\mathcal{H} = \mathcal{H}(\lambda_1, \lambda_2, \cdots, \lambda_n)$, and that Q is independent of λ_i. Then it easily follows that

$$\frac{\partial\langle Q\rangle}{\partial\lambda_i} = -\int_0^\beta du\left\langle e^{u\mathcal{H}} \frac{\partial\mathcal{H}}{\partial\lambda_i} e^{-u\mathcal{H}}Q\right\rangle + \beta\left\langle\frac{\partial\mathcal{H}}{\partial\lambda_i}\right\rangle\langle Q\rangle$$
$$= -\int_0^\beta du\left\langle e^{u\mathcal{H}}\Delta \frac{\partial\mathcal{H}}{\partial\lambda_i} e^{-u\mathcal{H}}\Delta Q\right\rangle, \quad (3.2)$$

where $\Delta Q \equiv Q - \langle Q\rangle$, etc. If we consider the case where the Hamiltonian has a perturbation λV added to an unperturbed part $\mathcal{H}_0$, so that $\mathcal{H} = \mathcal{H}_0 + \lambda V$, then Eq. (3.2) becomes

$$\frac{\partial\langle V\rangle}{\partial\lambda} = -\int_0^\beta du\langle e^{u\mathcal{H}}\Delta V e^{-u\mathcal{H}}\Delta V\rangle. \quad (3.3)$$

Assuming, for notational convenience, discrete energy levels $\mathcal{H}_i$ or $\mathcal{H}_j$, one easily obtains

$$\frac{\partial\langle V\rangle}{\partial\lambda} = -(\mathrm{Tr}\,e^{-\beta\mathcal{H}})^{-1}\sum_{i,j}|\langle i|\,\Delta V\,|j\rangle|^2$$
$$\times \int_0^\beta du \exp(-\beta\mathcal{H}_i + u\mathcal{H}_i - u\mathcal{H}_j), \quad (3.4)$$

which is seen to be nonpositive.[33] This result is the quantum-statistical analog of the well-known result that the second-order perturbation energy of the ground state is always negative. The latter result may be obtained from Eq. (3.4) as a special case by evaluating the integral in Eq. (3.4) and letting β become arbitrarily large.

Another application of Eq. (3.2) is to a system with dipole moment $\mathbf{M}$ subjected to an applied field $\mathbf{E}$, so that it is described by the Hamiltonian

$$\mathcal{H} = \mathcal{H}_0 - \mathbf{M}\cdot\mathbf{E}. \quad (3.5)$$

The field-dependent isothermal static susceptibility tensor $\chi_{\alpha\beta}(\mathbf{E})$ for a sample of unit volume is defined by

$$\chi_{\alpha\beta}(\mathbf{E}) \equiv \partial\langle M_\alpha\rangle/\partial E_\beta, \quad (3.6)$$

where $\alpha, \beta = x, y,$ or z. It follows from Eqs. (2) and (5) that

$$\chi_{\alpha\beta}(\mathbf{E}) = \int_0^\beta du\langle e^{u\mathcal{H}}\Delta M_\beta e^{-u\mathcal{H}}\Delta M_\alpha\rangle,$$

a result given by Kubo for the zero-field case.[34]

Before leaving this section, we note that thermodynamic perturbation theory may be conveniently based upon Eq. (2.1).[35] For lattice-dynamical systems, a diagrammatic analysis may be developed which is topologically the same as the ones given by Cowley for nonequilibrium quantum systems, and by the author for classical thermostatic systems.[36]

4. THE BAKER–CAMPBELL–HAUSDORFF FORMULA AND RELATED IDENTITIES

To derive the BCH formula and for later applications, we prefer to use the form

$$\partial e^Z/\partial\lambda = \int_0^1 dx e^{xZ} Z'(\lambda) e^{-xZ} e^Z \quad (4.1)$$

[31] See, e.g., Louisell, Ref. 3, p. 108, Eqs. (3.34).
[32] See, e.g., Louisell, Ref. 3, Sec. 1.11.

[33] C. Kittel, *Quantum Theory of Solids* (John Wiley & Sons, Inc., New York, 1963), p. 127, Problem 2.
[34] Kubo, Ref. 4, Eq. (2.48).
[35] L. D. Landau and E. M. Lifshitz, *Statistical Physics* (Addison-Wesley Publishing Company, Inc., Reading, Massachusetts, 1958), Chap. 3, Sec. 32, p. 93.
[36] R. A. Cowley, Advan. Phys. **12**, 421 (1963); R. M. Wilcox, Phys. Rev. **139**, A1281 (1965).

obtained from Eq. (2.1) by substituting $Z \equiv Z(\lambda)$ for $-H$, 1 for β, and $1 - x$ for u. We seek to express Z as a power series in λ such that

$$e^Z = e^{\lambda A} e^{\lambda B} \tag{4.2}$$

is identically satisfied. Thus,

$$Z = \sum_{n=1}^{\infty} \lambda^n Z_n, \quad Z'(\lambda) = \sum_{n=1}^{\infty} n\lambda^{n-1} Z_n, \tag{4.3}$$

where the Z_n are to be determined. Note that $Z = 0$ when $\lambda = 0$ as required by Eq. (4.2). Differentiating Eq. (4.2) with respect to λ and multiplying both sides from the right by $e^{-Z} = e^{-\lambda B} e^{-\lambda A}$, one obtains

$$\int_0^1 dx e^{xZ} Z'(\lambda) e^{-xZ} = A + e^{\lambda A} B e^{-\lambda A}. \tag{4.4}$$

The quantity $e^{\lambda A} B e^{-\lambda A}$ is easily expanded by Eq. (2.2) in the form

$$e^{\lambda A} B e^{-\lambda A} = \sum_{j=0}^{\infty} \lambda^j (j!)^{-1} \{A^j, B\}, \tag{4.5}$$

where the repeated commutator bracket is defined inductively by[37]

$$\{A^0, B\} = B, \quad \{A^{n+1}, B\} = [A, \{A^n, B\}]. \tag{4.6}$$

Similarly, since $\int_0^1 x^j\, dx = 1/(j+1)$, Eq. (4.5) implies that

$$\int_0^1 dx e^{xZ} Z' e^{-xZ} = \sum_{k=0}^{\infty} \frac{\{Z^k, Z'\}}{(k+1)!}. \tag{4.7}$$

Substituting Eqs. (4.3), (4.5), and (4.7) into Eq. (4.4), we obtain

$$\sum_{k=0}^{\infty} \left\{ \frac{1}{(k+1)!} \left(\sum_{m=1}^{\infty} \lambda^m Z_m \right)^k, \sum_{n=1}^{\infty} n\lambda^{n-1} Z_n \right\} = A + \sum_{j=0}^{\infty} \lambda^j (j!)^{-1} \{A^j, B\}. \tag{4.8}$$

Since Eq. (8) must be satisfied identically in λ, we equate coefficients of λ^j on the two sides of the equation. For $j = 0$, one obtains

$$Z_1 = A + B. \tag{4.9}$$

For $j = 1$, one obtains

$$\{Z^0, 2Z_2\} + \tfrac{1}{2}\{Z_1, Z_1\} = \{A, B\} \tag{4.10}$$

or

$$Z_2 = \tfrac{1}{2}[A, B]. \tag{4.11}$$

For $j = 2$, one obtains

$$\{Z^0, 3Z_3\} + \tfrac{1}{2}\{Z_1, 2Z_2\} + \tfrac{1}{2}\{Z_2, Z_1\} + \tfrac{1}{6}\{Z_1^2, Z_1\} = \tfrac{1}{2}\{A^2, B\}. \tag{4.12}$$

Equation (12) may be simplified by means of Eqs. (4.6), (4.9), and (4.11) to obtain

$$Z_3 = \tfrac{1}{12}[A, [A, B]] + \tfrac{1}{12}[[A, B], B]. \tag{4.13}$$

The BCH formula to third order is obtained by substituting Eqs. (4.3), (4.9), (4.11), and (4.13) into Eq. (4.2) and setting $\lambda = 1$:

$$e^A e^B = \exp\{A + B + \tfrac{1}{2}[A, B] + \tfrac{1}{12}[A, A, B] + \tfrac{1}{12}[[A, B], B] + \cdots\}. \tag{4.14}$$

The recursion scheme based upon Eq. (4.8) may, in principle, be carried out to arbitrarily high order. Weiss and Maradudin have manually calculated Z out to the fifth order,[6] while Richtmyer and Greenspan have calculated Z out to the tenth order by computer.[38] The expansion is not unique due to the existence of the Jacobi identity

$$[[A, B], C] + [[C, A], B] + [[B, C], A] = 0,$$

the identity

$$[[[A, B], C], D] + [[[B, C], D], A] + [[[C, D], A], B] + [[[D, A], B], C] = [[A, C], [B, D]],$$

and others.

It frequently happens that the commutator of A and B commutes with both A and B. In this case, Eq. (4.14) reduces to

$$e^A e^B = e^{A+B+\frac{1}{2}C} = e^{A+B} e^{\frac{1}{2}C} = e^{\frac{1}{2}C} e^{A+B}, \tag{4.15}$$

where $C \equiv [A, B]$. Equation (4.15) has been derived in various ways and is frequently employed in physical problems.[39] Another form of Eq. (4.15), which has been used by Moyal and by Sudarshan, is[10,40]

$$e^B e^{2A} e^B = e^{2A+2B}. \tag{4.16}$$

Equation (4.16) follows from Eq. (4.15) if one interchanges the order of A and B in Eq. (4.15),

$$e^B e^A = e^{A+B} e^{-\frac{1}{2}C}, \tag{4.17}$$

and then multiplies Eq. (17) by Eq. (15) from the right. Another derivation of Eq. (4.16) has been given by Sudarshan.[40]

To derive the Zassenhaus formula, we set

$$e^{\lambda(A+B)} = e^{\lambda A} e^{\lambda B} e^{\lambda^2 C_2} e^{\lambda^3 C_3} \cdots. \tag{4.18}$$

Differentiating both sides of Eq. (4.18) with respect to λ and multiplying it from the right by

$$e^{-\lambda(A+B)} = \cdots e^{-\lambda^3 C_3} e^{-\lambda^2 C_2} e^{-\lambda B} e^{-\lambda A},$$

[37] Note that our convention for the repeated-commutator bracket is opposite to that of Weiss and Maradudin, Ref. 6.

[38] R. D. Richtmyer and S. Greenspan, Commun. Pure Appl. Math. **18**, 107 (1965); The author is indebted to Dr. Greenspan for a private communication.

[39] A partial list of references includes Refs. 3, 8, 9, 10, 18, 19, 48, 50, 52, and 53.

[40] E. C. G. Sudarshan, in *Brandeis Summer Institute Lectures in Theoretical Physics* (W. A. Benjamin, Inc., New York, 1962), p. 181.

one obtains

$$A + B = A + e^{\lambda A}Be^{-\lambda A} + e^{\lambda A} + e^{\lambda B}(2\lambda C_2)e^{-\lambda B}e^{-\lambda A} + e^{\lambda A}e^{\lambda B}e^{\lambda^2 C_2}(3\lambda^2 C_3)e^{-\lambda^2 C_2}e^{-\lambda B}e^{-\lambda A} + \cdots. \quad (4.19)$$

The quantities $e^{\lambda A}Be^{-\lambda A}$, etc., and again expanded by means of Eq. (4.5) so that Eq. (4.19) becomes

$$0 = \sum_{n=1}^{\infty} \frac{\lambda^n}{n!}\{A^n, B\} + 2\lambda \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} \frac{\lambda^{m+n}}{m!\,n!}\{A^m, B^n, C_2\} + 3\lambda^2 \sum_{k=0}^{\infty}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty} \frac{\lambda^{k+m+2n}}{k!\,m!\,n!}\{A^k, B^m, C_2^n, C_3\} + \cdots. \quad (4.20)$$

The quantities $\{A^n, B\}$ are defined by Eq. (6), while the quantities $\{A^m, B^n, C_2\}$ are defined inductively as

$$\{A^0, B^n, C_2\} = \{B^n, C_2\}, \quad (4.21a)$$

$$\{A^{m+1}, B^n, C_2\} = [A, \{A^m, B^n, C_2\}]. \quad (4.21b)$$

Higher-order repeated-commutator brackets are similarly defined. Clearly the coefficients of λ^j must vanish in Eq. (20). Setting $j = 1$, one obtains

$$C_2 = -\tfrac{1}{2}[A, B]. \quad (4.22)$$

Setting $j = 2$, one obtains

$$0 = \tfrac{1}{2}\{A^2, B\} + 2\{A, B^0, C_2\} + 2\{A^0, B, C_2\} + 3\{A^0, B^0, C_2^0, C_3\}$$

or, upon using Eqs. (4.6), (4.21), and (4.22),

$$C_3 = \tfrac{1}{3}[B, [A, B]] + \tfrac{1}{6}[A, [A, B]]. \quad (4.23)$$

We note that both the BCH formula and the Zassenhaus formula could have been derived a little more simply by repeatedly differentiating Eqs. (4.2) and (4.18), respectively, and setting $\lambda = 0$ after each differentiation. Although Z_n and C_n may be obtained in a recursive manner by this procedure, this method does not manifestly display the general repeated-commutator nature of the expansion. This method has been used by Huang[41] to obtain the first three factors in the Zassenhaus formula. Huang has used the result to treat quantum deviations from the classical limit of the partition function for both a Bose–Einstein and a Fermi–Dirac gas.

5. WEYL'S PRESCRIPTION FOR QUANTIZING A CLASSICAL FUNCTION

Let p, q denote a conjugate pair of canonical variables of classical mechanics, and let P, Q denote the corresponding quantum operators,[42]

$$[Q, P] = i\hbar. \quad (5.1)$$

[41] K. Huang, *Statistical Mechanics* (John Wiley & Sons, Inc., New York, 1963), p. 217, Eq. (10.60).

[42] Only in Sec. 5 do small p and q denote classical variables.

Then, on the basis of group-theoretical considerations, Weyl has proposed that the quantum operator $F(P, Q)$ corresponding to a given classical function $f(p, q)$ be represented by the Fourier integral[43]

$$F(P, Q) = \iint_{-\infty}^{\infty} g(\sigma, \tau)e^{i(\sigma P + \tau Q)}\, d\sigma\, d\tau, \quad (5.2)$$

where $g(\sigma, \tau)$ is the Fourier transform of the classical function $f(p, q)$. The generalization of the Weyl prescription to the case of n independent pairs of canonical variables has been considered by Daughaday and Nigam (DN).[8] In effect, this amounts to interpreting the quantities occurring in Eq. (2) as

$$P = (P_1, P_2, \cdots, P_n),$$
$$\sigma = (\sigma_1, \sigma_2, \cdots, \sigma_n),$$
$$d\sigma = d\sigma_1\, d\sigma_2 \cdots d\sigma_n,$$
$$\sigma P = \sigma_1 P_1 + \sigma_2 P_2 + \cdots + \sigma_u P_u,$$

etc.

By a rather tortuous process, DN obtain the useful result that the quantum function $F(P, Q)$ corresponding to the classical function

$$f(p, q) = p_1^\alpha p_2^\beta \cdots p_u^\gamma \varphi(q_1, q_2, \cdots, q_n)$$

is given by[8]

$$2^{-(\alpha+\beta+\cdots+\gamma)}[\cdots[[\varphi, P_1]_{+\alpha}, P_2]_{+\beta} \cdots P_n]_{+\gamma}, \quad (5.3)$$

where $[\varphi, P_1]_{+\alpha}$ refers to the anticommutator bracket repeated α times. For example,

$$[\varphi, P_1]_{+2} = [\varphi P_1 + P_1\varphi, P_1]_{+1} = \varphi P_1^2 + 2P_1\varphi P_1 + P_1^2\varphi.$$

In DN, Eq. (3) has been used to obtain the quantum Hamiltonian for the case of two charged spinless particles interacting by retarded fields. We show here that Eq. (3) may be derived much more directly with the aid of Eq. (4.16) written in the form

$$e^{i(\sigma P + \tau Q)} = e^{\frac{1}{2}i\sigma P}e^{i\tau Q}e^{\frac{1}{2}i\sigma P}. \quad (5.4)$$

Equation (5.4) is valid, since σP and τQ both commute with their commutator. The Fourier transform of $f(p, q)$, $g(\sigma, \tau)$, is easily found to be given by

$$i^{\alpha+\beta+\cdots+\gamma}\delta^{(\alpha)}(\sigma_1)\delta^{(\beta)}(\sigma_2)\cdots\delta^{(\gamma)}(\sigma_n)u(\tau), \quad (5.5)$$

where, e.g., $\delta^{(\alpha)}(\sigma)$ denotes the αth derivative of the "Dirac δ function" and $u(\tau)$ is the Fourier transform of $\varphi(q)$. One easily obtains Eq. (5.3) by substituting

[43] H. Weyl, *The Theory of Groups and Quantum Mechanics* (E. P. Dutton & Co., Inc., New York, 1931), p. 274.

Eqs. (5.4) and (5.5) into Eq. (5.2), and using the well-known formula of distribution theory,[44]

$$\int_{-\infty}^{\infty} \delta^{(\alpha)}(\sigma')f(\sigma')\,d\sigma' = (-)^{\alpha}f^{(\alpha)}(0).$$

We state without proof some other interesting results involving the Weyl prescription which may be derived with the aid of the BCH formula and the Fourier integral theorem.

Theorem (McCoy[9])*:* Let $F(P, Q)$ be the quantum operator which corresponds to the classical function $f(p, q)$ according to the Weyl prescription, and let $F_Q(P, Q)$ be the function obtained from $F(P, Q)$ by ordering all Q factors to the left of all P factors with the aid of Eq. (5.1). Then $F_Q(P,Q)$ may be obtained by replacing p and q by P and Q with the Q's to the left of the P's in all terms of the power-series expansion of

$$\left[\exp\left(-\tfrac{1}{2}i\hbar\frac{\partial^2}{\partial p\partial q}\right)\right]f(p, q) = f(p, q) - \frac{i\hbar}{2}\frac{\partial^2 f(p, q)}{\partial p\partial q} - \left(\frac{\hbar}{2}\right)^2\frac{1}{2!}\frac{\partial^4 f(p, q)}{\partial p^2\partial q^2} + \cdots. \quad (5.6)$$

In DN, Eq. (5.6) is generalized to the case of more than one degree of freedom, and is used to derive Eq. (5.3).

Theorem (Moyal[10])*:* Let $F(P, Q)$, $G(P, Q)$, and $C(P, Q)$ be defined in the Weyl manner in terms of the classical functions $f(p,q)$, $g(p,q)$, and $c(p,q)$, respectively, and let

$$[F(P, Q), G(P, Q)] = C(P, Q). \quad (5.7)$$

Then

$$c(p, q) = 2i\left[\sin\frac{\hbar}{2}\left(\frac{\partial}{\partial q_1}\frac{\partial}{\partial p_2} - \frac{\partial}{\partial p_1}\frac{\partial}{\partial q_2}\right)\right] \times f(p_1, q_1)g(p_2, q_2), \quad (5.8)$$

evaluated at $p_1 = p_2 = p$ and $q_1 = q_2 = q$.

In the limit as $\hbar \to 0$, this reduces to the well-known relation between the quantum commutator and the classical Poisson bracket. This result and the corresponding law for operator multiplication have been treated by Mehta[45] with the aid of the BCH formula. Moyal's result originated in a paper which formulates quantum mechanics in terms of phase-space distribution functions, and occurs also in Sudarshan's study of the structure of dynamical theories.[40]

Theorem (Wigner[10])*:* Let $G(P, Q)$ be any operator defined in the Weyl manner, and let

$$\langle G\rangle \equiv \langle\psi|\, G(P, Q)\,|\psi\rangle \quad (5.9)$$

be the expectation value of G in the state $|\psi\rangle$. Then $\langle Q\rangle$ may be calculated from the phase-space distribution function $f(p, q)$ by means of

$$\langle G\rangle = \iint dp\, dq g(p, q)f(p, q), \quad (5.10)$$

where

$$f(p, q) \equiv \frac{1}{2\pi}\int \psi^*(q - \tfrac{1}{2}\hbar\tau)e^{-i\tau p}\psi(q + \tfrac{1}{2}\hbar\tau)\,d\tau, \quad (5.11)$$

with $\psi(q) \equiv \langle q \mid \psi\rangle$.

As shown by Moyal,[10] this result may be easily proved with the aid of Eqs. (2.11), (4.16), and the Fourier integral theorem.

6. LIE ALGEBRAIC SIMILARITY TRANSFORMATIONS

In quantum physics, one frequently encounters sets of operators $X_1, X_2, \cdots, X_n$ such that the commutator of any pair is a linear combination of members of the set according to the rule

$$[X_i, X_j] = c_{ij1}X_1 + c_{ij2}X_1 + \cdots + c_{ijn}X_n. \quad (6.1)$$

The X_i's are said to be elements of a Lie algebra, while the c_{ijk} are called the "structure constants" of the algebra.[46] For our purposes here, we do not require any knowledge of this highly abstract and technical subject. The "closure property" expressed by Eq. (6.1) is sufficient. We seek to perform a similarity transformation on X_j of the form $e^Z X_j e^{-Z}$, where Z is a given linear combination of the X_i's,

$$Z \equiv d_1X_1 + d_2X_2 + \cdots + d_nX_n. \quad (6.2)$$

Now from Eqs. (6.1), (6.2), and (2.2) it follows that $e^Z X_j e^{-Z}$ is also a linear combination of the X_i's,

$$e^Z X_j e^{-Z} = \sum_{i=1}^{n} g_{ji}X_i \equiv \mathbf{g}_j \cdot \mathbf{X}. \quad (6.3)$$

From the basic property of a similarity transformation, it then follows that any function of the X_i's, $F \equiv F(X_1, X_2, \cdots, X_n)$, is transformed to

$$e^Z F e^{-Z} = F(\mathbf{g}_1 \cdot \mathbf{X}, \mathbf{g}_2 \cdot \mathbf{X}, \cdots, \mathbf{g}_n \cdot \mathbf{X}). \quad (6.4)$$

Although the g_{ij}'s may in principle be determined from Eqs. (6.1), (6.2), and (2.2), in practice the infinite summation may become very complicated to perform. In this case, a better approach is to introduce a

[44] M. S. Lighthill, *Introduction to Fourier Analysis and Generalized Functions* (Cambridge University Press, Cambridge, England, 1959), p. 19, Eq. (17).

[45] Mehta, Ref. 10.

[46] See, e.g., H. J. Lipkin, *Lie Groups for Pedestrians*, (John Wiley & Sons, Inc., New York, 1965), or Jacobson, Ref. 5.

parameter x into the exponentials and determine the differential equation which $e^{xZ}X_ie^{-xZ}$ must satisfy. It is seen that this procedure generally leads to a coupled set of linear homogeneous first-order differential equations which, as is well known, may be solved as an eigenvalue problem.

The lowest-dimensional Lie algebra of physical interest is the non-Abelian two-dimensional algebra with elements $\{X, Y\}$ satisfying

$$[X, Y] = Y. \tag{6.5}$$

This algebra has been treated by Sack[11] in connection with his "Taylor's Theorem for Shift Operators" and by Wei and Norman.[15] The latter authors have shown that this algebra occurs in two master-equation problems: (a) a system of simple harmonic oscillators with Landau–Teller transition probabilities; (b) the deuterium exchange reaction with only nearest-neighbor transition probabilities. Other realizations of this algebra are known in quantum mechanics. The set $\{q/\mu, e^{-i\mu p/\hbar}\}$ satisfies Eq. (6.5), as may be seen from Eq. (2.10). Some realizations which involve annihilation and creation operators are $\{-a^\dagger a, a\}$, $\{a^\dagger a, a^\dagger\}$, $\{-\gamma aq, a^2\}$, $\{\gamma a^\dagger q, (a^\dagger)^2\}$, $\{\gamma aq, q^2\}$, and $\{-\gamma a^\dagger q, q^2\}$, where $a = \gamma(q + i\omega^{-1}p)$, $a^\dagger = \gamma(q - i\omega^{-1}p)$, $\gamma = (\omega/2\hbar)^{\frac{1}{2}}$, and $[a, a^\dagger] = 1$. This algebra also occurs as a subalgebra of larger Lie algebras. For example, in the algebra SU_3 there are 12 distinct pairs of elements which satisfy Eq. (6.5).[46]

To illustrate the parameterization method alluded to above, let

$$Z = \alpha X + \beta Y, \tag{6.6}$$

$$G = aX + bY, \tag{6.7}$$

$$G(x) = e^{xZ}Ge^{-xZ} \tag{6.8}$$

$$= a(x)X + b(x)Y. \tag{6.9}$$

Then $G(x)$ satisfies the differential equation

$$G'(x) = [Z, G(x)], \tag{6.10}$$

subject to the initial condition

$$G(0) = G. \tag{6.11}$$

Substituting Eqs. (6.6) and (6.9) into Eq. (6.10) and using Eq. (6.5), one finds that

$$a'(x)X + b'(x)Y = [\alpha b(x) - \beta a(x)]Y. \tag{6.12}$$

Since X and Y are independent operators, as is easily proved from Eq. (6.5), we must have

$$a'(x) = 0, \quad b'(x) = \alpha b(x) - \beta a(x) \tag{6.13}$$

subject to the initial condition

$$a(0) = a, \quad b(0) = b. \tag{6.14}$$

The solution of Eqs. (6.13) and (6.14) is easily found to be given by

$$a(x) = a, \quad b(x) = \beta a/\alpha + (b - \beta a/\alpha)e^{\alpha x}. \tag{6.15}$$

From Eqs. (6.6)–(6.9) and (6.15), we then find that

$$e^{\alpha X+\beta Y}(aX + bY)e^{-\alpha X-\beta Y} = aX + [\beta a\alpha^{-1} + (b - \beta a\alpha^{-1})e^{\alpha}]Y. \tag{6.16}$$

Note that it could have been foreseen from Eqs. (2.2) and (6.5) that $a(x) = a$. In future calculations, we make such possible simplifications at the outset without comment. From Eqs. (6.4) and (6.16), it follows that

$$e^{\alpha X+\beta Y}F(X, Y)e^{-\alpha X-\beta Y} = F[X + \beta\alpha^{-1}(1 - e^{\alpha})Y, e^{\alpha}Y]. \tag{6.17}$$

Special cases of Eq. (6.17) are[47]

$$e^{\alpha X}F(X, Y)e^{-\alpha X} = F(X, e^{\alpha}Y), \tag{6.18}$$

$$e^{\beta Y}F(X, Y)e^{-\beta Y} = F(X - \beta Y, Y). \tag{6.19}$$

A frequently occurring three-dimensional Lie algebra is spanned by the operators $\{P, Q, I\}$ with the commutation relations

$$[P, Q] = cI, \quad [P, I] = [Q, I] = 0. \tag{6.20}$$

It is exemplified by the coordinate-momentum or annihilation-creation operator commutation rules. Since all results for this algebra are well known, we do not explicitly derive them here. However, all such results may be obtained as a special case of the four-dimensional Lie algebra which we consider next.

A Lie algebra of interest for harmonic oscillator problems is spanned by the operators $\{P, Q, W \equiv P^2 + Q^2, cI\}$ with the commutation relations defined by Eq. (6.20) and by[15]

$$[W, P] = -2cQ, \quad [W, Q] = 2cP, \quad [W, I] = 0. \tag{6.21}$$

A physical realization of this algebra is provided by the set $\{p, \omega q, p^2 + \omega^2 q^2, -i\hbar\omega I\}$. An alternative and more convenient set to use is $\{W, X, Y, sI\}$, where

$$X = Q - iP, \quad Y = Q + iP,$$
$$W = XY - \tfrac{1}{2}sI, \quad s = 2ic. \tag{6.22}$$

Equations (6.21) and (6.22) imply the commutation relations

$$[W, X] = -sX, \quad [W, Y] = sY, \quad [X, Y] = sI. \tag{6.23}$$

[47] Examples of Eqs. (6.18) and (6.19) occur in Louisell, Ref. 3, Theorems 9 and 6, respectively.

A physical realization of this algebra is provided by the set $\{a^\dagger a, a, a^\dagger, I\}$. Let

$$Z = \gamma W + \delta X + \rho Y, \quad (6.24)$$

$$G = gW + dX + rY, \quad (6.25)$$

and let $G(x)$ be defined by Eq. (6.8). Then Eqs. (6.10) and (6.11) are again satisfied. Letting

$$G(x) = gW + d(x)X + r(x)Y + u(x)I,$$

one finds the differential equations

$$d'(x) = -s\gamma\, d(x) + s\delta g,$$
$$r'(x) = s\gamma r(x) - s\rho g,$$
$$u'(x) = s\delta r(x) - s\rho\, d(x),$$

subject to $d(0) = d$, $r(0) = r$, and $u(0) = 0$. The solution is easily found to be given by

$$d(x) = g\delta\gamma^{-1} + (d - g\delta\gamma^{-1})e^{-s\gamma x},$$
$$r(x) = g\rho\gamma^{-1} + (r - g\rho\gamma^{-1})e^{s\gamma x},$$
$$u(x) = \delta\gamma^{-1}(r - g\rho\gamma^{-1})(e^{s\gamma x} - 1) + \rho\gamma^{-1}(d - g\delta\gamma^{-1})(e^{-s\gamma x} - 1). \quad (6.26)$$

From Eqs. (6.4), (6.8), (6.24), (6.25), and (6.26), one finds

$$e^{Z}F(X, Y)e^{-Z} = F(U, V), \quad (6.27)$$

where

$$U = e^{-s\gamma}X + \rho\gamma^{-1}(e^{-s\gamma} - 1)I, \quad (6.28a)$$

$$V = e^{s\gamma}Y + \delta\gamma^{-1}(e^{s\gamma} - 1)I. \quad (6.28b)$$

Expressed in terms of Q and P by Eqs. (6.22), one finds, with $Z = \alpha P + \beta Q + \gamma W$,

$$e^{Z}F(P, Q)e^{-Z} = F(R, S), \quad (6.29)$$

where

$$R = P\cos 2c\gamma + Q\sin 2c\gamma - \tfrac{1}{2}I\gamma^{-1}[\alpha(1 - \cos 2c\gamma) - \beta\sin 2c\gamma], \quad (6.30a)$$

$$S = -P\sin 2c\gamma + Q\cos 2c\gamma - \tfrac{1}{2}I\gamma^{-1}[\alpha\sin 2c\gamma + \beta(1 - \cos 2c\gamma)]. \quad (6.30b)$$

Another well-known Lie algebra is that of the angular momentum operators (or rotation generators) $\{J_x, J_y, J_z\}$, where

$$[J_x, J_y] = iJ_z, \quad [J_y, J_z] = iJ_x, \quad [J_z, J_y] = iJ_x. \quad (6.31)$$

(We use units in which $\hbar = 1$.) Let

$$\mathbf{b}(x)\cdot\mathbf{J} \equiv b_x(x)J_x + b_y(x)J_y + b_z(x)J_z = e^{-ix\mathbf{a}\cdot\mathbf{J}}(\mathbf{b}\cdot\mathbf{J})e^{ix\mathbf{a}\cdot\mathbf{J}}, \quad (6.32)$$

where a and b are constant vectors. Then

$$\mathbf{b}'(x)\cdot\mathbf{J} = -i[\mathbf{a}\cdot\mathbf{J}, \mathbf{b}(x)\cdot\mathbf{J}] = [\mathbf{a}\times\mathbf{b}(x)]\cdot\mathbf{J}.$$

Hence $\mathbf{b}'(x) = \mathbf{a}\times\mathbf{b}(x)$ subject to $\mathbf{b}(0) = \mathbf{b}$. The solution is easily found to be given by

$$\mathbf{b}(x) = (\hat{a}\cdot\mathbf{b})\hat{a}(1 - \cos ax) + \mathbf{b}\cos ax + \hat{a}\times\mathbf{b}\sin ax, \quad (6.33)$$

where $a \equiv |\mathbf{a}|$ and $\hat{a} = \mathbf{a}/a$. Hence

$$e^{-i\mathbf{a}\cdot\mathbf{J}}F(J_x, J_y, J_z)e^{-i\mathbf{a}\cdot\mathbf{J}} = F(K_x, K_y, K_z), \quad (6.34)$$

where

$$\mathbf{K} = \hat{a}(\hat{a}\cdot\mathbf{J})(1 - \cos a) + \mathbf{J}\cos a + \mathbf{J}\times\hat{a}\sin a. \quad (6.35)$$

Equations (6.34) and (6.35) specify how a general operator function of J must transform under an arbitrary rotation of the coordinate axes characterized by the vector $\mathbf{a}$. An interesting special case is where $a_x = a$ and $a_y = a_z = 0$. Then Eqs. (6.34) and (6.35) reduce to[48]

$$\exp(-iaJ_x)F(J_x, J_y, J_z)\exp(iaJ_x) = F(J_x, J_y\cos a + J_z\sin a, J_z\cos a - J_y\sin a). \quad (6.36)$$

Another three-dimensional Lie algebra of wide interest is the "split three-dimensional simple algebra" characterized by[15]

$$[E, F] = H, \quad [E, H] = 2E, \quad [F, H] = -2F. \quad (6.37)$$

A physical realization of the set $\{E, F, H\}$ is given by $\{iJ_-, iJ_+, 2J_z\}$, where J_+ and J_- are the angular momentum raising and lowering operators, respectively, $J_+ \equiv J_x + iJ_y$, $J_- \equiv J_x - iJ_y$. These operators occur, not only for ordinary spin, but also for isotopic spin and for quasi-spin in many-fermion systems.[49] Another guise in which these operators occur is where

$$J_- = c^\dagger b, \quad J_+ = b^\dagger c, \quad J_z = \tfrac{1}{2}(b^\dagger b - c^\dagger c), \quad (6.38)$$

and $b^\dagger$, $c^\dagger$, b, and c are the creation and annihilation operators of a two-dimensional harmonic oscillator,

$$[b, b^\dagger] = [c, c^\dagger] = 1, \quad [b, c] = [b, c^\dagger] = 0. \quad (6.39)$$

Another physical realization of the set $\{E, F, H\}$ is given by $\{P^2/2c, Q^2/2c, (QP + PQ)/2c\}$, where $[P, Q] = cI$.[15] Let

$$Z = \alpha E + \beta F + \gamma H, \quad G = aE + bF + gH, \quad (6.40)$$

and let $G(x)$ once more be defined by Eq. (8). Letting

$$G(x) = a(x)E + b(x)F + g(x)H, \quad (6.41)$$

[48] Special cases of Eq. (6.36) are as follows: A. Messiah, *Quantum Mechanics* (John Wiley & Sons, Inc., New York, 1962), Vol. II, p. 578, Ex. 8; C. P. Slichter, *Principles of Magnetic Resonance* (Harper and Row, Inc., New York, 1963), p. 26, Eq. (13).

[49] See, e.g., Schwinger, Ref. 17; Heffner and Louisell, Ref. 16; Messiah, Ref. 48; Lipkin, Ref. 46.

one finds the coupled equations

$$\begin{aligned} a'(x) &= -2\gamma a(x) + 2\alpha g(x), \\ b'(x) &= 2\gamma b(x) - 2\beta g(x), \\ g'(x) &= -\beta a(x) + \alpha b(x). \end{aligned} \quad (6.42)$$

The solution of Eqs. (6.42) subject to $a(0) = a$, $b(0) = b$, $g(0) = g$, is found to be given by

$$a(x) = (a\beta + b\alpha - 2g\gamma)\alpha\rho^{-2}\sinh^2\rho x + a\cosh 2\rho x + (g\alpha - a\gamma)\rho^{-1}\sinh 2\rho x,$$

$$b(x) = (a\beta + b\alpha - 2g\gamma)\beta\rho^{-2}\sinh^2\rho x + b\cosh 2\rho x + (b\gamma - g\beta)\rho^{-1}\sinh 2\rho x,$$

$$g(x) = (a\beta\gamma + b\alpha\gamma - 2g\alpha\beta)\rho^{-2}\sinh^2\rho x + g + \tfrac{1}{2}(b\alpha - a\beta)\rho^{-1}\sinh 2\rho x,$$

where

$$\rho \equiv [\gamma^2 - \alpha\beta]^{\frac{1}{2}}.$$

Thus, with Z given by Eq. (40), one finds

$$e^Z f(E, F, H)e^{-Z} = f(J, K, L), \quad (6.43)$$

where J, K, and L are defined as

$$\begin{aligned} J &\equiv u(\alpha, \beta, \gamma)E + \beta^2 wF + v(\alpha, \beta, \gamma)H, \\ K &\equiv \alpha^2 wE + u(\alpha, \beta, -\gamma)F - v(\beta, \alpha, -\gamma)H, \\ L &\equiv -2v(\beta, \alpha, \gamma)E + 2v(\alpha, \beta, -\gamma)F + (1 - 2\alpha\beta w)H, \end{aligned} \quad (6.44)$$

$$\begin{aligned} w &\equiv \rho^{-2}\sinh^2\rho, \\ u(\alpha, \beta, \gamma) &\equiv \cosh 2\rho + \alpha\beta w - \gamma\rho^{-1}\sinh 2\rho, \\ v(\alpha, \beta, \gamma) &\equiv \beta\gamma w - \tfrac{1}{2}\beta\rho^{-1}\sinh 2\rho. \end{aligned} \quad (6.45)$$

In case $\gamma = 0$, w, u, and v simplify to

$$\begin{aligned} w &= (\alpha\beta)^{-1}\sin^2(\alpha\beta)^{\frac{1}{2}}, \\ u(\alpha, \beta, 0) &= \cos^2(\alpha\beta)^{\frac{1}{2}}, \\ v(\alpha, \beta, 0) &= -\tfrac{1}{2}(\beta/\alpha)^{\frac{1}{2}}\sin 2(\alpha\beta)^{\frac{1}{2}}. \end{aligned} \quad (6.46)$$

Some other special cases,

$$\begin{aligned} e^{\alpha E}f(E, F, H)e^{-\alpha E} &= f(E, F + \alpha H + \alpha^2 E, H + 2\alpha E), \\ e^{\beta F}f(E, F, H)e^{-\beta F} &= f(E - \beta H + \beta^2 F, F, H - 2\beta F), \\ e^{\gamma H}f(E, F, H)e^{-\gamma H} &= f(e^{-2\gamma}E, e^{2\gamma}F, H), \end{aligned} \quad (6.47)$$

may also be easily obtained directly from the commutator expansion, Eq. (6.22).

Consider now the six-dimensional Lie algebra whose elements are I, P, Q, P^2, QP, and Q^2, with $[P, Q] = cI$. The most general second-degree polynomial in P and Q is a linear combination of these elements. Let

$$Z = \alpha P^2 + \beta Q^2 + \gamma QP + \delta P + \epsilon Q, \quad (6.48)$$

and let

$$e^{xZ}Pe^{-xZ} = d(x)P + e(x)Q + f(x)I. \quad (6.49)$$

Then $d \equiv d(x)$, $e \equiv e(x)$, and $f \equiv f(x)$ satisfy

$$d' = 2c\alpha e - c\gamma d, \quad e' = c\gamma e - 2c\beta d, \quad f' = c\delta e - c\epsilon d,$$

subject to $d(0) = 1$, $e(0) = f(0) = 0$. The solution is given by

$$\begin{aligned} d(x) &= \cosh\lambda x - \gamma c\lambda^{-1}\sinh\lambda x, \\ e(x) &= -2\beta c\lambda^{-1}\sinh\lambda x, \\ f(x) &= -\epsilon c\lambda^{-1}\sinh\lambda x + (c/\lambda)^2(\epsilon\gamma - 2\beta\delta)(\cosh\lambda x - 1), \end{aligned} \quad (6.50)$$

where

$$\lambda \equiv c[\gamma^2 - 4\alpha\beta]^{\frac{1}{2}}. \quad (6.51)$$

The expression for $e^{xZ}Qe^{-xZ}$ may be obtained from Eqs. (6.49) and (6.50) by making the following substitutions:

$$P \rightleftarrows Q, \quad C \to -c, \quad \alpha \rightleftarrows \beta, \quad \delta \rightleftarrows \epsilon.$$

We conclude this section by considering an infinite-dimensional Lie algebra. This set, which occurs in the work of Kermack and McCrea,[19] consists of P and all functions of Q, where $[P, Q] = cI$. Clearly this set satisfies the closure condition since $[P, \varphi(Q)] = c\varphi'(Q)$ is in the set. Let $\varphi(Q)$ and $f(Q)$ be arbitrary functions, and let

$$(\exp\{x[\alpha P + \varphi(Q)]\})[\beta P + f(Q)] \times (\exp\{-x[\alpha P + \varphi(Q)]\}) \equiv \beta P + F(Q, x), \quad (6.52)$$

where α, β, and x are parameters. Then $F(Q, x)$ must satisfy the differential equation

$$\begin{aligned} \partial F(Q, x)/\partial x &= [\alpha P + \varphi(Q), \beta P + F(Q, x)] \\ &= \alpha c\,\partial F(Q, x)/\partial Q - \beta c\varphi'(Q), \end{aligned} \quad (6.53)$$

subject to the condition that $F(Q, 0) = f(Q)$. The solution is easily found to be given by

$$F(Q, x) = f(Q + \alpha cx) - \beta\alpha^{-1}[\varphi(Q + \alpha cx) - \varphi(Q)]. \quad (6.54)$$

Three special cases of interest are obtained by letting $f(Q)$, β, and α, respectively, go to zero:

$$(\exp\{x[P + \varphi(Q)]\})P(\exp\{-x[P + \varphi(Q)]\}) = P - \varphi(Q + cx) + \varphi(Q), \quad (6.55)$$

$$(\exp\{x[P + \varphi(Q)]\})f(Q)(\exp\{-x[P + \varphi(Q)]\}) = f(Q + cx), \quad (6.56)$$

$$e^{\varphi(Q)}Pe^{-\varphi(Q)} = P - c\varphi'(Q). \quad (6.57)$$

7. PRODUCT OF LIE EXPONENTIALS

Let A and B be LCLE's and let $e^A e^B = e^Z$. Then from the BCH formula, Eq. (4.14), and the "closure property," Eq. (6.1), it follows that Z is also a LCLE. In this section, we determine the form of Z, given A and B, for some of the Lie algebras introduced in the previous section. We parametrize the problem by setting

$$e^Z \equiv e^{Z(\lambda)} = e^{\lambda A} e^B, \quad (7.1)$$

subject to $Z(0) = B$. Then differentiating Eq. (7.1) with respect to λ by means of Eq. (4.1) and multiplying from the right by $e^{-Z} = e^{-B}e^{-\lambda A}$, one obtains

$$\int_0^1 dx e^{xZ} Z'(\lambda) e^{-xZ} = A. \quad (7.2)$$

We again consider first the non-Abelian two-dimensional Lie algebra of Eq. (6.5), $[X, Y] = Y$. Let $A = \alpha_1 X + \beta_1 Y$, $B = \alpha_2 X + \beta_2 Y$, and $Z(\lambda) = \alpha X + \beta(\lambda) Y$, where $\alpha = \alpha_2 + \lambda\alpha_1$ and $\beta(0) = \beta_2$. From Eq. (6.16), the quantity $e^{xZ}Z'(\lambda)e^{-xZ}$ is seen to be given by

$$\alpha_1 X + [\beta\alpha_1\alpha^{-1} + (\beta' - \beta\alpha_1\alpha^{-1})e^{\alpha x}]Y.$$

Then integrating over x in Eq. (7.2) and equating coefficients of Y, one finds that $\beta(\lambda)$ satisfies

$$\alpha_1\beta\alpha^{-1} + (\beta' - \alpha_1\beta\alpha^{-1})\alpha^{-1}(e^\alpha - 1) = \beta_1. \quad (7.3)$$

Defining $u \equiv u(\lambda) = \beta\alpha^{-1}$, Eq. (7.3) becomes

$$(\beta_1 - \alpha_1 u)^{-1}u' = (e^\alpha - 1)^{-1} = e^{-\alpha}(1 - e^{-\alpha})^{-1}, \quad (7.4)$$

which may also be written

$$-\partial[\ln(\alpha_1 u - \beta_1)]/\partial\lambda = \partial[\ln(1 - e^{-\alpha})]/\partial\lambda. \quad (7.5)$$

Integrating Eq. (7.5) and solving for $\beta(\lambda)$, one obtains

$$\beta(\lambda) = \lambda\beta_1\varphi(\lambda\alpha_1, \alpha_2) + \beta_2\varphi(-\alpha_2, -\lambda\alpha_1), \quad (7.6)$$

where

$$\varphi(x, y) \equiv (1 + x^{-1}y)(e^x - 1)(e^{x+y} - 1)^{-1}. \quad (7.7)$$

Hence

$$[\exp(\alpha_1 X + \beta_1 Y)][\exp(\alpha_2 X + \beta_2 Y)] = \exp[(\alpha_1 + \alpha_2)X + \beta(1)Y], \quad (7.8)$$

where $\beta(1)$ is obtained by setting $\lambda = 1$ in Eq. (7.6).

Some special cases of Eq. (7.8) have been derived by Sack by means of his "Taylor's Theorem for Shift Operators" [11]:

$$\exp[\alpha(X + \lambda Y)] = e^{\alpha X}\exp[\lambda(1 - e^{-\alpha})Y] = \{\exp[\lambda(e^\alpha - 1)Y]\}e^{\alpha X}. \quad (7.9)$$

Sack has applied Eqs. (7.9) to the last four realizations of this algebra listed above Eq. (6.6) in order to obtain a formula for the matrix elements of a Gaussian potential.[50]

[50] Sack, Ref. 11. Matrix elements for generalized Gaussian potentials and other potentials which may be represented as Fourier integrals are obtained in R. M. Wilcox, J. Chem. Phys. **45**, 3312 (1966).

Next, consider the four-dimensional Lie algebra defined by Eqs. (6.23). Let $A = \gamma_1 W + \delta_1 X + \rho_1 Y$, $B = \gamma_2 W + \delta_2 X + \rho_2 Y$, and $Z(\lambda) = \gamma W + \delta(\lambda) X + \rho(\lambda) Y + \sigma(\lambda) I$, where $\gamma = \gamma_2 + \lambda\gamma_1$, $\delta(0) = \delta_2$, $\rho(0) = \rho_2$, and $\sigma(0) = 0$. Then from Eqs. (7.2) and (6.26) one finds, after integrating over x and equating coefficients of X, Y, and I, respectively,

$$\gamma_1\delta\gamma^{-1} + (\delta' - \gamma_1\delta\gamma^{-1})(-\gamma s)^{-1}(e^{-\gamma s} - 1) = \delta_1, \quad (7.10a)$$

$$\gamma_1\rho\gamma^{-1} + (\rho' - \gamma_1\rho\gamma^{-1})(\gamma s)^{-1}(e^{\gamma s} - 1) = \rho_1, \quad (7.10b)$$

$$\sigma' + \delta\gamma^{-1}(\rho' - \gamma_1\rho\gamma^{-1})[(\gamma s)^{-1}(e^{\gamma s} - 1) - 1] + \rho\gamma^{-1}(\delta' - \gamma_1\delta\gamma^{-1})[(-\gamma s)^{-1}(e^{-\gamma s} - 1) - 1] = 0. \quad (7.10c)$$

Equations (7.10a) and (7.10b) are of the same form as Eq. (7.3), so that their solutions may be obtained from Eq. (7.6) by appropriate changes of variables:

$$\delta(\lambda) = \lambda\delta_1\varphi(-\lambda\gamma_1 s, -\gamma_2 s) + \delta_2\varphi(\gamma_2 s, \lambda\gamma_1 s), \quad (7.11)$$

$$\rho(\lambda) = \lambda\rho_1\varphi(\lambda\gamma_1 s, \gamma_2 s) + \rho_2(-\gamma_2 s, -\lambda\gamma_1 s). \quad (7.12)$$

From Eqs. (7.10a), (7.10b), and (7.10c), one finds that

$$\sigma'(\lambda) = \gamma^{-1}[\partial(\rho\delta)/\partial\lambda - \rho_1\delta - \delta_1\rho]. \quad (7.13)$$

Equation (7.13) is integrated with the aid of Eqs. (7.11) and (7.12) by putting the terms in a form similar to the right side of Eq. (7.5). Setting

$$\tau_1 = \rho_1/\gamma_1, \quad \tau_2 = \rho_2/\gamma_2, \quad \mu_1 = \delta_1/\gamma_1, \quad \mu_2 = \delta_2/\gamma_2, \quad (7.14)$$

one obtains finally

$$\sigma(1) = (\gamma_1 + \gamma_2)^{-1}\rho(1)\delta(1) - \gamma_1\tau_1\mu_1 - \gamma_2\tau_2\mu_2 + \theta, \quad (7.15)$$

where

$$\theta \equiv 2s^{-1}(\tau_1 - \tau_2)(\mu_1 - \mu_2)\sinh(\tfrac{1}{2}s\gamma_1) \times \sinh(\tfrac{1}{2}s\gamma_2)\operatorname{csch}[\tfrac{1}{2}s(\gamma_1 + \gamma_2)]. \quad (7.16)$$

This result may be stated in terms of the X and Y operators as follows: Let $[X, Y] = sI$. Then the equation

$$\exp[\gamma_1(X + \tau_1 I)(Y + \mu_1 I)]\exp[\gamma_2(X + \tau_2 I)(Y + \mu_2 I)] = \exp[(\gamma_1 + \gamma_2)(X + \tau I)(Y + \mu I) + \theta I] \quad (7.17)$$

is identically satisfied provided θ is defined by Eq. (7.16), and provided τ and μ are defined by

$$\tau \equiv \tau_1\psi(\gamma_1, \gamma_2) + \tau_2\psi(-\gamma_2, -\gamma_1), \quad (7.18)$$

$$\mu \equiv \mu_1\psi(-\gamma_1, -\gamma_2) + \mu_2\psi(\gamma_2, \gamma_1), \quad (7.19)$$

where $\psi(x, y)$ is defined by

$$\psi(x, y) \equiv [e^{sx} - 1][e^{s(x+y)} - 1]^{-1}. \quad (7.20)$$

The result may alternatively be stated in terms of the P and Q operators: Let $[P, Q] = cI$. Then the equation

$$\exp\{\gamma_1[(P+\nu_1 I)^2 + (Q+\omega_1 I)^2]\} \times \exp\{\gamma_2[(P+\nu_2 I)^2 + (Q+\omega_2 I)^2]\} = \exp\{(\gamma_1+\gamma_2)[(P+\nu I)^2 + (Q+\omega I)^2] + \theta I\} \quad (7.21)$$

is identically satisfied provided

$$\theta \equiv c^{-1}[(\nu_1+\nu_2)^2 + (\omega_1-\omega_2)^2]\lambda(\gamma_1,\gamma_2), \quad (7.22)$$

$$\nu \equiv \nu_1\chi(\gamma_1,\gamma_2) + \nu_2\chi(\gamma_2,\gamma_1) + (\omega_2-\omega_1)\lambda(\gamma_1,\gamma_2), \quad (7.23)$$

$$\omega \equiv \omega_1\chi(\gamma_1,\gamma_2) + \omega_2\chi(\gamma_2,\gamma_1) + (\nu_1-\nu_2)\lambda(\gamma_1,\gamma_2), \quad (7.24)$$

where

$$\chi(x,y) \equiv \sin(cx)\cos(cy)\csc[c(x+y)], \quad (7.25)$$

$$\lambda(x,y) \equiv \sin(cx)\sin(cy)\csc[c(x+y)]. \quad (7.26)$$

Some special cases of Eqs. (7.17) and (7.21) are of interest:

$$\ln[\exp(\alpha X+\beta Y)\exp(\gamma XY)] = \gamma[X+\beta s(e^{s\gamma}-1)^{-1}][Y+\alpha s(1-e^{-s\gamma})^{-1}] - \tfrac{1}{2}\alpha\beta s\coth(\tfrac{1}{2}s\gamma), \quad (7.27)$$

$$\ln[\exp\gamma(Q^2+P^2)\exp(\alpha P+\beta Q)] = \gamma\{P+\tfrac{1}{2}c[\alpha\cot(\gamma c)+\beta]\}^2 + \gamma\{Q+\tfrac{1}{2}c[\beta\cot(\gamma c)-\alpha]\}^2 - \tfrac{1}{4}(\alpha^2+\beta^2)c\cot(\gamma c). \quad (7.28)$$

Equation (7.28) with $\gamma = 1$ has been obtained by Weiss and Maradudin,[6] who derive the result directly from the BCH formula by a rather intricate summation procedure.

As an easy application of Eq. (7.28), we state a corollary to Bloch's theorem concerning the characteristic function of a harmonic oscillator in thermal equilibrium.[12]

Theorem: Let the thermal average be defined by Eq. (3.1) with $\mathcal{H} = \frac{1}{2}p^2 + \frac{1}{2}\omega^2 q^2$ and $[q, p] = i\hbar$. Then

$$\langle e^{i(\sigma p+\tau q)}\rangle = e^{-\frac{1}{2}\tau^2\langle q^2\rangle} e^{-\frac{1}{2}\sigma^2\langle p^2\rangle}, \quad (7.29)$$

where

$$\langle p^2\rangle = \omega^2\langle q^2\rangle = \tfrac{1}{2}\hbar\omega\coth(\tfrac{1}{2}\beta\hbar\omega).$$

By means of Eq. (5.2), this result may be used to obtain thermal averages for general observables represented in the Weyl manner.[51] Related corollaries to Bloch's theorem have occurred in connection with the scattering of x rays or neutrons by molecules or harmonic lattices,[52] as well as in treatments of the coherent states of the radiation field.[53]

We conclude this section by treating a special case of the infinite-dimensional Lie algebra whose elements are P and all functions of Q, where $[P, Q] = cI$. We seek to find a function $Z \equiv Z(Q, \lambda)$ which satisfies

$$e^Z = e^{\lambda A}e^{-\lambda P}, \quad (7.30)$$

where $A \equiv P + \varphi(Q)$ and $\varphi(Q)$ is an arbitrary given function. Then by differentiating Eq. (7.30) with respect to λ, multiplying both sides from the right by $e^{-Z} = e^{\lambda P}e^{-\lambda A}$, and applying Eq. (6.55), one finds, after some cancellations, that

$$\partial Z/\partial\lambda = \varphi(Q + c\lambda). \quad (7.31)$$

Since Z must vanish when λ does,

$$Z(Q,\lambda) = \int_0^\lambda dx\,\varphi(Q+cx). \quad (7.32)$$

From Eqs. (7.32) and (7.30), one obtains

$$\exp\{\lambda[P+\varphi(Q)]\} = \left[\exp\int_0^\lambda dx\,\varphi(Q+cx)\right]e^{\lambda P}. \quad (7.33)$$

This result is used in Sec. 10 to obtain a normal-ordering expansion of Kermack and McCrea, Eqs. (10.42).

8. SOLUTIONS OF $dY(t)/dt = A(t)Y(t)$

The operator differential-equation system

$$dY(t)/dt = A(t)Y(t), \quad Y(0) = I \quad (8.1)$$

has been extensively studied by mathematicians because of its relevance to the theory of coupled or higher-order ordinary differential equations. Some examples of this equation which occur in quantum physics are the equation of motion for the time-evolution operator, Eq. (9.3), the Bloch equation, $-\partial e^{-\beta\mathcal{H}}/\partial\beta = \mathcal{H}e^{-\beta}$, and master or rate equations.

8.1. Expansions of Magnus and Fer

Instead of dealing with Eq. (8.1) directly, we introduce the iteration parameter λ as

$$dY_\lambda(t)/dt = \lambda A(t)Y_\lambda(t), \quad Y_\lambda(0) = I, \quad (8.1_\lambda)$$

and seek to join $Y_0(t) = I$ to $Y_1(t) \equiv Y(t)$. To derive

[51] Equation (29) may also be derived easily from the condition that both sides satisfy the same first-order differential equation with respect to a parameter. Still another derivation of Eq. (29) is obtained by first calculating the matrix elements of $\exp(i\sigma p + i\tau q)$ in the harmonic oscillator representation (as one may do by employing the method which the author used in Ref. 50 for the case where $\sigma = 0$) and then carrying out the trace sum with the aid of the generating function for the Laguerre polynomials.

[52] A. C. Zemach and R. J. Glauber, Phys. Rev. **101**, 118 (1956); Weiss and Maradudin, Ref. 6; A. A. Maradudin, E. W. Montroll, and G. H. Weiss, Solid State Phys. Suppl. **3**, 239 (1963); N. D. Mermin, J. Math. Phys. **7**, 1038 (1966).

[53] R. J. Glauber, Phys. Rev. **131**, 2766 (1963); Louisell, Ref. 3, p. 244.

the Magnus formula, we assume a solution of the form

$$Y_\lambda(t) = \exp[\Omega(\lambda, t)] \equiv e^{\Omega}, \tag{8.2}$$

where

$$\Omega(\lambda, t) \equiv \sum_{n=1}^{\infty} \lambda^n \Delta_n(t). \tag{8.3}$$

From Eqs. (8.1_λ), (8.2), and (4.1), it follows that

$$\int_0^1 dx e^{x\Omega} \dot{\Omega} e^{-x\Omega} = \lambda A(t), \tag{8.4}$$

where $\dot{\Omega} \equiv \partial\Omega(\lambda, t)/\partial t$. Using the commutator expansion and integrating over x, as in Eq. (4.7), and substituting in Eq. (8.3), one obtains

$$\left\{\sum_{k=0}^{\infty} \frac{1}{(k+1)!}\left(\sum_{n=1}^{\infty} \lambda^n \Delta_n(t)\right)^k, \sum_{m=1}^{\infty} \lambda^m \dot{\Delta}_m(t)\right\} = \lambda A(t). \tag{8.5}$$

A recursive procedure again results from equating coefficients of λ^j on the two sides of Eq. (8.5). For $j = 1$, one obtains $\dot{\Delta}_1(t) = A(t)$. Hence,

$$\Delta_1(t) = \int_0^t A(\tau)\, d\tau. \tag{8.6}$$

For $j = 2$ one obtains

$$\dot{\Delta}_2(t) + \tfrac{1}{2}[\Delta_1(t), \dot{\Delta}_1(t)] = 0.$$

Hence,

$$\Delta_2(t) = \frac{1}{2}\int_0^t d\sigma \int_0^\sigma d\tau [A(\sigma), A(\tau)]. \tag{8.7}$$

For $j = 3$ one obtains

$$\dot{\Delta}_3 + \tfrac{1}{2}[\Delta_1, \dot{\Delta}_2] + \tfrac{1}{2}[\Delta_2, \dot{\Delta}_1] + \tfrac{1}{6}[\Delta_1, [\Delta_1, \dot{\Delta}_1]] = 0.$$

After carrying out the integration and putting the results in "time-ordered" form, one obtains

$$\Delta_3(t) = \frac{1}{6}\int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 \times \{[[A_1, A_2], A_3] + [[A_3, A_2], A_1]\}, \tag{8.8}$$

where $A_1 \equiv A(t_1)$, etc. The fourth-order term is similarly calculated. We find

$$\Delta_4(t) = \frac{1}{12}\int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 \int_0^{t_3} dt_4 \times \{[[[A_3, A_2], A_4], A_1] + [[[A_3, A_4], A_2], A_1] + [[[A_1, A_2], A_3], A_4] + [[[A_4, A_1], A_3], A_2]\}. \tag{8.9}$$

The solution of Eqs. (8.1) to fourth order is given by Eqs. (8.2), (8.3), and (8.6)–(8.9) with $\lambda = 1$.[54] This result is said to be the continuous analog of the BCH formula.

We now derive the Fer formula,[13] which may be said to be the continuous analog of the Zassenhaus formula. Let the solutions of Eqs. (8.1_λ) be given by

$$Y_\lambda(t) = e^{\lambda S_1} e^{\lambda^2 S_2} e^{\lambda^3 S_3} \cdots, \tag{8.10}$$

where $S_1 \equiv S_1(t)$, etc. Substituting Eq. (8.10) into (8.1_λ), multiplying from the right by

$$e^{-\lambda^3 S_3} e^{-\lambda^2 S_2} e^{-\lambda S_1} = [Y_\lambda(t)]^{-1},$$

and expanding in terms of repeated commutators as in Eq. (4.20), one obtains

$$\sum_{n=0}^{\infty} \frac{\lambda^{n+1}}{(n+1)!}\{S_1^n, \dot{S}_1\} + \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} \frac{\lambda^{m+2n+2}}{m!\,(n+1)!} \times \{S_1^m, S_2^n, \dot{S}_2\} + \sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\sum_{k=0}^{\infty} \frac{\lambda^{m+2n+3k+3}}{m!\,n!\,(k+1)!} \times \{S_1^m, S_2^n, S_3^k, \dot{S}_3\} + \cdots = \lambda A(t), \tag{8.11}$$

where the repeated commutators are again defined by Eqs. (4.21). The recursion scheme based upon Eq. (8.11) leads to

$$S_1(t) = \int_0^t A(\tau)\, d\tau, \tag{8.12}$$

$$S_2(t) = \frac{1}{2}\int_0^t d\sigma \int_0^\sigma d\tau [A(\sigma), A(\tau)], \tag{8.13}$$

$$S_3(t) = \frac{1}{3}\int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 \times \{[A_2, [A_3, A_1]] + [A_3, [A_2, A_1]]\}. \tag{8.14}$$

Equations (8.10), (8.12), (8.13), and (8.14), with $\lambda = 1$, give the first three factors in the infinite-product solution to Eqs. (8.1). The paper by Fer discusses the convergence of the infinite product and derives recursion relations, but does not obtain explicit expressions for the S_j's.[13]

$$A(t) \equiv e^{-at} b e^{at}, \quad Y_\lambda(t) \equiv e^{-at} U(t), \tag{8.15}$$

where a and b are independent of t. Then $U(t)$ must satisfy

$$dU(t)/dt = (a + \lambda b) U(t), \quad U(0) = I, \tag{8.16}$$

which implies that

$$U(t) = e^{(a+\lambda b)t}. \tag{8.17}$$

Kumar's expansion for $e^{(a+\lambda b)t}$ as an infinite product is given by[14]

$$e^{(a+\lambda b)t} = e^{at} Y_\lambda(t), \tag{8.18}$$

where $Y_\lambda(t)$ is given by Eqs. (8.10), (8.12), (8.13), (8.14), $\cdots$, and (8.15). An alternative expansion for $e^{(a+\lambda b)t}$ as a product of only two exponentials may

[54] Magnus, Ref. 7, and Weiss and Maradudin, Ref. 6, have carried out the calculation to third order. Their third-order terms, though not given in such a symmetrical form, may be shown to be equivalent to ours. A special case of this formula has also been calculated by Kumar, Ref. 14, to third order.

be more suitable for some purposes. It is obtained from the Magnus solution to Eqs. (8.1_λ) and is given by Eqs. (8.18), (8.2), (8.3), (8.6)–(8.9), $\cdots$, and (8.15). These expansions are more complicated than the Zassenhaus expansion, Eq. (4.18), but appear to be more useful when λb is "small" compared with a. They also appear to be more useful for large values of t, provided $U(t)$ is unitary. A fuller heuristic comparison of the two infinite-product forms for the case where $t \to \infty$ has been given by Kumar.[14]

8.2. Lie Algebraic Solutions

We now consider the case where $A(t)$ in Eq. (8.1) may be expressed as a LCLE,

$$A(t) = a_1(t)X_1 + a_2(t)X_2 + \cdots + a_n(t)X_n.$$

Then if a solution of the form

$$Y(t) = e^{\Omega(t)} \tag{8.19}$$

exists, the repeated-commutator form for Ω and the "closure property" of the Lie algebra imply that $\Omega(t)$ is also a linear combination of the X_j's. We will find some closed-form solutions for two Lie algebras of physical interest by a method similar to those employed in previous sections. Our method is also basically the same as the method employed by Wei and Norman to obtain solutions in the product form[15]

$$Y(t) = \exp[g_1(t)X_1]\cdots\exp[g_n(t)X_n] \tag{8.20}$$

if one ignores the technical group-theoretical considerations of that treatment. In practice, however, the single-exponential solutions are more difficult to obtain.

We again consider first the two-dimensional algebra where $[X, Y] = Y$. In Eqs. (8.1), let

$$A(t) \equiv a(t)X + b(t)Y, \tag{8.21}$$

where $a(t)$ and $b(t)$ are arbitrary functions of t, and let

$$\Omega(t) \equiv \alpha(t)X + \beta(t)Y \tag{8.22}$$

in Eq. (8.19). Substituting Eqs. (8.21) and (8.22) into Eq. (8.4) with $\lambda = 1$, using Eq. (6.16), integrating over x, and equating coefficients of X and Y, one obtains

$$\dot\alpha = a(t), \quad \dot\alpha u + \dot u(e^\alpha - 1) = b(t), \tag{8.23}$$

where

$$u(t) \equiv \beta(t)/\alpha(t). \tag{8.24}$$

Integrating Eqs. (8.23), one obtains

$$\alpha(t) = \int_0^t a(\tau)\,d\tau, \tag{8.25}$$

$$\beta(t) = [1 - e^{-\alpha(t)}]^{-1}\alpha(t)\gamma(t), \tag{8.26}$$

where

$$\gamma(t) = \int_0^t d\tau b(\tau)e^{-\alpha(\tau)}\,d\tau. \tag{8.27}$$

For the case where $A(t)$ is given by Eq. (8.21), Eqs. (8.19), (8.22), (8.25), (8.26), and (8.27) constitute the solution of Eq. (8.1). By means of Eq. (7.9), this result may be shown to be equivalent to the product form of Wei and Norman,[55]

$$Y(t) = e^{\alpha(t)X}e^{\gamma(t)Y}. \tag{8.28}$$

A solution may also be obtained for the four-dimensional harmonic-oscillator algebra of Eqs. (6.23). In Eqs. (8.1) and (8.19), let

$$A(t) \equiv g(t)W + d(t)X + r(t)Y + u(t)I \tag{8.29a}$$

$$\equiv g(t)[X + w(t)I][Y + v(t)I] + f(t)I, \tag{8.29b}$$

$$\Omega(t) \equiv \gamma(t)W + \delta(t)X + \rho(t)Y + \mu(t)I \tag{8.30a}$$

$$\equiv \gamma(t)[X + \omega(t)I][Y + \nu(t)I] + \varphi(t)I. \tag{8.30b}$$

Then proceeding in the same way as before, using either Eqs. (6.26) or Eq. (6.27), one obtains the differential equations

$$\dot\gamma = g,$$
$$g\nu + \dot\nu(1 - e^{-s\gamma})s^{-1} = d = gv,$$
$$g\omega + \dot\omega(e^{s\gamma} - 1)s^{-1} = r = gw,$$
$$\dot\varphi = g(w - \omega)(v - \nu) + f(t),$$

where $\gamma \equiv \gamma(t)$, $g \equiv g(t)$, etc. The solution, subject to the conditions $\gamma(0) = \delta(0) = \rho(0) = \mu(0) = 0$, is given by

$$\gamma(t) = \int_0^t g(\tau)\,d\tau, \tag{8.31}$$

$$\nu(t) = [e^{s\gamma(t)} - 1]^{-1}s\alpha(t), \tag{8.32}$$

$$\omega(t) = [1 - e^{-s\gamma(t)}]^{-1}s\beta(t), \tag{8.33}$$

$$\varphi(t) = \int_0^t d\tau\{g(\tau)[w(\tau) - \omega(\tau)][v(\tau) - \nu(\tau)] + f(\tau)\}, \tag{8.34}$$

where

$$\alpha(t) \equiv \int_0^t d(\tau)e^{s\gamma(\tau)}\,d\tau, \tag{8.35}$$

$$\beta(t) \equiv \int_0^t r(\tau)e^{-s\gamma(\tau)}\,d\tau. \tag{8.36}$$

For the case where $A(t)$ is given by Eqs. (8.29), Eqs. (8.19) and (8.30)–(8.36) constitute the solution of Eq. (8.1). This may be compared with the product form of Wei and Norman,[55]

$$Y(t) = e^{\gamma(t)W}e^{\alpha(t)X}e^{\beta(t)Y}e^{\psi(t)I}, \tag{8.37}$$

[55] Wei and Norman, Ref. 15, derive differential equations, but do not explicitly give their solution since they are mainly interested in determining whether or not solutions exist.

where $\alpha(t)$, $\beta(t)$, and $\gamma(t)$ are given by Eqs. (8.35), (8.36), and (8.31), respectively, and where

$$\psi(t) \equiv \int_0^t d\tau[u(\tau) - s\alpha(\tau)r(\tau)e^{-s\gamma(\tau)}]. \quad (8.38)$$

One may use either of these solutions to solve the problem of the driven harmonic oscillator, without the necessity of first transforming to the interaction representation as is usually done.[56]

9. SOLUTIONS OF $i\hbar\partial\rho(t)/\partial t = [\mathcal{H}(t), \rho(t)]$

Consider the equation for the time evolution of the density matrix $\rho(t)$, for a system described by a Hamiltonian $\mathcal{H}(t)$,[57]

$$i\hbar\partial\rho(t)/\partial t = [\mathcal{H}(t), \rho(t)]. \quad (9.1)$$

(Aside from a sign, the same equation of course applies to any Heisenberg operator.) In case $\mathcal{H}(t)$ is an LCLE and $\rho(t)$ is initially an LCLE, then Eqs. (9.1) and (6.1) imply that $\rho(t)$ will remain an LCLE for all time. A solution may then be readily obtained, as in Sec. 6. However, the condition that an arbitrary density matrix be expressible as an LCLE is very restrictive, so that not many cases occur in practice. A case where an arbitrary density matrix may be expressed in terms of an LCLE occurs in the problem of a spin $-\frac{1}{2}$ magnetic moment in a time-varying magnetic field.[58]

However, as is well known, even if $\rho(0)$ is not an LCLE, a solution of Eq. (9.1) is given by

$$\rho(t) = U(t)\rho(0)U^\dagger(t), \quad (9.2)$$

where $U(t)$ is a solution of

$$i\hbar\partial U(t)/\partial t = \mathcal{H}(t)U(t), \quad U(0) = I, \quad (9.3)$$

the problem discussed in Sec. 8.

A case of much interest is where the density matrix is initially in thermal equilibrium[59]:

$$\rho(0) = e^{-\beta\mathcal{H}(0)}/\mathrm{Tr}\,[e^{-\beta\mathcal{H}(0)}]. \quad (9.4)$$

It follows from the basic lemma given at the end of Sec. 2 that a solution to Eqs. (9.1) and (9.4) is given by

$$\rho(t) = e^{-\beta H(t)}/\mathrm{Tr}\,[e^{-\beta\mathcal{H}(0)}], \quad (9.5)$$

where $H(t)$ satisfies

$$i\hbar\partial H(t)/\partial t = [\mathcal{H}(t), H(t)], \quad H(0) = \mathcal{H}(0). \quad (9.6)$$

Since $H(t)$ satisfies the same differential equation as $\rho(t)$, it may appear that nothing has been gained. However, it may be easier to apply the boundary conditions to $H(0)$ than to $\rho(0)$. In particular, $H(0) \equiv \mathcal{H}(0)$ may be an LCLE although $\rho(0)$ is not. Considering the various methods available for handling exponential operators, Eqs. (9.5) and (9.6) may also be a useful starting point for dealing with practical many-body systems for which exact solutions are impossible.

Since $\mathrm{Tr}\,\rho(t) = 1$ at all times, as is implied by Eq. (9.4), Eq. (9.1), and the cyclic property of the trace, Eq. (9.5) may also be written in the form

$$\rho(t) = e^{-\beta H(t)}/\mathrm{Tr}\,[e^{-\beta H(t)}]. \quad (9.7)$$

Equation (9.7) shows that at all times the system behaves as though its temperature remains constant with a "canonical distribution" determined by the instantaneous value of the fictitious Hamiltonian $H(t)$. It may thus be possible to treat nonequilibrium situations by the methods of equilibrium statistical mechanics.

A simple illustrative example is the problem of an arbitrary spin magnetic moment in an arbitrary time-varying magnetic field with a Hamiltonian

$$\begin{aligned}\mathcal{H}(t) &= \gamma\mathbf{h}(t)\cdot\mathbf{J}\\ &\equiv \gamma[h_x(t)J_x + h_y(t)J_y + h_z(t)J_z]. \quad (9.8)\end{aligned}$$

Then $H(t)$ is of the form

$$H(t) = \gamma\mathbf{b}(t)\cdot\mathbf{J}. \quad (9.9)$$

It easily follows from Eqs. (9.6), (9.8), (9.9), and (6.31) that the fictitious field $\mathbf{b}(t)$ precesses about the instantaneous direction of $h(t)$ according to the equation

$$\dot{\mathbf{b}}(t) = \gamma\mathbf{h}(t)\times\mathbf{b}(t), \quad (9.10)$$

with $\mathbf{b}(0) \equiv \mathbf{h}(0)$.

10. NORMAL-ORDERING OF OPERATORS

Normal-ordering techniques are useful for solving operator differential equations,[60] evaluating matrix elements,[61] and finding the quantum operator corresponding to a given classical operator. We have already encountered an example of this last application in McCoy's theorem, Eq. (5.6). Using methods and formulas of previous sections, we may efficiently derive a number of related results.

The derivations are greatly facilitated with the aid of the "normal-ordering operator" $\mathcal{N}$ defined as

[56] See, e.g., Louisell, Ref. 3, p. 119, Sec. 3.5.

[57] See, e.g., Louisell, Ref. 3, Chap. 6. Other references are given there.

[58] See, e.g., F. A. Kaempffer, *Concepts in Quantum Mechanics* (Academic Press Inc., New York, 1965), Sec. 4.

[59] This situation has been treated by Kubo, Ref. 4.

[60] J. L. Anderson, Phys. Rev. **94**, 703 (1954); N. N. Bogoliubov and D. V. Shirkov, *Introduction to the Theory of Quantized Fields* (Interscience Publishers, Inc., New York, 1959), p. 486; see also Louisell, Ref. 3, and Heffner and Louisell, Ref. 16.

[61] G. Wick, Phys. Rev. **80**, 268 (1950); Bogoliubov and Shirkov, Ref. 60, Sec. 16; Louisell, Ref. 3; Wilcox, Ref. 50.

follows[62]: With $[P, Q] = cI$, let the function $f(P, Q)$ be defined by its formal power-series expansion,

$$f(P, Q) \equiv aI + bP + dQ + ePQ + gQP + \cdots. \tag{10.1}$$

Then the linear "superoperator" $\mathcal{N}$ acting on $f(P, Q)$ moves all P's to the right of the Q's *as though* P and Q commute; i.e.,

$$\mathcal{N}[f(P, Q)] \equiv aI + bP + dQ + (e + g)QP + \cdots. \tag{10.2}$$

Although other operator expressions may be obtained from $f(P, Q)$ by application of the commutation relation, we emphasize that their functional forms will be different. Thus, even though $f(P, Q) = g(P, Q)$ in the usual operator sense, it need not follow that $\mathcal{N}[f(P, Q)] = \mathcal{N}[g(P, Q)]$. Some useful properties of $\mathcal{N}$ are a direct consequence of its definition. If $f(P, Q)$ and $g(P, Q)$ are any two operator functions, then

$$\mathcal{N}[f(P, Q)g(P, Q)] = \mathcal{N}[g(P, Q)f(P, Q)]. \tag{10.3}$$

If $|P'\rangle$ and $|Q'\rangle$ are eigenstates of P and Q, $P|P'\rangle = P'|P'\rangle$ and $Q|Q'\rangle = Q'|Q'\rangle$, then

$$\{\mathcal{N}[f(P, Q)]\}|P'\rangle = f(P', Q)|P'\rangle, \tag{10.4a}$$

$$\langle Q'|\{\mathcal{N}[f(P, Q)]\} = \langle Q'|f(P, Q'^*), \tag{10.4b}$$

$$\langle Q'|\{\mathcal{N}[f(P, Q)]\}|P'\rangle = f(P', Q'^*)\langle Q' \mid P'\rangle. \tag{10.4c}$$

Equations (10.4) usually occur in practice for the case where P and Q correspond to the annihilation and creation operators a and $a^\dagger$, respectively, and the vacuum state $|0\rangle$ is involved, $a|0\rangle = 0$ or $\langle 0| a^\dagger = 0$. If the f in Eq. (10.1) also depends upon a parameter λ, $f \equiv f(P, Q, \lambda)$, then it is apparent that $\mathcal{N}$ commutes with $\partial/\partial\lambda$ since

$$\begin{aligned}\mathcal{N}[\partial f(P, Q, \lambda)/\partial\lambda] &= \mathcal{N}[a'I + b'P + d'Q + e'PQ + g'QP + \cdots] \\ &= a'I + b'P + d'Q + (e' + g')QP + \cdots \\ &= \partial\{\mathcal{N}[f(P, Q, \lambda)]\}/\partial\lambda,\end{aligned} \tag{10.5}$$

where $a' \equiv \partial a(\lambda)/\partial\lambda$, etc. From the definition of the derivative with respect to an operator, Eq. (2.0), it readily follows that $\mathcal{N}$ also commutes with $\partial/\partial P$ and $\partial/\partial Q$.

An important problem of normal-ordering is to express the product of two normal-ordered products in normal form.[3,16]

Theorem: Let $F(P, Q)$ and $G(P, Q)$ be in normal form: $F(P, Q) \equiv \mathcal{N}[F(P, Q)]$; $G(P, Q) \equiv \mathcal{N}[G(P, Q)]$. Then the normal form of the product is given by

$$\mathcal{N}[F(P + c\partial/\partial Q, Q)G(P, Q)]. \tag{10.6}$$

Proof: We prove the result first for the special case where $F(P, Q)$ and $G(P, Q)$ have the forms

$$F(P, Q) = e^{wQ}e^{xP}, \quad G(P, Q) = e^{vQ}e^{zP}.$$

Then

$$\begin{aligned}F(P, Q)G(P, Q) &= e^{wQ}e^{xP}e^{vQ}e^{zP} \\ &= e^{xvc}e^{wQ}e^{vQ}e^{xP}e^{zP} \\ &= \mathcal{N}[e^{xvc}e^{wQ}e^{vQ}e^{xP}e^{zP}] \\ &= \mathcal{N}[e^{wQ}e^{x(P+cv)}e^{vQ}e^{zP}] \\ &= \mathcal{N}[e^{wQ}e^{x(P+c\partial/\partial Q)}e^{vQ}e^{zP}] \\ &= \mathcal{N}[F(P + c\partial/\partial Q, Q)G(P, Q)].\end{aligned}$$

The general case easily follows by the method of linear superposition. The theorem may be readily generalized to the case of more than one pair of conjugate variables.

As an application of this theorem, consider the case where $F(P, Q) = P^m$, $G(P, Q) = Q^n$. Then

$$\begin{aligned}P^mQ^n &= \mathcal{N}[(P + c\partial/\partial Q)^m Q^n] \\ &= \mathcal{N}\sum_{j=0}^{m} \frac{m!\, P^{m-j}c^j}{j!\,(m-j)!}\frac{\partial^j Q^n}{\partial Q^j} \\ &= \sum_{j=0}^{m} \frac{m!\, n!\, c^j Q^{n-j}P^{m-j}}{j!\,(m-j)!\,(n-j)!}.\end{aligned} \tag{10.7}$$

To show how the theorem may be used for solving differential equations, and to compare with the treatment of Heffner and Louisell,[16] we consider their example of a spin magnetic moment in a rotating magnetic field. The Hamiltonian is then of the form[16]

$$\mathcal{H} = \tfrac{1}{2}\hbar\omega_0(b^\dagger b - c^\dagger c) + \tfrac{1}{2}\hbar\gamma H_1(b^\dagger c e^{-i\omega t} + c^\dagger b e^{i\omega t}), \tag{10.8}$$

where the annihilation and creation operators b, $b^\dagger$, c, and $c^\dagger$ were defined in Eq. (6.39), and $\hbar$, ω_0, γ, H_1, and ω are costants. We assume that the solution of the equation

$$i\hbar\dot{U} \equiv i\hbar\partial U/\partial t = \mathcal{H}U \tag{10.9}$$

is of the form[63]

$$U = \mathcal{N}\{\exp[(A-1)b^\dagger b + (B-1)c^\dagger c + Db^\dagger c + Ec^\dagger b]\}, \tag{10.10}$$

where $\mathcal{N}$ orders b and c to the right of $b^\dagger$ and $c^\dagger$, and

[62] Our definition of the "normal-ordering operator" is not the same as that given by Louisell, Ref. 3, and Heffner and Louisell, Ref. 16, but we believe it is more convenient.

[63] For convenience, we define U such that A, B, D, and E correspond to the notation of Ref. 16, but this, of course, is not essential for the solution of the problem.

the scalar functions A, B, D, and E are to be determined. It clearly follows that

$$\dot{U} = \dot{A}b^\dagger Ub + \dot{B}c^\dagger Uc + \dot{D}b^\dagger Uc + \dot{E}c^\dagger Ub. \quad (10.11)$$

From the above theorem, $2\mathcal{H}U/\hbar$ is given by

$$\mathcal{N}[(\omega_0 b^\dagger + \gamma H_1 e^{i\omega t}c^\dagger)(b + \partial/\partial b^\dagger)U + (-\omega_0 c^\dagger + \gamma H_1 e^{-i\omega t}b^\dagger)(c + \partial/\partial c^\dagger)U]. \quad (10.12)$$

Since

$$\partial U/\partial b^\dagger = U[(A-1)b + Dc] \quad (10.13)$$

and

$$\partial U/\partial c^\dagger = U[(B-1)c + Eb], \quad (10.14)$$

it follows from Eqs. (10.9)–(10.14), by equating coefficients of $b^\dagger Ub$, $c^\dagger Uc$, $b^\dagger Uc$, and $c^\dagger Ub$, respectively, that

$$\begin{aligned} i\partial A/\partial t &= \tfrac{1}{2}\omega_0 A + \tfrac{1}{2}\gamma H_1 e^{-i\omega t}E,\\ i\partial B/\partial t &= -\tfrac{1}{2}\omega_0 B + \tfrac{1}{2}\gamma H_1 e^{i\omega t}D,\\ i\partial D/\partial t &= \tfrac{1}{2}\omega_0 D + \tfrac{1}{2}\gamma H_1 e^{-i\omega t}B,\\ i\partial E/\partial t &= -\tfrac{1}{2}\omega_0 E + \tfrac{1}{2}\gamma H_1 e^{i\omega t}A. \end{aligned} \quad (10.15)$$

We refer the reader to Ref. 16 for the solution of these equations. Note that the treatment given here avoids the necessity of transforming the annihilation–creation operator space onto a space of commuting algebraic variables, and back again.

We next derive a general result which is primarily of interest for cases where P and Q are annihilation and creation operators. Let

$$e^{zP}e^{xQP}e^{yQ} = \mathcal{N}[\exp(fQP + gP + hQ + sI)]. \quad (10.16)$$

In Eq. (10.16), we regard f, g, h, and s to be scalar functions of x which depend parametrically upon z and y. Differentiating Eq. (10.16) with respect to x and substituting Eq. (10.16) into the result, one obtains

$$e^{zP}QPe^{xQP}e^{yQ} = Qe^{zP}e^{xQP}e^{yQ}(f'P + h') + e^{zP}e^{xQP}e^{yQ}(g'P + s'I). \quad (10.17)$$

Multiplying Eq. (10.17) from the right by $e^{-yQ}e^{-xQP} \times e^{-zP}$, carrying out the similarity transformations, and equating coefficients of QP, P, Q, and I, respectively, on the two sides of the equation, one obtains

$$\begin{aligned} f' &= e^{cx},\\ g' &= cze^{cx},\\ h' &= cyf' = cye^{cx},\\ s' &= cyg' = c^2yze^{cx}. \end{aligned} \quad (10.18)$$

Integrating Eqs. (10.18) subject to the conditions $f(0) = 0$, $g(0) = z$, $h(0) = y$, and $s(0) = cyz$ and substituting the results into Eq. (10.16), one obtains

$$e^{zP}e^{xQP}e^{yQ} = \mathcal{N}\{\exp[c^{-1}(e^{cx} - 1)QP + e^{cx}(zP + yQ + cyzI)]\}. \quad (10.19)$$

A special case of interest is obtained by setting $z = 0$, $P = a$, $Q = a^\dagger$, and $c = 1$ in Eq. (10.19):

$$e^{xa^\dagger a}e^{ya^\dagger} = \exp(ye^x a^\dagger)\mathcal{N}\{\exp[(e^x - 1)a^\dagger a]\}. \quad (10.20)$$

By the method of linear superposition on y, it follows from Eq. (10.20) that

$$e^{xa^\dagger a}f(a^\dagger) = f(e^x a^\dagger)\mathcal{N}\{\exp[(e^x - 1)a^\dagger a]\}. \quad (10.21)$$

A special case of Eq. (10.20) or (10.21) has been derived in Ref. 3 by a different method:

$$e^{xa^\dagger a} = \mathcal{N}\{\exp[(e^x - 1)a^\dagger a]\} \quad (10.22a)$$

$$= \sum_{r=0}^{\infty}(e^x - 1)^r(r!)^{-1}a^{\dagger r}a^r. \quad (10.22b)$$

This result is also a special case of a theorem due to McCoy. [See Eqs. (10.38) and (10.41).] Another result given in Ref. 3 is easily obtained from Eq. (10.22b) by using the binomial expansion,

$$(e^x - 1)^r = \sum_{s=0}^{r}\frac{(-)^{r-s}r!\,e^{sx}}{s!\,(r-s)!},$$

and employing the method of linear superposition on x:

$$f(a^\dagger a) = \sum_{r=0}^{\infty}\sum_{s=0}^{r}\frac{(-)^{r-s}f(s)}{s!\,(r-s)!}a^{\dagger r}a^r. \quad (10.23)$$

It is sometimes useful to put expressions in antinormal form. Let $\bar{N}$ be the antinormal-ordering operator defined similarly to $\mathcal{N}$ except that it puts the a's to the left of the $a^\dagger$'s. Thus the antiequation of (10.22a) is given by

$$e^{xa^\dagger a} = e^{-x}\bar{N}\{\exp[(1 - e^{-x})a^\dagger a]\}. \quad (10.24)$$

Substituting Eq. (10.24) into Eq. (10.21) and letting $(1 - e^{-x}) = z$, one obtains a result derived by Schwinger in a different manner[17]:

$$\bar{N}[e^{za^\dagger a}]f(a^\dagger) = \frac{1}{1-z}f\left(\frac{a^\dagger}{1-z}\right)\mathcal{N}\left[\exp\left(\frac{za^\dagger a}{1-z}\right)\right]. \quad (10.25a)$$

Another formula given by Schwinger is similarly derived:

$$f(a)\bar{N}e^{za^\dagger a} = \mathcal{N}\left[\exp\left(\frac{za^\dagger a}{1-z}\right)\right]\frac{1}{1-z}f\left(\frac{a}{1-z}\right). \quad (10.25b)$$

Using these formulas with $a^\dagger = x$ and $a = \partial/\partial x$, Schwinger has derived some interesting operator identities and classical formulas involving cylinder functions and associated Laguerre polynomials. A corollary of one of these is the formula

$$a^m(a^\dagger)^{m+r} = m!\,(a^\dagger)^r \mathcal{N}[L_m^r(-a^\dagger a)], \quad (10.26)$$

a result which one may also obtain directly from Eq. (10.7) by using the definition of the associated Laguerre polynomial.

The next derivation shows how the exponential of an arbitrary second-degree polynomial may be put into normal form. This result generalizes a theorem of McCoy.[18]

Theorem: Let

$$e^Z = \mathcal{N}(e^W), \quad (10.27)$$

where

$$Z \equiv \alpha P^2 + \beta Q^2 + \gamma QP + \delta P + \epsilon Q, \quad (10.28)$$

$$W \equiv AP^2 + BQ^2 + GQP + DP + EQ + FI. \quad (10.29)$$

Then Eq. (10.27) is identically satisfied provided

$$\begin{aligned} \alpha^{-1}A = \beta^{-1}B = H &\equiv (\lambda J)^{-1}\sinh\lambda, \\ G &= c^{-1}(J^{-1}-1), \\ D &= \rho^2(\tau G + 2\mu A), \\ E &= \rho^2(\mu G + 2\tau B), \\ F &= -\tfrac{1}{2}\ln J - \tfrac{1}{2}c\gamma + \rho^2(\varphi - \gamma\delta\epsilon) + \rho^4\tau\mu G \\ &\quad + \rho^4(4\alpha\beta\varphi + \gamma^2\varphi - 8\alpha\beta\gamma\delta\epsilon)H, \end{aligned} \quad (10.30)$$

where

$$\begin{aligned} J &\equiv \cosh\lambda - \rho\gamma\sinh\lambda, \quad \rho \equiv \lambda^{-1}c, \\ \lambda &= c[\gamma^2 - 4\alpha\beta]^{\frac{1}{2}}, \quad \varphi \equiv \alpha\epsilon^2 + \beta\delta^2, \\ \tau &\equiv \gamma\delta - 2\alpha\epsilon, \quad \mu \equiv \gamma\epsilon - 2\beta\delta. \end{aligned} \quad (10.31)$$

Proof: Instead of Eq. (10.27), consider

$$e^{xZ} = \mathcal{N}[e^{W(x)}], \quad (10.32)$$

where $W(0) = 0$. In Eq. (10.29), W, A, B, G, D, E, and F are now considered to be functions of x. Differentiating Eq. (10.32) with respect to x, one obtains

$$\begin{aligned} Ze^{xZ} &= \mathcal{N}[W'(x)e^{W(x)}] \\ &= A'e^{xZ}P^2 + B'Q^2e^{xZ} + G'Qe^{xZ}P \\ &\quad + D'e^{xZ}P + E'Qe^{xZ} + F'e^{xZ}, \end{aligned} \quad (10.33)$$

where $A' \equiv \partial A/\partial x$, etc. Multiplying Eq. (10.33) from the right by e^{-xZ}, one obtains

$$\begin{aligned} Z = A'e^{xZ}P^2e^{-xZ} &+ (G'Q + D')e^{xZ}Pe^{-xZ} \\ &+ B'Q^2 + E'Q + F'I. \end{aligned} \quad (10.34)$$

The quantities $e^{xZ}Pe^{-xZ}$ and

$$e^{xZ}P^2e^{-xZ} = [e^{xZ}Pe^{-xz}]^2$$

are obtained from Eqs. (6.48)–(6.51). Equating coefficients of P^2, QP, Q^2, P, Q, and I, respectively, on the two sides of Eq. (10.34) leads to the differential equations

$$\begin{aligned} \alpha &= A'd^2, \quad \gamma = 2A'de + G'd, \\ \beta &= A'e^2 + B' + G'e, \quad \delta = 2A'df + D'd, \\ \epsilon &= 2A'ef + G'f + D'e + E', \\ 0 &= A'f^2 + cA'de + D'f + F', \end{aligned} \quad (10.35)$$

where $d \equiv d(x)$, $e \equiv e(x)$, and $f \equiv f(x)$ are defined by Eqs. (6.50). Equations (10.35) simplify to

$$\begin{aligned} A'/\alpha &= B'/\beta = d^{-2}, \quad G' = -c^{-1}d^{-2}d', \\ D' &= \rho^2(\tau G' + 2\mu A'), \quad E' = \rho^2(\mu G' + 2\tau B'), \\ F' &= -\tfrac{1}{2}d'd^{-1} + \rho^2(\varphi - \gamma\delta\epsilon) + \rho^4\tau\mu G' \\ &\quad -\tfrac{1}{2}c\gamma + \rho^4(4\alpha\beta\varphi + \gamma^2\varphi - 8\alpha\beta\gamma\delta\epsilon)d^{-2}. \end{aligned} \quad (10.36)$$

Integrating Eqs. (10.36) subject to $A(0) = \cdots = F(0) = 0$ and setting $x = 1$, one obtains Eqs. (10.30) for $A \equiv A(1)$, $B \equiv B(1)$, etc. Q.E.D.

Using Eq. (2.8), one may verify that both sides of Eq. (10.27) satisfy the pair of partial differential equations

$$\partial U/\partial P = 2AUP + GQU + DU, \quad (10.37a)$$

$$\partial U/\partial Q = GUP + 2BQU + EU. \quad (10.37b)$$

Some special cases of Eqs. (10.27)–(10.31) are of interest. If $\delta = \epsilon = 0$, then $D = E = 0$ and

$$\begin{aligned} &\exp(\alpha P^2 + \beta Q^2 + \gamma QP) \\ &\quad = [Je^{c\gamma}]^{-\frac{1}{2}}\mathcal{N}[\exp(AP^2 + BQ^2 + GQP)], \end{aligned} \quad (10.38)$$

where A, B, G, and J are given by Eqs. (10.30) and (10.31). This result may be shown to be equivalent to McCoy's theorem.[18] We note that McCoy gave an ingenious derivation based upon a pair of partial differential equations like Eqs. (10.37) with $D = E = 0$. If we set $\gamma = 0$ in Eq. (10.28) and define

$$S \equiv P + \theta I, \quad R \equiv Q + \sigma I, \quad y \equiv 2c(\alpha\beta)^{\frac{1}{2}}, \quad (10.39)$$

then

$$\begin{aligned} &\exp(\alpha S^2 + \beta R^2) \\ &\quad = (\sec y)^{\frac{1}{2}}\mathcal{N}\{\exp[(y^{-1}\tan y)(\alpha S^2 + \beta R^2) \\ &\qquad + c^{-1}(\sec y - 1)RS]\}. \end{aligned} \quad (10.40)$$

If we set $\alpha = \beta = 0$ in Eq. (10.28) and define S and R by Eqs. (10.39), then

$$e^{\gamma RS} = \mathcal{N}\{\exp[c^{-1}(e^{c\gamma} - 1)RS]\}. \quad (10.41)$$

Equations (10.40) and (10.41) may also be derived from Eq. (10.38) by using the fact that S and R satisfy the same commutation relation as P and Q.

An expansion of Kermack and McCrea, which provided the starting point for Sach's derivation of his "Taylor's theorem for shift operators,"[11] is as follows[19]:

$$F[P+\varphi(Q)] = \mathcal{N}\left\{\left[\exp\int_0^{\partial/\partial P} dx\varphi(Q+cx)\right]F(P)\right\} \quad (10.42a)$$

$$= \mathcal{N}\{\exp[\varphi(Q)\partial/\partial P + \tfrac{1}{2}c\varphi'(Q)\partial^2/\partial P^2 + \tfrac{1}{6}c^2\varphi''(Q)\partial^3/\partial P^3 + \cdots]\}F(P). \quad (10.42b)$$

For the special case where $F(P) = e^{\lambda P}$, Eq. (10.42a) easily follows from Eq. (7.33), while the general case follows by the method of linear superposition. Equation (10.42b) follows from Eq. (10.42a) by Taylor-expanding $\varphi(Q+cx)$ about $x=0$ and carrying out the integration over x.

A result recently obtained by Cohen is readily obtained by setting $\varphi(Q) = Q$ and $F(P) = P^n$ in Eq. (10.42b).

$$\begin{aligned}(P+Q)^n &= \mathcal{N}[\exp(Q\partial/\partial P + \tfrac{1}{2}c\partial^2/\partial P^2)]P^n \\ &= \mathcal{N}\left[\exp\left(\frac{Q\partial}{\partial P}\right)\sum_{k=0}^{\infty}\frac{(\frac{1}{2}c)^k\partial^{2k}P^n/\partial P^{2k}}{k!}\right] \\ &= \sum_{k=0}^{[\frac{1}{2}n]}\frac{(\frac{1}{2}c)^k n!}{k!\,(n-2k)!}\sum_{s=0}^{\infty}\frac{Q^s(\partial^s P^{n-2k}/\partial P^s)}{s!} \\ &= \sum_{k=0}^{[\frac{1}{2}n]}\sum_{s=0}^{n-2k}\frac{(\frac{1}{2}c)^k n!\,Q^sP^{n-2k-s}}{k!\,s!\,(n-2k-s)!}.\end{aligned} \quad (10.43)$$

Equation (10.43) may be easily shown to be equivalent to Cohen's result which he obtained as an application of his "Expansion Theorem for Functions of Operators."[20] In contrast to the normal-ordering theorems considered above, this theorem requires for its application that one knows the solution to an eigenvalue problem. A slightly more general statement of Cohen's theorem and a briefer proof of it follow.

Theorem: Let $F(q,p)$ be a Hermitian operator function of q and p, with $[q,p] = i\hbar$, which satisfies the eigenvalue equation

$$F|k\rangle = \alpha_k|k\rangle. \quad (10.44)$$

Then any operator function $g(F)$ may be represented by

$$g(F) = \sum_{k=0}^{\infty} g(\alpha_k)\psi_k(q)\int_{-\infty}^{\infty}\psi_k^*(q+\theta)e^{i\theta p/\hbar}d\theta, \quad (10.45)$$

where $\psi_k(q') \equiv \langle q' \mid k\rangle$. If the eigenvalue spectrum of F is continuous, the summation is to be replaced by an integration.

Proof: Equation (10.45) may be verified by showing that the matrix elements of both sides are the same between states $\langle q'|$ and $|q''\rangle$. Since $g(F)$ has the same eigenstates as F, the left-hand side of Eq. (10.45) may be written

$$g(F) = \sum_{k=0}^{\infty} g(\alpha_k)\,|k\rangle\langle k|. \quad (10.46)$$

Hence

$$\langle q'|\,g(F)\,|q''\rangle = \sum_{k=0}^{\infty} g(\alpha_k)\psi_k(q')\psi_k^*(q''). \quad (10.47)$$

The corresponding matrix element of the right-hand side of Eq. (10.45) is given by

$$\sum_{k=0}^{\infty} g(\alpha_k)\psi_k(q')\int_{-\infty}^{\infty}\psi_k^*(q'+\theta)\langle q'|\,e^{i\theta p/\hbar}\,|q''\rangle\,d\theta. \quad (10.48)$$

From Eq. (2.11), we have

$$\langle q'|\,e^{i\theta p/\hbar}\,|q''\rangle = \langle q' \mid q''-\theta\rangle = \delta(q'-q''+\theta). \quad (10.49)$$

Substituting Eq. (10.49) into Eq. (10.48), one obtains Eq. (10.47). Q.E.D.

11. HIGHER DERIVATIVES

Higher derivatives of exponential operators may be obtained straightforwardly by repeated application of Eq. (2.1). The results obtained, however, are not in the most concise and symmetrical form possible. Although they may be put into a symmetrical "time-ordered" form by a change of integration variables, we prefer to proceed in a different manner which makes use of an integral representation due to Poincaré[21]:

$$f(H) = (2\pi i)^{-1}\int_c f(z)(zI-H)^{-1}\,dz. \quad (11.1)$$

In Eq. (11.1), it is assumed that the contour of integration encloses a region of the complex z plane where all the eigenvalues of H lie and throughout which $f(z)$ is analytic. Equation (11.1) may be verified by taking matrix elements of both sides in a representation in which H is diagonal, and employing the Cauchy integral formula. For convenience, we assume that H is a positive-definite Hermitian operator with a discrete eigenvalue spectrum although the results obtained are often valid under less restrictive conditions.

We consider first the case where $f(z) = e^{-\beta z}$, and rotate 90° to the x plane defined by $x \equiv iz$. From Eq. (11.1), it then follows that

$$E(\beta) \equiv (2\pi i)^{-1}\int_{-\infty}^{\infty} e^{i\beta x}(x-iH)^{-1}\,dx \quad (11.2a)$$

$$= \begin{cases} e^{-\beta H}, & \beta > 0, \\ 0, & \beta < 0. \end{cases} \quad (11.2b)$$

The cases $\beta > 0$ and $\beta < 0$, respectively, are obtained by choosing the contours of integration to be infinite semicircles in the upper- and lower-half x plane. For the special case where $H \equiv H(\lambda)$ is of the form $H = \mathcal{H} + \lambda V$, one finds that the nth derivative of $E(\beta)$ with respect to λ, $\partial^n E(\beta)/\partial\lambda^n \equiv E^{(n)}(\beta)$, is given by

$$\frac{n!\, i^n}{2\pi i}\int_{-\infty}^{\infty} dx e^{i\beta x}(x - iH)^{-1}[V(x - ih)^{-1}]^n. \quad (11.3)$$

Equation (11.3) follows directly from Eq. (11.2a) by using the formula for the derivative of the inverse,

$$\partial[(x - iH)^{-1}]/\partial\lambda = i(x - iH)^{-1}V(x - iH)^{-1}.$$

A recursive formula for $E^{(n)}(\beta)$ which shows its "time-ordered" form is given by

$$E^{(n)}(\beta) = -n\int_0^\beta du E(\beta - u)VE^{(n-1)}(u). \quad (11.4)$$

Equation (11.4) follows from Eq. (11.3) by writing it in the form

$$\frac{n!\, i^n}{2\pi i}\iint_{-\infty}^{\infty} dx\, dy \delta(x - y)e^{i\beta x}(x - iH)^{-1}[V(y - iH)^{-1}]^n$$
$$= \frac{n!\, i^n}{4\pi^2 i}\iiint_{-\infty}^{\infty} du\, dx\, dy e^{iu(y-x)}e^{i\beta x} \times (x - iH)^{-1}[V(y - iH)^{-1}]^n$$
$$= -n\int_{-\infty}^{\infty} du E(\beta - u)VE^{(n-1)}(u). \quad (11.5)$$

In the integrations over x and y, we have used Eqs. (11.2) and (11.3), respectively. Equation (11.5) is the same as Eq. (11.4), since $E(\beta - u) = 0$ if $u > \beta$, and $E^{(n-1)}(u) = 0$ if $u < 0$. For the case where $n = 1$, since $E^{(0)}(u) \equiv E(u) = e^{-uH}$, Eq. (11.4) constitutes another derivation of Eq. (2.1). An equation like Eq. (11.4) has been derived by Kumar in a different manner, while the derivatives of the exponential evaluated at $\lambda = 0$ occur in a well-known expansion of $e^{\mathcal{H}+\lambda V}$. Of course, higher derivatives may also be calculated from Eqs. (11.2) in the same manner when H does not just depend linearly upon λ, but the results will be more complicated. For example, the second derivative, $E''(\beta) = \partial^2 e^{-\beta H}/\partial\lambda^2$, is then given by[64]

$$E''(\beta) = -\int_0^\beta du E(\beta - u)H''E(u) + 2\int_0^\beta du\int_0^u dv E(\beta - u)H'E(u - v)H'E(v), \quad (11.6)$$

where $H' \equiv \partial H/\partial\lambda$ and $H'' \equiv \partial^2 H/\partial\lambda^2$.

[64] An equivalent formula given by Snider, Ref. 23, Eq. (B7), is not as concise and symmetrical.

The Poincaré formula may also be used to efficiently obtain results of the type derived by Aizu for general operator functions.[2] A formula from which a number of sum rules can be derived is obtained by considering H to be a function of two parameters, λ and μ, and taking matrix elements of $\partial^2 f(H)/\partial\lambda\partial\mu$. Then from Eq. (11.1), one obtains

$$\langle m|\frac{\partial^2 f(H)}{\partial\lambda\partial\mu}|r\rangle = \langle m| A_{\lambda\mu} + A_{\mu\lambda} + B_{\lambda\mu}|r\rangle, \quad (11.7)$$

where

$$\langle m| A_{\lambda\mu}|r\rangle \equiv \sum_n \langle m|\frac{\partial H}{\partial\lambda}|n\rangle\langle n|\frac{\partial H}{\partial\mu}|r\rangle S_{mnr} \quad (11.8)$$

and

$$\langle m| B_{\lambda\mu}|r\rangle \equiv \langle m|\frac{\partial^2 H}{\partial\lambda\partial\mu}|r\rangle T_{mr}. \quad (11.9)$$

In Eqs. (11.8) and (11.9), S_{mnr} and T_{mr} are defined by

$$S_{mnr} \equiv \frac{1}{2\pi i}\int_c \frac{f(z)\, dz}{(z - H_m)(z - H_n)(z - H_r)}, \quad (11.10)$$

$$T_{mr} \equiv \frac{1}{2\pi i}\int_c \frac{f(z)\, dz}{(z - H_m)(z - H_r)}. \quad (11.11)$$

Performing the contour integrations, one obtains

$$T_{mr} = \Delta_{mr}f'(H_m) + \rho_{mr}\frac{f(H_m) - f(H_r)}{H_m - H_r} \quad (11.12)$$

and

$$S_{mnr} = \tfrac{1}{2}\Delta_{mn}\Delta_{nr}f''(H_m) + U_{mnr} + U_{rmn} + U_{nrm}, \quad (11.13)$$

where

$$\Delta_{mn} \equiv 1 - \rho_{mn} \equiv \begin{cases} 1, & H_m = H_n, \\ 0, & H_m \neq H_n, \end{cases} \quad (11.14)$$

$$U_{mnr} \equiv \frac{\rho_{mn}\rho_{nr}\rho_{rm}f(H_m)}{(H_m - H_n)(H_m - H_r)} + \Delta_{mn}\rho_{nr}\left[\frac{f(H_r) - f(H_m)}{(H_r - H_m)^2} - \frac{f'(H_m)}{H_r - H_m}\right]. \quad (11.15)$$

Equations (11.7)–(11.9) and (11.12)–(11.15) may be shown to be equivalent to [25] of Aizu.[2]

It is straightforward to obtain matrix elements of higher derivatives by the same method, but the results obtained are complicated. If one specializes the results so obtained to the case where $f(H) = f(\mathcal{H} + \lambda V) = \exp(\mathcal{H} + \lambda V)$ and compares with the matrix elements of Eq. (11.4), one finds that the latter results do not immediately have such a simple form. Comparison of the two forms reveals the existence of the curious identity

$$\sum_{j=0}^{N}\prod_{\substack{k=1\\k\neq j}}^{N}(x_j - x_k)^{-1} = 0, \quad (11.16)$$

where the variables $x_1, x_2, \cdots, x_N$, stand for H_m, H_n, H_l, etc., and it is assumed that no two are equal. Equation (11.6) may also be derived from the Lagrangian interpolation formula.[65]

Poincaré's formula is also well suited to derive [27] and [28] of Aizu, which depend upon the cyclic property of the trace. We indicate the proof for [27].

Theorem[2]*:*

$$\operatorname{Tr}\left[\varphi(H)\frac{\partial f(H)}{\partial\lambda}\frac{\partial g(H)}{\partial\mu}\right] = \operatorname{Tr}\left[\varphi(H)\frac{\partial g(H)}{\partial\lambda}\frac{\partial f(H)}{\partial\mu}\right],$$

where φ, f, and g are arbitrary functions.

[65] The author is indebted to Dr. P. F. Wacker for suggesting to him that this might be the case.

Proof:

$$\operatorname{Tr}\left[\varphi(H)\frac{\partial f(H)}{\partial\lambda}\frac{\partial g(H)}{\partial\mu}\right] = \frac{1}{(2\pi)^2}\int_c f(z)\,dz\int_c g(w)\,dw \times \operatorname{Tr}\left[\varphi(H)(z-H)^{-1}\frac{\partial H}{\partial\lambda} \times (z-H)^{-1}(w-H)^{-1}\frac{\partial H}{\partial\mu}(w-H)^{-1}\right].$$

Since $(z - H)^{-1}$, $(w - H)^{-1}$, and $\varphi(H)$ commute, z and w can effectively be interchanged in the trace, so that the theorem follows.

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