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Entropy of ideal quantum gases as a Lie function

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Received 2 February 1993, in final form 27 September 1993

Abstract. We investigate the Lie series representation of the canonical transformations in a complex phase space. It is shown that any canonical mapping in the complex domain can be labelled by two different functions. One of these functions corresponds to an observable in the sense of classical mechanics. The second one has special analytic properties and can be used to form quantities which are important in quantum statistical mechanics. In particular we show that the entropy of ideal quantum gases generates a special canonical transformation and, moreover, the entropy itself can be represented as a Lie function formed by a special characteristic function.

1. Introduction

In mathematics it is well known that investigation in the complex domain usually simplifies a problem, rather than making it more complicated. This is a motivation to study Hamiltonian mechanics in a complex formulation. Such a formulation seems to be very natural because one complex equation of motion is the same as two real ones. However, the complex treatment only of the harmonic oscillator makes its way into the physical textbooks. On the other hand, complex structures play an important role in quantum mechanics. For instance, Lahti and Maczynski [1] have shown that the Heisenberg inequality can only be derived in the complex field framework. In the classical limit of quantum mechanics one separates the Schrödinger equation into real and imaginary parts and only the real phase of the wavefunction is important for $\hbar \to 0$. But the connection between the commutators and Poisson brackets is difficult to explain in this limit. One may hope that the connection between quantum and classical mechanics becomes more apparent if the same number field for the mathematical apparatus is used in both theories. In fact, Strocchi [2] has shown that classical and quantum mechanics may be embedded in the same formulation by using complex coordinates. A similar treatment can also be found in [3], where the generator aspect of observables is emphasized.

The investigation of the generator aspect of observables is always connected with the study of the basic transformation properties of the corresponding theory. In this paper we are interested in the canonical transformation groups and their action on a complex phase space. In order to study the generator aspect of canonical transformations, the Lie series representation is more appropriate than the generating function which depends upon old and new coordinates. Compared to the standard result in a real phase space (cf [4, 5]) there are some differences because of the complex nature of the generating function. In particular, Lie transformations exist which are not canonical ones [6]. In this paper we demonstrate that any canonical transformation in the complex phase space can be marked by two different functions. One of these functions is a real generating function which corresponds to an observable in the sense of classical mechanics. The second one is a complex-valued function

with special analytic properties (holomorphic or antiholomorphic). Moreover, an example is given which shows that one can form quantities from this complex function which are important in quantum statistical mechanics. This suggest that the transformation apparatus of the classical theory contains more basic physical information than is generally supposed.

In order to make the paper self-contained some of the properties of Lie transformations in a complex phase space are given in section 2. In section 3 we discuss the condition which selects the canonical transformations from the Lie transformations and in section 4 some special transformations are considered. Finally, we show that the entropy of ideal quantum gases can be represented as a Lie function.

2. Lie transformations in complex phase space

We consider coordinate transformations in a finite dimensional complex vector space of the type

$$z_k \rightarrow w_k = w_k(z_j, z_j^*)$$

where $z_k (k = 1...N)$ are the old and w_k the new coordinates, respectively (* denotes the complex conjugate). Such a transformation is a canonical one if the new coordinates fulfil the conditions

$$\{w_j, w_k\} = 0 \qquad \{w_j, w_k^*\} = \delta_{jk} \tag{2.1}$$

where the Lie product of two complex-valued functions $A(z_k, z_k^*)$ and $B(z_k, z_k^*)$ is defined by the Poisson bracket operation

$$\{A, B\} = \sum_{k=1}^{N} \left(\frac{\partial A}{\partial z_k} \frac{\partial B}{\partial z_k^*} - \frac{\partial A}{\partial z_k^*} \frac{\partial B}{\partial z_k} \right).$$
(2.2)

Let A be a specified function depending upon z_k and z_k^* . Then associated with A is a linear differential operator (the Lie operator, the Hamiltonian vector field)

$$\hat{X}_{A} = \sum_{k=1}^{N} \left(\frac{\partial A}{\partial z_{k}} \frac{\partial}{\partial z_{k}^{*}} - \frac{\partial A}{\partial z_{k}^{*}} \frac{\partial}{\partial z_{k}} \right).$$
(2.3)

It is straightforward to calculate the commutator of two such operators

$$[\hat{X}_A, \hat{X}_B] = \hat{X}_{\{A,B\}}$$
(2.4)

i.e. the Lie operators form a Lie algebra under commutation which is homomorphic to the Poisson bracket algebra of the phase space functions.

Lie series are defined by infinite operator power series, where the exponential series

$$\exp(\hat{X}_A) = \sum_{n=0}^{\infty} \frac{1}{n!} (\hat{X}_A)^n \qquad (\hat{X}_A)^0 = 1$$

are of particular interest. We shall call the action of $\exp(\hat{X}_A)$ on phase space functions a Lie transformation associated with the complex valued generating function $A(z_k, z_k^*)$. There are

some basic properties of the Lie transformations which are important for their applications (β and γ are complex numbers)

$$(e^{\hat{X}_{A}})^{*}B = (e^{\hat{X}_{A}}B^{*})^{*} = e^{-\hat{X}_{A}^{*}}B \qquad e^{\hat{X}_{A}}(\beta B + \gamma C) = \beta e^{\hat{X}_{A}}B + \gamma e^{\hat{X}_{A}}C$$

$$e^{\hat{X}_{A}}(BC) = (e^{\hat{X}_{A}}B)(e^{\hat{X}_{A}}C) \qquad e^{\hat{X}_{A}}\{B, C\} = \{e^{\hat{X}_{A}}B, e^{\hat{X}_{A}}C\}$$

$$e^{\hat{X}_{A}}F(z_{k}, z_{k}^{*}) = F(e^{\hat{X}_{A}}z_{k}, e^{\hat{X}_{A}}z_{k}^{*}).$$
(2.5)

The proofs of these properties are based upon the power series definition and can be adopted from Steinberg [5]. There are some other exponential identities which are important for applications of Lie series. For example

$$e^{\hat{X}_{A}}\hat{X}_{B}e^{-\hat{X}_{A}} = \hat{X}_{e^{\hat{X}_{A}}B} \qquad e^{\hat{X}_{A}}e^{\hat{X}_{B}} = \exp(\hat{X}_{e^{\hat{X}_{A}}B})e^{\hat{X}_{A}}.$$
 (2.6)

The product of two Lie transformations is once more a single Lie transformation. The celebrated Baker-Campbell-Hausdorff (BCH) theorem then shows how one must combine a product of exponentials into an exponential of a sum [4,5,7]. Then we can write

$$e^{\hat{X}_C} = e^{\hat{X}_A} e^{\hat{X}_B}$$

with

$$\hat{X}_{C} = \hat{X}_{A} + \hat{X}_{B} + \frac{1}{2}[\hat{X}_{A}, \hat{X}_{B}] + \frac{1}{12}[\hat{X}_{A-B}, [\hat{X}_{A}, \hat{X}_{B}]] + \cdots$$
(2.7)

Closed formulae can be given for certain Lie operators forming finite algebras [7]. Consequently, (2.4) provides a connection between the generating functions

$$C = A + B + \frac{1}{2} \{A, B\} + \frac{1}{12} \{A - B, \{A, B\}\} + \cdots .$$
(2.8)

We note that the mapping $A \rightarrow \hat{X}_A$ is linear and unique, but it is not invertible. If there are two operators with $\hat{X}_A = \hat{X}_B$ we can conclude only that the difference (A - B) has no functional dependence on the complex coordinates z_k, z_k^* , but it may depend upon some additional parameters. Therefore the function C in (2.8) is determined up to a constant only which may depend on these parameters. However, the constant is a trivial one because the phase space functions serve as generating functions and the Lie operator is always unique. We shall call the phase space function $C(z_k, z_k^*)$ which arises from the BCH formula (2.8) a Lie function formed by A and B. There are some cases in which the Lie function has special properties. For instance, let $A(z_k, z_k^*)$ be an arbitrary function and $B = A^*(z_k, z_k^*)$ the conjugate complex function. Then

$$e^{\hat{X}_C} = e^{\hat{X}_A} e^{\hat{X}_{A^*}}$$

and with

$$e^{-\hat{X}_{C^*}} = (e^{\hat{X}_C})^* = (e^{\hat{X}_A} e^{\hat{X}_{A^*}})^* = e^{-\hat{X}_{A^*}} e^{-\hat{X}_A} = e^{-\hat{X}_C}$$

one obtains

$$C = C^* \tag{2.9}$$

i.e. the Lie function is real (up to the trivial constant). Up to now, we have not discussed the convergence of Lie series expansions. This is a complicated matter; however, some estimates are known (cf [8]). Moreover, there are only very special cases in which the sum can be done in closed form. One of these cases is realized for holomorphic or antiholomorphic generating functions. These functions are defined by

$$\frac{\partial G}{\partial z_k^*} = \{z_k, G\} = 0 \quad \Leftrightarrow \quad G = G(z_k) = \text{holomorphic}$$
$$\frac{\partial F}{\partial z_k} = \{F, z_k^*\} = 0 \quad \Leftrightarrow \quad F = F(z_k^*) = \text{antiholomorphic}$$

and the corresponding Lie transformations become

$$e^{\hat{X}_{G(\omega)}} \begin{pmatrix} z_k \\ z_k^* \end{pmatrix} = \begin{pmatrix} z_k \\ z_k^* + \hat{X}_G z_k^* \end{pmatrix} = \begin{pmatrix} z_k \\ z_k^* + \partial G(z)/\partial z_k \end{pmatrix}$$
$$e^{\hat{X}_{F(\omega^*)}} \begin{pmatrix} z_k \\ z_k^* \end{pmatrix} = \begin{pmatrix} z_k + \hat{X}_F z_k \\ z_k^* \end{pmatrix} = \begin{pmatrix} z_k - \partial F(z^*)/\partial z_k^* \\ z_k^* \end{pmatrix}$$
(2.10)

i.e. the infinite sum reduces to a single term and the transformation is a gauge type one. Another case is given by the phase transformations of the complex coordinates. Let

$$J = \sum_{k=1}^{N} z_k^* z_k$$

be the unitary invariant and let α be a real parameter. The sum can be done in closed form and one finds ($i^2 = -1$)

$$\mathrm{e}^{\mathrm{i}\alpha\hat{X}_{j}}\begin{pmatrix}z_{k}\\z_{k}^{*}\end{pmatrix}=\begin{pmatrix}\mathrm{e}^{-\mathrm{i}\alpha}z_{k}\\\mathrm{e}^{\mathrm{i}\alpha}z_{k}^{*}\end{pmatrix}$$

Moreover, with $\alpha = \pi (+2k\pi)$ we have a reflection of all coordinates

$$e^{i\pi\hat{X}_{J}}\begin{pmatrix} z_{k}\\ z_{k}^{*} \end{pmatrix} = -\begin{pmatrix} z_{k}\\ z_{k}^{*} \end{pmatrix}.$$
(2.11)

3. Canonical transformations

In [6] we investigated two types of transformations of the complex coordinates given by

(i)
$$T_{\mathbf{B}}(\Phi): \qquad w_k = \exp(-\hat{X}_{\Phi})z_k$$
 (3.1)

(ii)
$$T_{\rm F}(\Psi)$$
: $w_k = \exp(\hat{X}_{\Psi}) z_k^*$

where Φ , Ψ are complex valued generating functions. Therefore the transformations (i), (ii) depend upon two real functions—the real and the imaginary part, respectively, of Φ or Ψ . Instead of $T_{\rm B}(\Phi)$ we sometime will use the notation $T_{\rm B}(S, \Omega)$ to indicate the dependence upon the real part $S \equiv \text{Re}(\Phi)$ and the imaginary part $\Omega \equiv \text{Im}(\Phi)$.

The first type (i) has an infinitesimal limit whereas (ii) is not connected with the identity. Also for the differential characterization given in [2] one obtains these two types, i.e. transformations which are connected with the identity and those which are not. The transformations (3.1) are canonical mappings if and only if the generating functions fulfil the conditions

(i)
$$\delta_{kj} = -e^{\hat{X}_{\Phi^*}} \hat{X}_{z_j^*} e^{-\hat{X}_{\Phi^*}} e^{-\hat{X}_{\Phi}} z_k$$
(3.2)

(ii)
$$\delta_{kj} = -e^{-\hat{X}_{\psi^*}}\hat{X}_{z_j}e^{\hat{X}_{\psi^*}}e^{\hat{X}_{\psi}}z_k^*.$$

These conditions directly follow from (2.1) by use of (2.5); however, they can be further simplified. Multiplication with $\exp(-\hat{X}_{\Phi^*})$ and $\exp(\hat{X}_{\Psi^*})$ from the left and application of $\hat{X}_{z_j^*} = -\partial/\partial z_j$ and $\hat{X}_{z_j} = \partial/\partial z_j^*$ yields

(i)
$$\delta_{kj} = \frac{\partial}{\partial z_j} \left(e^{-\hat{X}_{\Phi^*}} e^{-\hat{X}_{\Phi}} z_k \right)$$

(iI)
$$\delta_{kj} = -\frac{\partial}{\partial z_j^*} \left(e^{\hat{X}_{\Psi^*}} e^{\hat{X}_{\Psi}} z_k^* \right) \,.$$

We define the Lie functions $\xi(z_k, z_k^*)$ and $\eta(z_k, z_k^*)$ by setting

$$e^{-\hat{X}_{\xi}} \equiv e^{-\hat{X}_{\Phi^*}} e^{-\hat{X}_{\Phi}} \qquad e^{\hat{X}_{\eta}} \equiv e^{\hat{X}_{\Psi^*}} e^{\hat{X}_{\Psi}}$$
(3.3)

and obtain after integration with respect to the coordinates

(i)
$$\exp(-\hat{X}_{\xi})z_k = z_k + F_k(z_j^*)$$
 (3.4)

(ii)
$$\exp(\hat{X}_{\eta})z_k^* = -z_k^* + G_k(z_j)$$

where $F_k(z_j^*)$ and $G_k(z_j)$ are antiholomorphic and holomorphic functions, respectively. In the next step we show that the N functions $F_k(z_j^*)$ can be derived from a single function $F(z_j^*)$. Differentiation of (3.4)(i) with respect to z_j^* provides

$$\frac{\partial F_k}{\partial z_j^*} = \frac{\partial}{\partial z_j^*} \left(e^{-\hat{X}_k} z_k \right) = \{ z_j, e^{-\hat{X}_k} z_k \}$$

and therefore

$$\frac{\partial F_k}{\partial z_j^*} - \frac{\partial F_j}{\partial z_k^*} = \{z_j, e^{-\hat{X}_{\xi}} z_k\} + \{e^{-\hat{X}_{\xi}} z_j, z_k\}.$$

On the right-hand side we add a zero given by

$$0 = -\{z_j, z_k\} - e^{-\hat{X}_{\xi}}\{z_j, z_k\}$$

and use the properties of the Poisson bracket and the bracket preservation property of Lie series in (2.5) to find

$$\frac{\partial F_k}{\partial z_j^*} - \frac{\partial F_j}{\partial F_k} = -\{(\mathbf{e}^{-\hat{\mathbf{X}}_k} - 1)z_j, (\mathbf{e}^{-\hat{\mathbf{X}}_k} - 1)z_k\} = -\{F_j, F_k\}$$

where the last equality follows from (3.4)(i). The Poisson bracket of F_j and F_k vanishes because all F_k are antiholomorphic functions. Therefore we obtain

$$\frac{\partial F_k}{\partial z_j^*} - \frac{\partial F_j}{\partial z_k^*} = 0 \qquad \Rightarrow \qquad F_k(z_j^*) = \frac{\partial F(z_j^*)}{\partial z_k^*} \tag{3.5}$$

i.e. the F_k are gradient type functions. An analogous calculation is also possible for the functions $G_k(z_j)$ in (3.4)(ii) and yields

$$\frac{\partial G_k}{\partial z_j} - \frac{\partial G_j}{\partial z_k} = 0 \qquad \Rightarrow \qquad G_k(z_j) = \frac{\partial G(z_j)}{\partial z_k}.$$
(3.6)

With (3.5) and (3.6), equation (3.4) becomes

(i)
$$\exp(-\hat{X}_{\xi})z_{k} = z_{k} + \frac{\partial F(z_{j}^{*})}{\partial z_{k}^{*}}$$
(3.7)

. . .

(ii)
$$\exp(\hat{X}_{\eta})z_k^* = -z_k^* + \frac{\partial G(z_j)}{\partial z_k}$$

We shall call the functions $F(z_j^*)$ and $G(z_j)$ the characteristic functions. Note that the generating functions Φ , Ψ and the characteristic functions F, G are not independent. The connection is given just by (3.3) and (3.7). In order to find this connection in a more direct form, we study the action of $\exp(-\hat{X}_{\xi})$ on the conjugate complex coordinates z_k^* . We start with the complex conjugate of (3.7)(i),

$$z_k^* + \frac{\partial F^*(z_j^*)}{\partial z_k} = \exp(\hat{X}_{\xi^*}) z_k^* = \exp(\hat{X}_{\xi}) z_k^*$$

where we have used the fact that $\xi(z_k, z_k^*)$ is a real Lie function which arises from (3.3) and (2.9). Consequently,

$$\mathrm{e}^{-\hat{X}_{i}}z_{k}^{*}=z_{k}^{*}-\mathrm{e}^{-\hat{X}_{i}}\frac{\partial F^{*}(z_{j}^{*})}{\partial z_{k}}$$

and with

$$e^{-\hat{X}_{\ell}}\left(\frac{\partial F^{*}(z_{j}^{*})}{\partial z_{k}}\right) = e^{-\hat{X}_{\ell}}\tilde{F}_{k}(z_{j}) = \tilde{F}_{k}(e^{-\hat{X}_{\ell}}z_{j}) = \tilde{F}_{k}(z_{j} + \frac{\partial F(z^{*})}{\partial z_{j}^{*}}) = \frac{\partial}{\partial z_{k}}F^{*}\left(z_{j}^{*} + \frac{\partial F^{*}(z^{*})}{\partial z_{j}}\right)$$
(3.8)

we have

$$e^{-\hat{X}_{k}}z_{k}^{*} = z_{k}^{*} - \frac{\partial}{\partial z_{k}}F^{*}\left(z_{j}^{*} + \frac{\partial F^{*}(z^{*})}{\partial z_{j}}\right).$$
(3.9)

A similar treatment for the type (ii) transformations yields

$$e^{\hat{X}_{\eta}}z_{k} = -z_{k} - \frac{\partial}{\partial z_{k}^{*}}G^{*}\left(-z_{j} + \frac{\partial G^{*}(z)}{\partial z_{j}^{*}}\right).$$
(3.10)

It is easy to show that (3.7), (3.8) and (3.9) are equivalent to

(i)
$$e^{-\hat{X}_{\xi}} \begin{pmatrix} z_k \\ z_k^* \end{pmatrix} = e^{-\hat{X}_{F(z^*)}} e^{-\hat{X}_{F^*(z^*)}} \begin{pmatrix} z_k \\ z_k^* \end{pmatrix}$$
 (3.11)

(ii)
$$e^{\hat{X}_{\eta}} \begin{pmatrix} z_k \\ z_k^* \end{pmatrix} = e^{-\hat{X}_{G(z)}} e^{i\pi \hat{X}_J} e^{-\hat{X}_{G^*(z)}} \begin{pmatrix} z_k \\ z_k^* \end{pmatrix}$$

The proof can be found by a straightforward calculation which starts from (3.10) and uses (2.5), (2.10) and (2.11).

With (3.10) we know the action of $\exp(-\hat{X}_{\xi})$ and $\exp(\hat{X}_{\eta})$ on the complex coordinates and therefore we also know the action on an arbitrary phase space function

$$e^{-\hat{X}_{\xi}}A(z_{k}, z_{k}^{*}) = e^{-\hat{X}_{F(z^{*})}} e^{-\hat{X}_{F^{*}(z^{*})}}A(z_{k}, z_{k}^{*}) \qquad e^{\hat{X}_{\eta}}A(z_{k}, z_{k}^{*}) = e^{-\hat{X}_{G(z)}} e^{i\pi\hat{X}_{J}} e^{-\hat{X}_{G^{*}(z)}}A(z_{k}, z_{k}^{*}).$$
(3.12)

Since this is true for any function $A(z_k, z_k^*)$, we have the operator relations

(i)
$$e^{-\hat{X}_{\xi}} = e^{-\hat{X}_{\phi^*}} e^{-\hat{X}_{\phi}} = e^{-\hat{X}_{F(x^*)}} e^{-\hat{X}_{F^*(x^*)}}$$

(3.13)

(ii)
$$e^{\hat{X}_{\eta}} = e^{\hat{X}_{\psi^*}} e^{\hat{X}_{\psi}} = e^{-\hat{X}_{G(x)}} e^{i\pi \hat{X}_J} e^{-\hat{X}_{G^*(x)}}$$

i.e. the Lie transformations (3.1) providing they converge, are canonical mappings if there exist characteristic functions $F(z^*)$ and G(z) such that the generating functions $\Phi(z, z^*)$ and $\Psi(z, z^*)$ satisfy (3.12). The occurrence of the reflection operator in (3.12)(ii) is a direct indication that the type (ii) transformations are not connected with the identity.

Because of (3.11) the following identities are valid for the Lie functions $\xi(z, z^*)$ and $\eta(z, z^*)$:

$$\xi(z_k, z_k^*) = e^{-\hat{X}_{F(z^*)}} e^{-\hat{X}_{F^*(z^*)}} \xi(z_k, z_k^*) \qquad \eta(z_k, z_k^*) = e^{-\hat{X}_{G(z)}} e^{i\pi \hat{X}_J} e^{-\hat{X}_{G^*(z)}} \eta(z_k, z_k^*)$$

One finds a more explicit form after application of (2.5) and (2.10) on the right-hand side. These are identities for the Lie functions; however, we are mainly interested in the properties of the generating functions. Therefore we investigate the action of the transformation operator $\exp(-\hat{X}_{\Phi})$ on the complex conjugate coordinates z_k^* . The complex conjugate of (3.7) is given by

$$e^{\hat{X}_{\Phi}}e^{\hat{X}_{\Phi^*}}z_k^*=z_k^*+\frac{\partial F^*(z_j^*)}{\partial z_k^*}$$

or

 $\mathrm{e}^{-\hat{X}_{\Phi}}z_k^* = \mathrm{e}^{\hat{X}_{\Phi^*}}z_k^* - \mathrm{e}^{-\hat{X}_{\Phi}}\frac{\partial F^*(z_j^*)}{\partial z_k}\,.$

With

$$w_k^* = \mathrm{e}^{\hat{X}_{\Phi^*}} z_k^*$$

and

$$e^{-\hat{X}_{\Phi}}\left(\frac{\partial F^{*}(z_{j}^{*})}{\partial z_{k}}\right) = \frac{\partial F^{*}(w_{j}^{*})}{\partial w_{k}}$$

one obtains

$$e^{-\hat{X}_{\phi}}z_{k}^{*} = w_{k}^{*} - \frac{\partial F^{*}(w_{j}^{*})}{\partial w_{k}}.$$
 (3.14)

Equations (3.1) and (3.13) then determine the action of the transformation operator on the complex coordinates

$$\mathbf{e}^{-\hat{X}_{\Phi}} \begin{pmatrix} z_k \\ z_k^* \end{pmatrix} = \begin{pmatrix} w_k \\ w_k^* - \partial F^*(w_j^*) / \partial w_k \end{pmatrix}.$$
(3.15)

For the type (ii) transformations a similar treatment yields

$$e^{\hat{X}_{\Psi}} \begin{pmatrix} z_k \\ z_k^* \end{pmatrix} = \begin{pmatrix} -w_k^* + \partial G^*(w_j^*) / \partial w_k \\ w_k \end{pmatrix}.$$
(3.16)

With (3.14) and (3.15) we also know the action of the transformation operators on arbitrary phase space functions $A(z_k, z_k^*)$. In particular, one finds for the generating function

$$\Phi(z_k, z_k^*) = \mathrm{e}^{-\hat{X}_{\Phi}} \Phi(z_k, z_k^*) = \Phi(\mathrm{e}^{-\hat{X}_{\Phi}} z_k, \mathrm{e}^{-\hat{X}_{\Phi}} z_k^*)$$

and, with (3.14),

$$\Phi(z_k, z_k^*) = \Phi\left(w_k, w_k^* - \frac{\partial F^*(w_j^*)}{\partial w_k}\right).$$
(3.17)

Moreover, considering the type (ii) transformations,

$$\Psi(z_k, z_k^*) = \Psi\left(-w_k^* + \frac{\partial G^*(w_j^*)}{\partial w_k}, w_k\right).$$
(3.18)

Equation (3.16) clearly shows that the generating function Φ is not an invariant function for all non-trivial F. This seems to be a contradiction to the Lie series representation of canonical transformations in a real phase space because in that case the (real) generating function is always an invariant one. We discuss the solution of this problem in section 4. The investigation of (3.17) is a more complicated matter because there is an additional exchange of the slots of the independent variables in this function. There is at least one example with $G \neq 0$, such that Ψ is an invariant (cf section 5). However, we expect that this is not the generic case.

4. Special types of canonical mappings

In order to study the meaning of the generating and characteristic functions, respectively, we consider some special canonical transformations. First of all we look for type (i) transformations which have an invariant generating function. With (3.16) we conclude that these mappings are characterized by

$$F(z_k^*) = c(=0) \tag{4.1}$$

where c is an arbitrary constant which can be chosen equal to zero. Moreover, (3.12)(i) reduces to

$$\mathrm{e}^{-\hat{X}_{\Phi^*}}\,\mathrm{e}^{-\hat{X}_{\Phi}}=1$$

i.e. the complex conjugate function Φ^* generates the inverse transformation. This is realized by

$$\Phi^* = -\Phi \Leftrightarrow \Phi(z, z^*) = i\Omega(z, z^*) \qquad \Omega = \Omega^*$$
(4.2)

i.e. the generating function is a pure imaginary one. Note that we have neglected a trivial constant in (4.2). Then the real function Ω is an invariant under the transformation which they generate. Of course, this type of transformation is the counterpart to that in a real phase space (cf [4]) and the function Ω is an observable in the sense of classical mechanics. Particularly, the motion of a classical physical system is determined by the unfolding-in-time of a canonical transformation. The generating function of this special type of transformations is the real Hamiltonian $H(z_k, z_k^*)$. By setting

$$\Phi = i\Omega = -itH$$

and taking the infinitesimal limit $t \rightarrow 0$ in (3.1)(i), one obtains the equations of motion

$$\dot{z}_k = i\hat{X}_H z_k = -i\frac{\partial H}{\partial z_k^*}$$
(4.3)

where the overdot indicates differentiation with respect to the time parameter. Of course, equation (4.3) are the famous Hamiltonian equations in a complex form (cf [2]).

Canonical transformations are one of the cornerstones of classical mechanics; however, our consideration shows that a very small part of the full group is usually used. All mappings with $F(z^*) \neq 0$ and all mappings of the type (ii) do not play any role in classical mechanics. Then the most interesting question is whether these other transformations have an application in other fields of physics. Before we attempt an answer to this question, the transformations with $F \neq 0$ must be studied. Let $\Phi(z, z^*)$ and $F(z^*)$ be sufficiently small. Then (3.12)(i) in the neighbourhood of the identity reduces to

$$1 - \hat{X}_{\Phi^*} - \hat{X}_{\Phi} + \cdots = 1 - \hat{X}_{F(z^*)} - \hat{X}_{F^*(z^*)} + \cdots$$

and therefore

$$S(z, z^*) \equiv \operatorname{Re}[\Phi(z, z^*)] = \frac{1}{2}(F(z^*) + F^*(z^*)) + \cdots$$
(4.4)

i.e. the characteristic function F determines the real part $S(z, z^*)$ of the generating function in the limit of infinitesimal transformations. This is valid in the case of some global transformations too. Let

$$\Phi(z, z^*) = S(z, z^*) + i\Omega(z, z^*)$$

and

$$\{\Phi, \Phi^*\} = 0 \quad \Leftrightarrow \quad \{S, \Omega\} = 0$$

then it is easy to see that (3.12)(i) yields

$$\xi(z_k, z_k^*) = 2S(z_k, z_k^*) \tag{4.5}$$

i.e. the Lie function ξ formed by F and F^* provides the real part S of the generating function. Moreover, the imaginary part Ω of the generating function is not fixed by means of (3.12)(i) and therefore it can be arbitrarily chosen. We see that there are two possibilities for characterizing the canonical transformations of the type (i). Suppose that S and Ω are given and therefore $T_B(S, \Omega)$ is known. Then one has to check whether there exists a function F such that condition (3.12) is fulfilled. On the other hand, given an arbitrary antiholomorphic F and a real function Ω , one has to calculate the real part S according to (3.12). After that one can form the transformation by computation of the Lie series. The analysis of (3.12) may be a complicated matter in both cases, however, we have, at least in principle,

$$(F, \Omega) \Leftrightarrow (S, \Omega) \Rightarrow T_{\mathrm{B}}(\Phi)$$
 (4.6)

i.e. we can mark the transformations by the pair (S, Ω) or (F, Ω) . A similar statement is also valid in the case of the type (ii) transformations.

A very important question is connected with the combination of the type (i) and (ii) transformations, respectively. We consider the following special case only. Let Φ and Ψ be the generating functions of the type (i) and (ii) respectively. Then we consider all transformations which have the same characteristic function, i.e.

$$G^*(z_j) = F(z_j^*)$$
 (4.7)

Hence, (3.12) becomes

 $e^{-\hat{X}_{\xi}} = e^{-\hat{X}_{F}} e^{-\hat{X}_{F^{*}}} \qquad e^{\hat{X}_{\pi}} = e^{-\hat{X}_{F^{*}}} e^{i\pi\hat{X}_{f}} e^{-\hat{X}_{F}}$

moreover, after elimination of $\exp(-\hat{X}_{F^*})$

$$e^{-\hat{X}_{\xi}} = e^{-\hat{X}_{F}} e^{\hat{X}_{\eta}} e^{\hat{X}_{F}} e^{-i\pi\hat{X}_{J}}$$

Using (2.6) and (2.10) one obtains

$$\mathrm{e}^{-\hat{X}_{\xi}}\,\mathrm{e}^{\mathrm{i}\pi\,\hat{X}_{J}}=\exp\hat{X}_{\eta(z_{k}+\partial\,F/\partial z_{k}^{*},z_{k}^{*})}$$

and with (2.7) and (2.8)

$$\eta(z_k + \frac{\partial F}{\partial z_k^*}, z_k^*) = -\xi + i\pi J - \frac{i\pi}{2} \{\xi, J\} + \cdots$$
(4.8)

i.e. the Lie functions ξ and η are not independent for $G^* = F$. We note that (4.8) is not unique because the generating function of the reflection operator is not unique. This defect can be removed by the substitution $i\pi \to i\pi + i2\pi n$, $n = 0, \pm 1, \ldots$ in (4.8).

In the remaining part of this section we give some heuristic arguments which show that the real part of the generating function can possibly be connected with the entropy. We begin with the observation that there are equivalent transformations with

$$T_{\rm B}(S,\,\Omega=0) = T_{\rm B}(S=0,\,\Omega).$$
 (4.9)

which means that different generating functions generate the same mapping of the complex coordinates. A very simple example of this type is given by the functions

$$\Phi_1 = \sum_{j=1}^N a_j \operatorname{Re}(z_j) \qquad \Phi_2 = -i \sum_{j=1}^N a_j \operatorname{Im}(z_j) \qquad a_j \in \mathbb{R}^N$$

where both functions generate the same shift of the complex coordinates z_k given by

$$w_k = e^{-\hat{X}_{\Phi_1}} z_k = e^{-\hat{X}_{\Phi_2}} z_k = z_k + \frac{a_k}{2}$$

Of course, condition (3.12)(i) is fulfilled in the case of Φ_2 with a trivial characteristic function $F_2 = 0$. On the other hand, Φ_1 corresponds to a transformation with a characteristic function $F_1(z^*) = \sum_k a_k z_k^*$. We note that \hat{X}_{F_1} and $\hat{X}_{F_1^*}$ commute and the evaluation of the BCH series in (3.12) is a simple task.

Suppose that (4.9) is also true for other functions, in particular for $\Omega = -tH$. Then we have

$$\exp(-\hat{X}_S)z_k = \exp(\mathrm{i}t\hat{X}_H)z_k \,.$$

In order to compare the two series we assume S = S(H). Hence,

$$\exp\left(-\frac{\mathrm{d}S}{\mathrm{d}H}\hat{X}_H\right)z_k=\exp(\mathrm{i}t\hat{X}_H)z_k\,.$$

Then the comparison shows that the series are linked by the substitution

$$it \longrightarrow \frac{dS}{dH}$$
 (4.10)

where the negative sign is not important because it can be absorbed in the definition of the parameter t. A similar transition from quantum mechanics to statistics is well known and can be realized by

$$it \longrightarrow \frac{1}{k_{\rm B}T}$$
 (4.11)

where $k_{\rm B}$ is the Boltzmann constant and T is the thermodynamic temperature. In the case that we accept (4.11), the comparison with (4.10) yields

$$\frac{\mathrm{d}S}{\mathrm{d}H} \sim \frac{1}{k_{\mathrm{B}}T} \tag{4.12}$$

which shows the thermodynamic relation between entropy (represented by S), energy (represented by H) and the temperature T. Of course, this is not an exact proof, however, the consideration shows the direction in the search for an interpretation of the real part $S(z_k, z_k^*)$.

One of the most fundamental properties of the entropy is the increase during an irreversible physical process. A similar property can be found for the real part of the generating function too. Let Φ , F be the generating and characteristic function, respectively, of an infinitesimal canonical transformation.

$$\Phi(z, z^*) = \delta \varepsilon S - i \delta t H \qquad F(z^*) = \delta \varepsilon f(z^*) \tag{4.13}$$

where $\delta \varepsilon$ and δt are small real parameters. Using (4.4) we get

$$S(z, z^*) = \frac{1}{2}(f(z^*) + f^*(z^*))$$
 $H = \text{arbitrary}$

and the infinitesimal transformation of the coordinates is given by the linear terms in the parameters $\delta \varepsilon$ and δt

$$\delta z_k = w_k - z_k = \delta \varepsilon \frac{\partial S}{\partial z_k^*} - i \delta t \frac{\partial H}{\partial z_k^*} = \frac{\delta \varepsilon}{2} \frac{\partial f}{\partial z_k^*} - i \delta t \frac{\partial H}{\partial z_k^*}.$$

Now we calculate the increment of $S(z_k, z_k^*)$ with respect to this transformation

$$\delta S = \sum_{k=1}^{N} \left(\frac{\partial S}{\partial z_k} \delta z_k + \frac{\partial S}{\partial z_k^*} \delta z_k^* \right) \,.$$

Inserting the infinitesimal transformations δz_k , δz_k^* one obtains

$$\delta S = 2\delta \varepsilon \sum_{k=1}^{N} \left(\frac{\partial S}{\partial z_k} \frac{\partial S}{\partial z_k^*} \right) - i\delta t \{S, H\}.$$
(4.14)

Hence, in the special case S = S(H) the Poisson bracket $\{S, H\}$ vanishes, i.e. the function S is a conserved quantity with respect to the time evolution (variation of δt). Nevertheless, we find with $\delta \varepsilon > 0$ an increment of S under the transformation given by

$$\delta S = \frac{\delta \varepsilon}{2} \sum_{k=1}^{N} \left| \frac{\partial f}{\partial z_{k}^{*}} \right|^{2} \ge 0$$
(4.15)

where the connection $S = \frac{1}{2}(f(z^*) + f^*(z^*))$ is used on the right-hand side. More precisely, (4.15) shows the property of monotony only because the sign of $\delta \varepsilon$ can be arbitrarily chosen. It must be underlined that the validity of (4.15) is not secured for $\{S, H\} \neq 0$ and in the case of global transformations. Of course, the infinitesimal transformation with $\delta \varepsilon \neq 0$ also changes the imaginary part of the generating function. The corresponding increment is given by

$$\delta H = \frac{\delta \varepsilon}{2} \sum_{k=1}^{N} \left(\frac{\partial H}{\partial z_k} \frac{\partial f}{\partial z_k^*} + \frac{\partial H}{\partial z_k^*} \frac{\partial f^*}{\partial z_k} \right) .$$
(4.16)

We close this section with the remark that by elimination of $\delta \varepsilon$ in (4.15) and (4.16) a direct connection between δS and δH can be obtained.

5. Entropy of ideal quantum gases

The discussion of section 4 indicates that there are some hints that the canonical transformations with a non-trivial characteristic function can be connected with important physical quantities. Then the real problem is the realization of examples of exact global transformations. In [6,9] we have investigated two special types of transformations, where the generating function is determined by the entropy of an ideal quantum gas. However, the connection between the generating and characteristic functions has not been analysed up to now. Here we shall fill this gap. In order to make this section self-contained, a modified derivation of the transformations in question is given which is based on the content of section 3.

At first we consider the type (i) transformations and choose the following characteristic function

$$F(z_k^*) = \sum_{k=1}^{N} a_k \ln(z_k^*)$$
(5.1)

where the a_k are real parameters. The logarithmic function $\ln(z^*)$ is considered as the principal branch of the general logarithmic function. Let $\Phi(z_k, z_k^*)$ be the generating function with

$$\{\Phi, \Phi^*\} = 0. \tag{5.2}$$

Then the real part $\operatorname{Re}(\Phi) = S_{(i)}(z_k, z_k^*)$ of the generating function is given by the Lie function ξ formed by F and F^* (cf (4.5))

$$e^{-\hat{X}_{t}} = e^{-2\hat{X}_{s_{0}}} = e^{-\hat{X}_{F}} e^{-\hat{X}_{F^{*}}}.$$
(5.3)

Instead of (5.2) the simple assumption $Im(\Phi) = 0$ can also be used to reduce (3.12) to (5.3). Taking notice of (2.8) and (5.1), the first few terms of the BCH expansion are given by

$$2S_{(i)} = F^* + F + \frac{1}{2}\{F^*, F\} + \frac{1}{12}\{(F^* - F), \{F^*, F\}\} + \cdots$$

where

$$F^{*} + F = \sum_{k} a_{k} \ln I_{k} \qquad \frac{1}{2} \{F^{*}, F\} = \frac{1}{2} \sum_{k} \frac{a_{k}^{2}}{I_{k}}$$

$$\frac{1}{12} \{(F^{*} - F), \{F^{*}, F\}\} = -\frac{1}{6} \sum_{k} \frac{a_{k}^{3}}{I_{k}^{2}} \cdots$$
(5.4)

where we have defined the abbreviation $I_k = z_k^* z_k$. The form of (5.4) shows that the BCH series can be considered as a power series in the parameter a_k (cf [4]), i.e. in the sense of perturbation theory the first few terms determine an approximation of $S_{(i)}(z_k, z_k^*)$ for all sufficiently small a_k . Furthermore we observe that the right-hand side of (5.4) depends upon the I_k only. This dependence suggest an ansatz of the form

$$S_{(i)} = S_{(i)}(z_k, z_k^*) = S_{(i)}(I_k) \quad .$$
(5.5)

In order to determine the function $S_{(i)}(I_k)$ we use (3.7)(i) which can be considered as a consequence of (3.12)(i). Inserting the characteristic function (5.1) equation (3.7)(i) becomes

$$\exp(-\hat{X}_{\xi})z_k = \exp(-2\hat{X}_{S_{(1)}})z_k = z_k + \frac{a_k}{z_k^*}$$

where

$$\hat{X}_{S_{(1)}(I_k)} = \sum_{j=1}^N \frac{\partial S_{(1)}}{\partial I_j} \hat{X}_{I_j}.$$

The infinite series can be summed up by means of the fact that z_k is an eigenfunction of the operator \hat{X}_{l_k} . Hence,

$$\exp\left(2\frac{\partial S_{(i)}}{\partial I_k}\right)z_k = z_k + \frac{a_k}{z_k^*}$$

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$$\exp\left(2\frac{\partial S_{(i)}}{\partial I_k}\right)I_k = I_k + a_k.$$
(5.6)

The last integration is easy to perform and yields

$$\xi = 2S_{(i)} = \sum_{k=1}^{N} a_k \left[\left(1 + \frac{I_k}{a_k} \right) \ln \left(1 + \frac{I_k}{a_k} \right) - \frac{I_k}{a_k} \ln \frac{I_k}{a_k} \right]$$
(5.7)

where an additional constant of integration is possible. Obviously, (5.7) is the important entropy formula of Planck [10] which stands at the beginning of quantum mechanics. In order to check their nature as a Lie function, we calculate the power series representation with respect to the parameter a_k and compare the result with the BCH series (5.4). Without any restriction the special case of one degree of freedom is considered. The Taylor expansion of $\xi(a)$ reads

$$\xi(a) = \xi(0) + \left. \frac{\partial \xi}{\partial a} \right|_0 a + \frac{1}{2} \left. \frac{\partial^2 \xi}{\partial a^2} \right|_0 a^2 + \frac{1}{6} \left. \frac{\partial^3 \xi}{\partial a^3} \right|_0 a^3 + \cdots$$

where

$$\xi(0) = 0 \qquad \frac{\partial \xi}{\partial a} = \ln(I+a) - \ln a$$

$$\frac{\partial^2 \xi}{\partial a^2} = \frac{1}{(a+I)} - \frac{1}{a} \qquad \frac{\partial^3 \xi}{\partial a^3} = \frac{-1}{(a+I)^2} + \frac{1}{a^2} \cdots$$
(5.8)

i.e. in the limit $a \rightarrow 0$ and $I \neq 0$ all (non-trivial) terms of the series are divergent. Moreover, the order of the divergence increases as the order of the expansion increases. For a moment this seems to be a serious problem but there is a simple renormalization procedure. We use the fact that the transition from (2.7) to (2.8) is not unique and the Lie function is determined up to a constant only. Therefore a shift

$$\tilde{\xi}(z, z^*, a) = \xi(z, z^*, a) + c(a)$$

with a suitable c(a) can remove the divergence. It is easy to show that in our case the constant must be chosen to be

$$c(a) = a(\ln a - 1).$$

Then the Taylor series is regular and, moreover, it corresponds exactly to the BCH series (5.4). At this stage of the considerations one may suppose that the appearence of the entropy of an ideal Bose gas is an accident; however, let us consider the type (ii) transformations. We choose the same characteristic function as for the type (i) transformation

$$G(z_k) = F^*(z_k^*) = \sum_{k=1}^N a_k \ln(z_k)$$
(5.9)

and make a similar ansatz as (5.5), i.e.

$$\operatorname{Re}[\Psi(z_k, z_k^*)] = S_{(ii)}(z_k, z_k^*) = S_{(ii)}(I_k).$$

Using (3.7)(ii) one can calculate the function $S_{(ii)}(I_k)$. The result is

$$\eta = 2S_{\text{(ii)}} = -\sum_{k=1}^{N} a_k \left[\left(1 - \frac{I_k}{a_k} \right) \ln \left(1 - \frac{I_k}{a_k} \right) + \frac{I_k}{a_k} \ln \left(\frac{I_k}{a_k} \right) \right]$$
(5.10)

which is, of course, the entropy of an ideal Fermi gas. In order to check the nature of the Fermi-entropy as a Lie function we investigate (3.12)(ii). Using (2.6) and (2.11) in (3.12)(ii) we get

$$e^{\hat{X}_{\eta}} e^{-i\pi \hat{X}_{J}} = e^{-\hat{X}_{G(z_{k})}} e^{-\hat{X}_{G^{*}(-z_{k})}}$$

The operators \hat{X}_{η} and \hat{X}_{J} commute as a consequence of the dependence $\eta(I_k)$ in (5.10) and the BCH theorem provides

$$\eta - i\pi J + c(a_k) = -G(z_k) - G^*(-z_k) + \frac{1}{2} \{G(z_k), G^*(-z_k)\} + \frac{1}{12} \{G^*(-z_k) - G(z_k), \{G(z_k), G^*(-z_k)\}\} + \cdots$$
(5.11)

where $c(a_k)$ is a suitable renormalization constant which is independent of z_k and z_k^* . The right-hand side is easy to calculate by means of (5.9) and one obtains

$$\eta - i\pi J + c(a_k) = \sum_{k=1}^{N} \left(-a_k \ln(-I_k) + \frac{1}{2} \frac{a_k^2}{I_k} + \frac{1}{6} \frac{a_k^3}{I_k^2} + \cdots \right) \,.$$

On the left-hand side one can perform the Taylor expansion with respect to the parameters a_k , where the relations $i\pi = \ln(-1)$, $c(a_k) = -\sum_k a_k(\ln a_k - 1)$ and (5.10) must be used. We note that this Taylor expansion gives the same result as the BCH series. Of course, we have only calculated the first three terms of the series, but we expect that there is also an agreement for the higher order powers of the parameters a_k . Because we have chosen the same characteristic function (5.9) for the type (i) and the type (ii) transformation, the relation (4.8) must be valid. The Poisson bracket $\{\xi, J\}$ and all higher order brackets vanish as a consequence of the dependence $\xi = \xi(I_k)$ and with (5.1) we obtain

$$\eta(I_k + a_k) = -\xi(I_k) + i\pi J$$
(5.12)

where J is the unitary invariant. Equation (5.11) is easy to confirm by means of a direct calculation which makes use of (5.7) and (5.10). Moreover, one proves the validity of (3.16) and (3.17) in the case of the special generating functions $\Phi = S_{(i)}$ and $\Psi = S_{(i)}$.

One of the most important aspects of the functions $S_{(i)}(I_k)$ and $S_{(ii)}(I_k)$ is their generator property with respect to the canonical transformations, i.e. the entropy plays an active role similar to the energy H. The associated transformations of the complex coordinates are given by

(i)
$$T_{B}(S_{(i)}, 0)$$
: $w_{k} = e^{-\hat{X}_{S_{(i)}}} z_{k} = \sqrt{1 + \frac{a_{k}}{I_{k}}} z_{k}$ (5.13)

(ii) $T_{\rm F}(S_{\rm (ii)}, 0): \qquad w_k = {\rm e}^{\hat{X}_{S_{\rm (ii)}}} z_k^* = \sqrt{\frac{a_k}{I_k} - 1} z_k^*$

and, moreover, for the square of the modulus of the coordinates

(i)
$$w_k w_k^* = z_k z_k^* + a_k$$
 (5.14)

(ii)
$$w_k w_k^* = a_k - z_k z_k^*.$$

Hence, the Bose-entropy (5.7) generates a translation wheras the Fermi-entropy (5.10) generates a glide reflection in the I_k -space. More precisely, the half of the corresponding entropies generates the transformation. The mapping (5.13)(ii) has a fixed point lying at $z_k^* z_k = a_k/2$ and, moreover, the Fermi-entropy is an invariant function with respect to the transformation (5.13)(ii), i.e.

$$\eta(w_k^* w_k) = \eta(a_k - I_k) = \eta(I_k) = \eta(z_k^* z_k).$$
(5.15)

A two-fold application of the type (ii) transformations yields the original coordinates z_k , i.e.

$$T_{\rm F}^2(S_{\rm (ii)},0) = 1$$

and therefore $T_{\rm F}$ allows only two numerical values I_k and $a_k - I_k$ for the square of the modulus. This is a typical spin $\frac{1}{2}$ property when the I_k are identified with measurable quantities, for example with the energy in the harmonic oscillator picture. We suppose that the connection between spin and statistics can be attributed to the more direct connection between entropy and associated transformations. This seems to be a very fundamental level of physics.

6. Summary

We have shown in this paper that the canonical transformations in the complex phase space can be labelled by two functions, e.g. by the pair $\Omega(z_k, z_k^*)$, $F(z_k^*)$ for the type (i) mappings. This is contrary to the Lie series representation of the canonical transformations in a real phase space because in that case there is only a single real function which generates the mappings. The main difference to the transformations in a real phase space is caused by the existence of non-trivial characteristic functions $F(z_k^*)$. The function F is a complex-valued one and therefore it cannot be a physical observable. Nevertheless, by using the BCH theorem one can form quantities from these complex functions which have an immediate physical meaning. Section 5 clearly shows that the entropy of ideal quantum gases is such a Lie function formed by the special characteristic function (5.1). Moreover, it must be underlined that the entropy plays an active role because it generates a canonical transformation similar to the energy which generates the time evolution of the system. Obviously, the characteristic function is the central point of interest because it determines both the Bose-entropy and the Fermi-entropy. Up to now we have no principle which provides those characteristic functions (e.g. (5.1)) which are important in physics. However, we believe that the study of continuous families of canonical transformations yields some hints to the meaning of the characteristic function. A discussion of the relationship between finite and infinitesimal representations of a one-parameter subgroup of the canonical transformations (cf [11]) may be helpful in this connection. On the other hand, the special functional dependence of the functions $F(z_k^*)$ or $G(z_k)$ suggests that there may be a connection to the elements of the Bargmann space of the entire analytic functions [12]. A similar direction comes from the correspondence of the transformations (5.13) to the action of raising and lowering operators in quantum mechanics.

Of course, there are many other important questions concerning the canonical transformations in the complex phase space. However, our study has shown that the investigation of the classical transformation apparatus in the complex domain provides unexpected physical results. This seems to support the view of Moshinsky and Seligman [13] that classical mechanics is not, as usually assumed, a simple asymptotic form of quantum mechanics.

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