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Dissipation in quantum physics

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A compact description of the evolution of a many-body quantum system, e.g., a dilute gas, is provided by the generalization of the usual reaction U matrix to a system U matrix. Using this tool, it is demonstrated that in such systems (i) time-reversal-invariant states are unstable and cannot exist in nature or be "constructed in the laboratory;" (ii) the time-reversal invariance of the Hamiltonian leads inexorably to relaxation towards thermal equilibrium of arbitrary nonequilibrium states, i.e., to dissipation, which thus allows the definition of a quantum arrow of time; (iii) the second law of thermodynamics, and hence the complete field of thermodynamics, is a consequence of quantum physics. These results have at their basis the Hermiticity of the Hamiltonian and the Heisenberg uncertainty relations.

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I. INTRODUCTION

Macroscopic quantum systems not at thermal equilibrium, for example, a well-insulated glass of hot water with an ice cube in it, certainly thermalize, i.e., exhibit dissipation. In quantum physics the motion of the system is governed by a Hamiltonian that is time-reversal invariant and the spectrum of the system may be discrete. On the surface, time-reversal-invariant equations of motion and time-directed evolution, i.e., dissipation, seem contradictory. However, a symmetry of the Hamiltonian does not imply that all states of the system will exhibit that symmetry; still, time-reversal-invariant states must actually exist. We will identify all these states that turn out to be also time-displacement invariant and demonstrate that all other states do exhibit dissipation. We also will demonstrate that the time-reversal-invariant states not only are highly improbable, as is generally accepted [1], but, more strongly, cannot exist in nature in principle; they will be shown to have probability measure zero. The underlying reason for this will be seen to be the Heisenberg uncertainty relation.

For simplicity and for conceptual transparency, we shall investigate the case of a dilute gas. Depending on the system, it could consist of atoms, molecules, phonons, quasiparticles, etc. In such a gas the dynamics consists mostly of a succession of two-body interactions; it can be described by a cluster expansion. Thus, in preparation for the treatment of the many-body system we begin the development in Sec. II by discussing the case of two-body scattering, principally to fix the notation and to introduce the method of our treatment, which is based on the Tomonaga-Schwinger evolution operator, the U matrix. In particular, we identify the time-reversal-invariant states as the eigenstates of the U matrix.

Treating the time evolution of the many-body quantum system by means of the Tomonaga-Schwinger equation leads to the U matrix describing the evolution of the complete system, which we denote as "the system U matrix." We now identify the time-reversal-invariant states of the system as the eigenstates of the system U matrix. We then show that all the other states exhibit a characteristic that can be loosely denoted as "infinite Poincaré time." This characteristic is essential for, but in itself does not imply, dissipation, i.e., relaxation. The central result of Sec. II is that the exceptional states, viz., the time-reversal-invariant states, cannot exist in nature as they have probability measure zero. That this indeed is the basis for the existence of dissipation in quantum physics is explained in Sec. III. (Of course, the fact that one can write down formally mathematical expressions for the exceptional states is of no importance; it does not make them realizable.)

The essential point of this paper is the demonstration that every possible state of a quantum system undergoes relaxation, i.e., exhibits the effect of dissipation, simply as the consequence of its evolution being governed by quantum dynamics. This is done in Sec. III. In detail, we will demonstrate that the state of the system evolves toward equal occupation probability for the accessible phase space cells. This way the axiom of statistical thermodynamics, viz., the assumption of equal *a priori* probability for the occupation of the phase space cells at thermal equilibrium, turns out to be a consequence of the quantum physics evolution. Hence all results of statistical thermodynamics turn out to be correct; in particular, the second law of thermodynamics is fulfilled.

It is now easy to define an expression for the entropy in terms of quantum physics variables. This is done in Sec. IV. Being part of quantum physics, this definition allows the evaluation of the entropy for arbitrarily off-equilibrium situations. At the same time the entropy can be used to define the arrow of time in nonequilibrium systems. No arrow of time can be defined in systems at equilibrium.

Some mathematical details concerning zero measure as needed in the present paper are collected in the Appendix. A discussion of the physical interpretation of zero measure is also given.

We now summarize the logical chain of steps leading to the conclusions of the paper. (i) Owing to the time-reversal invariance of the Hamiltonian, time-reversal-

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invariant states must exist. A "physical" scattering state has an incoming wave in one channel and outgoing waves in all channels. The time-reversed state has phase- and amplitude-related incoming waves in all channels and an outgoing wave in one channel. The time-reversed physical state is unstable in that any change, even only in one of the incoming waves, leads to outgoing waves in all channels. (ii) We identify the time-reversal-invariant states as the eigenstates of the system U matrix; for an $N \times N$ U matrix there are exactly N such states. We show that linear combinations of these eigenstates are not time-reversal invariant; more specifically, such linear combinations are nonperiodic. (iii) In the language of mathematics, the time-reversal symmetric and the time-reversal-invariant states and also the time-reversed physical states have probability measure zero; this means that they do not exist in nature and also cannot be generated "in the laboratory." (iv) In the last step we demonstrate that all physically possible states evolve toward uniform density in phase space, which is known to be the characteristic of thermal equilibrium. This thus demonstrates that the axiom of equipartition of classical physics is a consequence in quantum physics. The two main results of this paper are that it is in principle impossible to actually construct time-reversed states and all possible states evolve toward uniform occupation of the accessible phase space.

II. TIME-REVERSAL-INVARIANT STATES

Since the Hamiltonian (by assumption) is time-reversal invariant, then for any solution of the equations of motion, say, $\psi(t)$, which does not have to be an eigenstate of the Hamiltonian, the time-reversed state $\phi(t)$ reached from the original state $\psi(t)$ by the time-reversal transformation $\phi(t) = [\psi(-t)]^*$ is also a solution. Consequently

$$\mathcal{N}\ \Psi(t) = \psi(t) + \phi(t) \tag{1}$$

($\mathcal{N}$ is a normalization constant) is also a solution. This state is time-reversal symmetric in that it allows the reflection in time with respect to $t = 0$. Our first task is to identify not only the time-reversal symmetric states but also the time-reversal-invariant states; then we will show that both these kinds of states do not exist in nature and why — even though, evidently, they are formally possible, i.e., the appropriate expressions can be written down. We shall derive our results by studying the evolution of a dilute gas. Since the dynamics of that system can be described by a sequence of two-body interactions, we shall first recall the evolution in time of an isolated two-body collision and then tackle the case of the dilute gas.

The prototype elastic two-body scattering system at energy E is described as consisting in the asymptotic region of an incoming plane wave and an outgoing spherical wave. This description has two related difficulties: the waves fill all space and generate unphysical interference patterns and there is no before or after the collision: they collide all the time [2]. The system is delocalized in space and time.

To avoid these difficulties we shall employ the Weyl eigendifferential method, which can be used to discretize any continuous spectrum. The Weyl eigendifferential states are defined as [3]

$$\Psi_W(E_k; x, t) = \mathcal{N} \int_{E_k-\epsilon}^{E_k+\epsilon} dE\ \Psi(E; x, t), \tag{2}$$

where the limit $\epsilon \to 0$ yields the δ-function normalization $\langle\Psi(E)|\Psi(E')\rangle = \delta(E-E')$. We shall use the more general case of ϵ small; in (2), $\mathcal{N}$ is the normalization constant.

The Weyl states have several useful characteristics: they are as close to being eigenstates of the Hamiltonian as can be while being localized in space and time; the original continuous spectrum has been discretized, i.e., the number of Weyl states is denumerably infinite and thus only summations and not integrations are encountered; they are Kronecker orthonormal; they have simple mathematical properties; and they are minimum uncertainty wave packets and can be directly used to define the phase space cells. Indeed, replacing in the wave function Ψ of Eq. (2) the coordinate x by $x - x_l$, then in the classification of phase space the indices k and l play the roles of the commonly used coordinates p and q, respectively. We shall use this labeling of the phase space. Also, in our development we will not need the more general description by density matrices, which would be needed if impure, i.e., mixed, states were required [4].

Now let $\Psi(E)$ be the complete wave function of our two-body system, i.e., it includes all channels and the actual collision region. Then, using Weyl states, one can achieve that for large negative t the colliding systems in a physical scattering state are far apart — they are in the asymptotic in-states — and they are approaching each other; at $t = 0$ they collide and at positive t the reaction products fly apart (they are then in the asymptotic out-states). A time-reversal-symmetric Weyl scattering state, constructed from this physical state according to Eq. (1), at $t \ll 0$ would have in addition to the original asymptotic incoming state, in which the colliding particles approach each other in the input channel, also the time-reversed original outgoing state, i.e., particles approaching each other in the original asymptotic output channels, all of them to meet at $t = 0$ at the origin. All these components must be phase and amplitude related. As we will see below, for any system that has more than one open channel the time-reversed physical states cannot be realized in the laboratory; they have probability measure zero (see the Appendix).

Since in Weyl states the collision partners at $t = -\infty$ are infinitely far apart and do not interact, the inner structure (e.g., the self-energy) of each of the colliding partners can be computed (prediagonalized) without interference by the other partner. (Actually $t = -\infty$ is not required; the collision partners only must be sufficiently far apart so as to render their mutual interaction negligibly small; see below.) We shall employ as asymptotic states such prediagonalized states. Thus the incoming particles may be atoms or molecules, etc., in some well-defined states, not necessarily in the ground states. We shall denote the representation constructed with these states as "the asymptotic representation." This is in contrast to the "full state representation," for which the states are the full wave functions of the colliding system, each of which encompasses the incoming and all the outgoing waves and also the reaction volume. Hence, given the initial state in terms of the asymptotic states, then the final state, again in terms of the asymptotic states, is computed exactly by multiplying the state vector of the initial state by the S matrix or by the U matrix if the starting point is at some finite time [5]. The difference between these two forms is that the U matrix contains the closed channels, i.e., the channels that contain off-the-mass-shell particles, while the S matrix ignores them. Since the closed channels decrease in amplitude exponentially as the systems move apart, the difference between the elements of the U and the S matrix is important only very close to the actual collision. For larger separation distances the elements of the S matrix and the U matrix have the same value. Also, only stable states can be used in the S matrix formalism since it is defined as the limit $t = -\infty$; since the U matrix is defined with finite times the required quasiasymptotic states can contain decaying states. Which lifetimes are acceptable for these decaying states then is determined by the time constants of the considered system. The U matrix can be defined to encompass the spreading of the (minimum uncertainty) Weyl packets.

In describing a many-body system we shall use as asymptotic states Weyl packets of products of single-particle states that are (delocalized) eigenstates (or quasieigenstates for the above mentioned decaying states) of the Hamiltonian, i.e., where the internal structure has been fully treated.

Let us now discuss the general characteristics of a two-body collision. We will see below that *mutatis mutandis* they hold also for many-body systems. In hyperspherical coordinates [6] that contain only one radial coordinate, for a given (non-Weyl) state of definite energy $\Psi(E)$, all channels c asymptotically for $r_c \to \infty$ have the form (omitting the angular and hyperangular parts)

$$\psi_c = a_c\, e^{i(k_c r_c - E_c t)} - b_c\, e^{-i(k_c r_c + E_c t)} . \tag{3}$$

Here a_c is the amplitude "before" and b_c "after" the collision. In general, the states have $|a_c| \neq |b_c|$, i.e., in a given channel c the in-current is not equal to the out-current; thus they are not time-reversal invariant. There do exist time-reversal-invariant states, viz., the eigenchannel states [7], which are the eigenstates of the U matrix. In an $N \times N$ U matrix there are N such states. Since the eigenchannel states form a complete set of states, any state, for example, a physical scattering state, can be written as a superposition of eigenchannel states. In general, all N eigenchannel states are needed for this superposition.

For a system in a pure eigenchannel state there holds (the index n denotes the eigenchannel)

$$b = U\, a = e^{-2i\eta_n}\, a \tag{4}$$

or, in detail,

$$b_c^{(n)} = a_c^{(n)}\, e^{-2i\eta_n} . \tag{5}$$

[Being unitary, the U matrix must have eigenvalues of absolute value 1; hence the eigenvalues, as written in Eq. (5), must have real eigenphases η_n.] Thus the channel functions are of the form

$$\psi_c^{(n)} = a_c^{(n)}\, e^{-i(E_c t + \eta_n)}\, \sin(k_c r_c + \eta_n) ; \tag{6}$$

they have standing waves in all channels c, which evidently is necessary for time-reversal invariance, and are phase and amplitude related. The eigenchannel states are delocalized continuum states. As we will see in a moment, the pure eigenchannel states are the only time-reversal-invariant states. Given a U matrix, the eigenchannel wave function can be written down; in reality, however, similarly as the time-reversed states, such states cannot be constructed as they have probability measure zero.

We now describe the reasons for this observation. Consider a given physical scattering state. Its time-reversed state has an outgoing wave in exactly one channel. This situation is, however, unstable, in that a change of the amplitude even for only one of the incoming waves, say, $a'_r = a_r + \Delta a_r$, will generate a solution containing outgoing waves in all channels. (Owing to the normalization condition, Δa_r can only produce a rotation of a_r in the complex plane.) This change can be thought of as the addition of a physical state that has its incoming wave in channel r with amplitude Δa_r; this then generates outgoing waves in all channels. In the same way, changing the amplitude only in one channel in an eigenchannel solution will unbalance the in- versus the out-currents in all channels. The demonstration that the time-reversed physical states and also the eigenchannel states have probability measure zero is given in the Appendix. This in fact is essential for the existence of dissipation in quantum physics.

We now proceed to the many-body system. We take the case of a dilute gas in a mathematically perfect box, where as previously the particles are described by Weyl states in the asymptotic-state representation. (The circumstance that in a box the spectrum is discrete makes no difference since an immense number of such states participate in a single Weyl state.) To describe the evolution of this system it is useful to introduce the system U matrix; it is defined similarly as the usual U matrix in terms of the Tomonaga-Schwinger equation [5], where the interaction-picture interaction is the sum of the individual interactions between the collision partners. It is a generalization of the familiar graph expansion methods of many-body theory [8]. A more detailed discussion is planned to be given in a separate paper [9]. The restriction to a dilute gas leads to a substantial simplification and to conceptual transparency of the problem since then the evolution of the system can be treated in terms of the cluster expansion, which can be visualized as a sequence of two- or three-body collisions. This then can be used to factorize the system U matrix into reaction U matrices. Of course, this simplification is not essential for the existence of a system U matrix; it only allows for easy visualization.

We now return to our problem. If there are M particles in the box, the overall wave function is contained in a $3M$-dimensional finite configuration space; at fixed total energy the phase space of the system is also finite and has, say, N cells. Then the overall system U matrix, labeled by the system phase space cell indices, is $N \times N$; it is sparse, but not disconnected. Except for its size, it has all the same attributes as the U matrix of a two-body system discussed above. In particular, it allows for the definition of eigenchannel states, which now concern the complete system. Again, these N eigenchannel states are time-reversal invariant and, as we will show below, are the only time-reversal-invariant states of the system. Importantly, the remarks made above that the time-reversal-invariant solutions for a two-body system have probability measure zero thus apply also for a many-body system.

We now give the promised demonstration that the eigenchannel states are the only time-reversal-invariant states. In the eigenchannel representation the U matrix is diagonal with diagonal elements $e^{-2i\eta_n}$. In this representation the state vector of the given eigenchannel, say, n, is $\delta_{n,m}$. On the other hand, in the asymptotic state representation the eigenchannel state has nonvanishing amplitudes in all components. Each action of the U matrix generates the "outgoing" wave (the state at time $t + \tau$) by multiplying each of the "incoming" wave components (of the state at t) by the factor $e^{-2i\eta_n}$, common to all these components; see Eq. (4). The ratio of the amplitudes thus is not altered by the "collision"; by definition the system is in a stationary state. If, however, only one more eigenchannel solution, say, m, is admixed, then after the collision the amplitude in channel c will be

$$b_c = a_c^{(n)} \, e^{-2i\eta_n} + a_c^{(m)} \, e^{-2i\eta_m} \; . \tag{7}$$

Since in view of the orthogonality of the eigenchannels in general the ratio $a_c^{(n)}/a_c^{(m)}$ is different for the different channels c, the state in the collision has undergone an essential change. Furthermore, as long as $(\eta_n - \eta_m)/\pi$ is not a rational number, the system will never return to the state it occupied before the first collision. As demonstrated in the Appendix, the probability measure of a rational phase difference is zero. Hence the return time is infinite; the states are nonperiodic. Admixing to our two states of Eq. (7) further eigenchannel states does not change the situation in any qualitative manner. Of course, in that case there exist more relative phases, irrational multiples of π, between the contributing eigenchannel states; this then allows for greater variety of trajectories in the asymptotic-representation Hilbert space. Furthermore, the physically possible states in general are linear combinations of all eigenchannel states.

More importantly, as also shown in the Appendix, even individual eigenchannel states, the same as time-reversed physical states, have probability measure zero. Hence time-reversal-symmetric states constructed according to Eq. (1) have probability measure zero.

Thus all physically possible states (i.e., states with nonzero probability measure) are nonperiodic; the quantum phase space trajectories are open. Considering the spreading of the minimum-uncertainty wave packets, one may say that all physically possible quantum states have infinite "Poincaré time."

To summarize the results of this section, we have shown that all time-reversal-invariant and time-reversal-symmetric states have probability measure zero and hence cannot exist in nature; they can be called "forbidden states." Conversely, every possible, "allowed" state in quantum physics has the character of no return, i.e., has infinite Poincaré time. This is one aspect needed for dissipation. The elucidation of the other aspect, viz., the determination of the state the system evolves into, will be the subject of the next section. That state will turn out to be the state of maximum entropy, i.e., a state in thermal equilibrium. As we will see, the results of the present section will turn out to be essential in arriving at this result.

III. DISSIPATION

In the preceding section we have shown that it is impossible to construct in nature time-reversal-invariant states and also time-reversed physical states, i.e., that is impossible to implement the time-reversal transformation even though it is a mathematically fully defined operation. The reason was shown to be the fact that such states have probability measure zero. In the present section we will show that all physically realizable initial states evolve in time toward thermal equilibrium. We conduct the discussion for the case of pure states, which can be represented by a wave function. The simplifications that arise for impure states are mentioned toward the end of this section.

The question we here address is the following: Starting from some arbitrary allowed, i.e., realizable initial state, what is the nature of the state the system evolves into? To answer this question we derive a difference equation for the time evolution of the system by investigating the change induced in the system by the next collision, which actually means the evolution of the system over a short time step $\tau = \Delta t$. (The limit $\Delta t \to 0$ would yield a differential equation.) We describe this time evolution as in Sec. II by means of the $(N \times N)$ system U matrix, labeled as previously by the system phase space cell indices.

Assume that before the considered time step, i.e., at time t, the amplitudes of the system wave function in the asymptotic representation are a_j. Then the amplitudes after the next time step are given by multiplication of the original amplitudes by the system U matrix. Writing the system U matrix as $U = 1 + R$, the amplitudes at time $t + \tau$, written as $\bar{a}_j$, will be

$$\bar{a}_1 = (1 + R_{11}) \, a_1 + R_{12} \, a_2 + R_{13} \, a_3 + \cdots , \tag{7a}$$

$$\bar{a}_2 = R_{21} \, a_1 + (1 + R_{22}) \, a_2 + R_{23} \, a_3 + \cdots , \tag{7b}$$

$$\vdots$$

$$\bar{a}_j = R_{j1} \, a_1 \;\cdots + (1 + R_{jj}) \, a_j \;\cdots + R_{jk} \, a_k + \cdots , \tag{7c}$$

$$\vdots$$

$$\bar{a}_k = R_{k1} \, a_1 \;\cdots + R_{kj} \, a_j + \cdots + (1 + R_{kk}) \, a_k + \cdots , \tag{7d}$$

$$\vdots$$

The elements R_{jk}, $j \neq k$, describe crossflow of probability amplitudes between the cells j and k and the elements R_{jj} reflect the net inflow (or outflow) into cell j.

Take as the measure of pairwise nonuniformity for the occupation of the phase space cells the expression

$$\Delta_{jk} = |a_j|^2 - |a_k|^2 \ . \tag{8}$$

From (7c) and (7d) we compute the change in the nonuniformity ($\bar{\Delta}_{jk}$ after the collision)

$$\begin{aligned}\bar{\Delta}_{jk} - \Delta_{jk} &= \left(|\bar{a}_j|^2 - |\bar{a}_k|^2\right) - \left(|a_j|^2 - |a_k|^2\right) \\ &= -|R_{jk}|^2 \ \Delta_{jk} + [F_{jk}] + [G_j] - [G_k] \ . \end{aligned} \tag{9}$$

This is the promised equation that describes the time evolution of the nonuniformity Δ_{jk}. It is a first-order difference equation. Within the validity of the description of the evolution by the system U matrix, this equation is exact. Of course, it is not a new equation; it simply reflects the dynamics of the Eqs. (7) and allows visualization of the evolution as given by those equations.

Since Eq. (9) is central to our development we shall discuss its ingredients one at a time. Ignore for now the terms $[F]$ and $[G]$; we will return to them below. Then, as is well known, the solutions of Eq. (9) are exponential functions that in view of the negative sign on the right-hand side fall off as $t \to \infty$. Hence we have the important result that in the absence of the terms $[F]$ and $[G]$ the nonuniformity Δ_{jk} relaxes exponentially toward zero. This is true for every pair j, k for every physically possible initial state.

In view of the results of Sec. II, the statements of the preceding paragraph terminate the development. It nonetheless is instructive to look as an illustration at the difference between the mathematical time-reversal operation and its actually possible approximate implementation, i.e., to see how the impossibility of time-reversed physical states as discussed in Sec. II manifests itself in the solutions of Eq. (9). To wit, Eq. (9) of course is form invariant under a time-reversal transformation, i.e., the exchange $t \to -t$ together with the exchange $U \to U^{\dagger}$. In this time-reversed system the actually later difference $\bar{\Delta}_{jk}$ would be the "earlier" one. One thus may be tempted to follow the evolution of the system "forward" in this "new" time (actually backward in time) and to conclude that it proceeds in the form of derelaxation. However, this new state, ϕ in the terminology of Eq. (1), involves the replacement of physical processes by time-reversed physical processes. It is here that the results of Sec. II are essential: as demonstrated there, the time-reversed states of physical states have probability measure zero. That means that the time-reversal operation that is mathematically well defined cannot be implemented in nature; such a state cannot be realized. At best, an approximate realization is possible. In detail, the evolution of this approximate new "initial state" toward derelaxation is unstable; owing to the inaccuracies in the amplitudes $\bar{a}_j^*$ unavoidable in quantum physics (e.g., Heisenberg uncertainties; see the Appendix) after a short new time, the derelaxation will terminate and the evolution will revert toward relaxation, precisely in terms of this new time.

We now discuss the influence of the term $[F_{jk}]$ of Eq. (9) on the solutions. The developments of the preceding paragraph have bearing also on this discussion. The term $[F_{jk}]$ contains the interference terms, which are of the form $[R_{jr}a_r]^* R_{sk}a_k - R_{sj}a_j[R_{kr}a_r]^*$ and thus are phase sensitive. They contain only off-diagonal elements of the density matrix. In a fully impure state the term $[F]$ vanishes and the nonuniformities Δ_{jk} decay exponentially. Since interference terms in general do not influence the overall process (for example, total reaction cross sections) and for the reasons given in the preceding paragraph, the terms contained in $[F]$ can only induce fluctuations and not secular effects. The terms $[G_j]$ are diagonal in the state indices; their action is to maintain the unitarity of the transformation, i.e., the normalization of the state.

It is also informative to consider the case of an eigenchannel state. There the amplitude squares $|a_j|^2$, and thus also the differences Δ_{jk}, are constant in time; cf. Eq. (5). For this to be true requires that the right-hand side of Eq. (9) vanish exactly for all pairs j, k, which, according to the Appendix, is not possible. This observation provides an alternative way to see that the time-reversal-invariant states, i.e., the eigenchannel states, have probability measure zero.

For any arbitrary initial state the time evolution of both the fluctuations and the relaxation can be traced by repeated matrix multiplication. This then is fully exact as it represents one way of solving the time-dependent Schrödinger equation. If a fully exact treatment is not required, then, since exceptional states have been shown not to exist, this matrix multiplication can be carried out by statistical methods. One thus, at this point, arrives at statistical (nonequilibrium) thermodynamics. This, however, is totally irrelevant for the existence of dissipation as given by Eq. (9). Thus, if one so desires, one can investigate special cases of interest in full exactness.

We now discuss our result. Recall (cf. Sec. II) that the labels of the system U matrix denote the cells of the overall combined system phase space. Thus the amplitude a_j is directly the occupation amplitude for phase space cell j and thus the occupation probability for that cell is $|a_j|^2$. Hence, even though the Hamiltonian is time-reversal invariant, the dynamics of the system tends to achieve equal *a posteriori* probability for the occupation of the energetically accessible phase space cells. This is simply the consequence of the no-return character (infinite Poincaré time) of the evolution and of the nonzero value of some R_{jk}, together with the connectedness and the unitarity, i.e., time-reversal invariance, of the U matrix. This way our result obviates the need for the axiom basic to equilibrium statistical thermodynamics [10], which postulates equal *a priori* occupation probability of the accessible phase space cells.

If the U matrix should turn out to be quasidisconnected, then the equalization initially would take place within each strongly connected piece of the U matrix. A fully disconnected U matrix actually does not occur in nature; what does occur is that by virtue of the smallness of the relevant elements R_{jk}, some parts of the U matrix are only weakly connected to the rest of the U matrix.

In that case the overall equalization of the occupation probabilities would be slowed down; the overall system very well might, and actually usually does, have a set of different relaxation time constants, i.e., the system may consist of more or less well-insulated subsystems.

The above discussion concerns a system described by a wave function, for which the density matrix obeys $\rho^2 = \rho$. For an impure state the off-diagonal terms of the density matrix have smaller values and hence the influence of the fluctuation-inducing term $[F]$ of Eq. (9) is diminished. Furthermore, as already mentioned, for fully impure states having a purely diagonal density matrix the term $[F]$ is absent and the solution for $t \to \infty$ is unique, i.e., $\Delta_{jk} \to 0$.

IV. QUANTUM ENTROPY

After the results of the previous sections it is not difficult to find a workable definition for the entropy in quantum physics. To that end recall Boltzmann's definition

$$S = -\sum_j p_j \ln p_j \ . \tag{10}$$

In this expression the quantities p_j are the classical probabilities, arrived at by counting the available phase space cells. To achieve the corresponding quantum physics expression one must replace in Eq. (10) the classical probabilities by quantum probabilities, say, w_j. Now, given the amplitudes at $t = 0$, $a_k(0)$, in the asymptotic Weyl state representation, we have

$$w_j(t) = \sum_{k,k'} a^*_{k'}(0)\ U^*_{k'j}(t)\ U_{jk}(t)\ a_k(0), \tag{11}$$

which accounts for all possible interferences. If the initial state is impure it can be specified only in term of its density matrix. Denoting it, again in the asymptotic Weyl state representation, by $\omega(0)$, Eq. (11) must be replaced by

$$w_j(t) = \sum_k U_{jk}(t)\ \omega_{kl}(0)\ U^*_{lj}(t)\ . \tag{12}$$

Since for large systems the quantum probabilities approach the classical probabilities, the definitions (10)–(12) directly approach the Boltzmann entropy.

Finally, one can account for the selection of final states by a measuring device by augmenting Eq. (10) by an appropriate projection operator W_j representing the measurement or the filter used in the preparation of the state, say, a Stern-Gerlach setup. This then yields

$$S = -\sum_j W_j\ w_j \ln w_j\ . \tag{13}$$

The projection operator can act as a "refrigerator"; the filter may select a particular polarization, thus resulting in a beam having the spin temperature $T_s \simeq 0$.

Now some remarks concerning the experimental determination of the entropy of a quantum system are in order. Strictly, the thermodynamic quantities are defined only for infinitely large systems. On the other hand, no such demands are visible in the definitions of this section, e.g., Eq. (13). Thus, given a table of data for a system, one may evaluate the number S by means of Eq. (13). Also, if one has tables for two times, one can determine the time order by comparing the computed values of S, i.e., determine the "arrow of time." This, of course, is possible only for nonequilibrium conditions; in equilibrium S remains constant, except for fluctuations associated with the noninfinite size of the system.

The definition (10) or (13) is given in terms of the asymptotic states. It thus is applicable only for such times where no collision is in progress. It is not possible to generalize the definition so as to make it applicable also during the time of a collision. The reason for that is that the off-the-mass-shell states arising during the collision are given by propagators; they are not measurable. One thus cannot ask precisely at which point "entropy is produced" in the reaction. Only the entropy before and after the reaction is defined.

The definition (10) or (13) must be distinguished from the von Neumann definition

$$S_{vN} = -\mathrm{Tr}(\rho \ln \rho), \tag{14}$$

where ρ is the density matrix in the full-state representation (Sec. II). As is well known, S_{vN} is a constant of the motion, i.e., does not change in time. A pure state remains pure. Hence purity of the state seems not to be a useful concept for defining the entropy in quantum physics.

V. CONCLUSIONS

The central result of this paper is that quantum dynamics achieves directly relaxation toward a uniform occupation of the accessible phase space. Recall that all results of statistical thermodynamics are arrived at by axiomatically assuming for equilibrium equal *a priori* occupation probability of all accessible phase space cells and evaluating the resulting probability by counting the phase space cells. Our result shows that we have proven the correctness of that axiom for quantum dynamics. [Note that Eq. (9) concerns only the occupation probabilities $|a_{jk}|^2$; the amplitudes still may contain phase relations, which, however, has no importance for our result.] Hence, not only are the results of statistical thermodynamics correct but even more strongly, we have proven that statistical thermodynamics is a direct consequence of quantum physics. In particular, one of these consequences is the validity of the second law of thermodynamics; it arises as a direct consequence of the time-reversal invariance of the quantum physics Hamiltonian and the equations of motion derived from this Hamiltonian. At the same time this allows the definition of quantum entropy. In view of the fact that the first law of thermodynamics, being only the expression of energy conservation, is contained in quantum physics, the overall conclusion is that the field of thermodynamics, including dissipation, is simply part of quantum physics.

In this whole discussion the question of measurement in quantum physics did not arise and did not have to be addressed. Measurement evidently is irrelevant to the existence of dissipation. In particular, the well-known collapse of the wave function plays no role here. This is not to say that an analysis of the measurement process for a many-body system is of no interest; to the contrary, it is very worthwhile to give a careful discussion of that problem [11–13], in particular in the context of the definition of the observables representing the microscopic thermodynamic variables. Simply, it lies outside of the frame of the present paper. In our development no questions of general relativity, e.g., the expansion of the universe, have been addressed; we only note that dissipation does not depend on this expansion.

In summary, we have shown that in quantum physics thermalization, i.e., dissipation, is an inevitable process; all systems tend toward thermal equilibrium, while exhibiting quantum fluctuations. As long as thermal equilibrium has not been reached, the process of dissipation allows the definition of the arrow of time. No arrow of time can be defined for a system at thermal equilibrium. At that point the entropy, as defined in this paper, reaches its maximum value.

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APPENDIX

Because of its central position in the developments of this paper we collect here some aspects of the concept of measure zero. To begin we address the question of the probability measure of states with rational differences of eigenphases. To that end define

$$x = \pi(\eta^{(i)} - \eta^{(j)}) \ . \tag{A1}$$

The eigenphases are some regular, in general transcendental, functions of the parameters of the Hamiltonian and of the energy. In particular, they are not generalized functions, for example, δ functions. Thus, except for some special points, e.g., thresholds of reactions, in its dependence on the energy the function $x(E)$, Eq. (A1) is regular, i.e.,

$$\left| \frac{dx}{dE} \right| < \infty \tag{A2}$$

and

$$\frac{dx}{dE} \neq 0 \ . \tag{A3}$$

Consider now the normalization

$$N = \int F(E) \ dE \ . \tag{A4}$$

In view of (A2) and (A3), Eq. (A4) can be replaced by

$$M = \int G(x) \ dx \ . \tag{A5}$$

Take any rational number $x = P/Q$ (P and Q integers) and compute its contribution to the integral (A5). To that end integrate (A5) over the interval $P - 0.5 < Qx < P + 0.5$:

$$\begin{aligned} \int_{(P-.5)/Q}^{(P+.5)/Q} G(x) \ dx = \lim_{\epsilon \to 0} \Bigg\{ & \int_{(P-0.5)/Q}^{(P-\epsilon)/Q} G(x) \ dx \\ & + \int_{(P+\epsilon)/Q}^{(P+0.5)/Q} G(x) \ dx \\ & + \int_{(P-\epsilon/Q}^{(P+\epsilon)/Q} G(x) \ dx \Bigg\} \ . \end{aligned} \tag{A6}$$

Since the integrand is regular at $x = P/Q$, the contribution of the third integral vanishes in the limit. Thus the contribution of the rational point P/Q and hence of every rational point has probability measure zero.

In precisely the same manner one can demonstrate that the contribution of any single number, rational, irrational, or transcendental, has probability measure zero. Similarly, a time-reversed physical state has probability measure zero, as it requires the exact reproduction of $N - 1$ in general complex numbers, and so does each eigenchannel state.

The impossibility of constructing in nature a state with exact values of its parameters follows from the Heisenberg uncertainty relation: it would take an infinite time to construct two waves with an exact phase relation. In some detail, the uncertainty with which the phase relation can be established decreases as $1/t$, where t is the setup time of the experiment. On the other hand, the deviation from the desired behavior goes exponentially with time; cf. Eq. (9). Hence one must conclude that it is impossible in principle (not only in practice) to physically construct such a state and also that such states cannot exist in nature. This is one example for the physical meaning of the mathematical concept "probability measure zero."

On the other hand, the construction of Weyl packets has probability measure unity since it is stable against changes of the weight function, say, $f_k(E)$, used in the construction

$$\Psi_W(k; x, t) = \mathcal{N} \int dE \ f_k(E) \ \Psi(E; x, t) \ , \tag{A7}$$

which does not have to be the "square wave" function used in Eq. (2). A similar character has the construction of a discrete state, which is a special case of Eq. (A7) with $f_k(x)$ a perhaps very narrow resonance curve or even a δ function.

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