Statistical Mechanics for States with Complex Eigenvalues and Quasi-stable Semiclassical Systems

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Abstract

Statistical mechanics for states with complex eigenvalues, which are described by Gel'fand triplet and represent unstable states like resonances, are discussed on the basis of principle of equal \textit{a priori} probability. A new entropy corresponding to the freedom for the imaginary eigenvalues appears in the theory. In equilibriums it induces a new physical observable which can be identified as a common time scale. It is remarkable that in spaces with more than 2 dimensions we find out existence of stable and quasi-stable systems, even though all constituents are unstable. In such systems all constituents are connected by stationary flows which are generally observable and then we can say that they are semiclassical systems. Examples for such semiclassical systems are constructed in parabolic potential barriers. The flexible structure of the systems is also pointed out.

1. Introduction

It is well known that quantum mechanics including complex eigenvalues which represent unstable states like resonances are described by Gel'fand triplet \cite{1}. Since systems including such unstable states are usually unstable, it seems to be not suitable for constructing a theory like statistical mechanics for thermal equilibriums. We can, however, consider interesting situations, that is, the cases where the imaginary parts of energy eigenvalues of the states are so small that there are time enough to realize thermal equilibriums before the decay. In such situations statistical mechanics based on principle of equal \textit{a priori} probability can be meaningful and we can observe some decay properties of such systems. It will possibly be a representation for quasi-stable systems having long
life-times. Furthermore there is another noticeable feature of the complex eigenvalues such that they are represented by pairs of complex conjugates like $a \pm ib$ for $a, b \in \mathbb{R}$, that is, since Hamiltonians $\hat{H}$ are real, for any solutions $\psi$ satisfying the equation

$$\hat{H}\psi = (a - ib)\psi \quad \text{for } a, b \in \mathbb{R},$$

we always find solutions having complex conjugate eigenvalues such that

$$\hat{H}\psi^* = (a + ib)\psi^*.$$

An explicit example was presented for parabolic potential barrier [2,3,4]. It is quite interesting that in spaces with more than 2 dimensions real eigenvalue solutions can be obtained by using those pair solutions represented only by Gel’fand triplet and they are in infinite degrees of degeneracy [4]. In general they describe stationary states but they simultaneously have incoming- and outgoing-quantum stationary flows [4,5]. Actually the real eigenvalue solutions are interpreted as the states which have equal incoming- and outgoing-flows. It is quite natural to have questions; whether systems constructed with such real-eigenvalue states can really be stable and furthermore how they can physically be interpreted in realistic phenomena. In order to study these problems we shall make statistical mechanics for states including complex eigenvalues on the basis of the same principle for the usual statistical mechanics, that is, principle of equal $a$ priori probability.

In §2 statistical mechanics for complex eigenvalue states is performed. It is shown that the entropy of a system is represented by the sum of the usual entropy and a new one induced from the freedom of imaginary part and a new observable quantity appears in equilibriums, which will be identified as time scale of decay of the system. Explicit examples for stable and quasi-stable systems are presented in the case of parabolic potential barriers in §3, where those quasi-stable systems are connected by stationary flows [5]. Some realistic applications will be remarked in §4.
2. Statistical mechanics for complex-eigenvalue states

Let us construct a statistical mechanics corresponding to microcanonical ensemble for states having complex energies which are generally represented by

\[ \varepsilon_{ij} = \epsilon_i - i\gamma_{ji}, \quad \text{for } \epsilon_i, \gamma_{ji} \in \mathbb{R} \]  

(1)

where \( i, j_i \in \mathbb{Z}_+ \) (\( \mathbb{Z}_+ = \{0, 1, 2, \ldots\} \)) and the suffix \( i \) of \( j_i \) is needed when there is some relation between the real and imaginary energy eigenvalues. We consider a simple case described by a system composed of \( N \) independent particles being in complex-energy states. In this case the total energy of the \( N \)-particle system is given by the sum of energy eigenvalues of each particles such that

\[ \mathcal{E} = E - i\Gamma, \]  

(2)

where

\[ E = \sum_i \epsilon_i \quad \text{and} \quad \Gamma = \sum_{j_i} \gamma_{ji}. \]  

(3)

Here we shall investigate simple cases where the real and imaginary energy eigenvalues are independently determined and then we can take off the suffix \( i \) from \( j_i \). Such models will explicitly be presented in the next section. The basic principle is taken as same as that for the usual statistical mechanics, that is, principle of equal \textit{a priori} probability.

Then we start from counting the number of independent combinations of states for a fixed energy \( \mathcal{E} \). Since two freedoms concerning to the real and imaginary parts of energies are independent of each other, the number of the combination \( W(\mathcal{E}) \) is counted by the product of the number \( W^{\mathbb{R}}(E) \) for realizing the real part \( E \) and that \( W^{\mathbb{I}}(\Gamma) \) for realizing the imaginary part \( \Gamma \) such that

\[ W(\mathcal{E}) = W^{\mathbb{R}}(E)W^{\mathbb{I}}(\Gamma). \]  

(4)

Following the procedure of statistical mechanics, we now see that the entropy \( S(\mathcal{E}) = k_B \log W(\mathcal{E}) \) of the system is written in terms of the sum of two entropies such that

\[ S(\mathcal{E}) = S^{\mathbb{R}}(E) + S^{\mathbb{I}}(\Gamma), \]  

(5)
where \( S^R(E) = k_B \log W^R(E) \) and \( S^\Im(\Gamma) = k_B \log W^\Im(\Gamma) \) are, respectively, the Boltzmann entropy and the new entropy induced from the freedom of the imaginary part.

Let us consider equilibrium between two systems which can each other transfer only energies. The total energy \( \mathcal{E} = E - i \Gamma \) given by the sum of those for two systems \( \mathcal{E}_I = E_I - i \Gamma_I \) and \( \mathcal{E}_II = E_{II} - i \Gamma_{II} \) is fixed. The number of the available combinations is written by the product of those for the two systems as

\[
W(\mathcal{E}) = W_I(\mathcal{E}_I)W_{II}(\mathcal{E}_{II}),
\]

where \( W_I(\mathcal{E}_I) = W^R_I(E_I)W^\Im_I(\Gamma_I) \) and \( W_{II}(\mathcal{E}_{II}) = W^R_{II}(E_{II})W^\Im_{II}(\Gamma_{II}) \). Now we have the entropy expressed as the sum of four terms

\[
S(\mathcal{E}) = S^R_I(E_I) + S^\Im_I(\Gamma_I) + S^R_{II}(E_{II}) + S^\Im_{II}(\Gamma_{II}),
\]

where \( S^R_I(E_I) = k_B \log W^R_I(E_I) \) and so on. In the procedure maximizing the entropy \( S(\mathcal{E}) \) under the constraints that \( E = E_I + E_{II} \) and \( \Gamma = \Gamma_I + \Gamma_{II} \) are fixed, we obtain two independent relations corresponding to the two constraints such that

\[
\frac{\partial S^R_I(E_I)}{\partial E_I} = \frac{\partial S^R_{II}(E_{II})}{\partial E_{II}}, \quad (8)
\]

\[
\frac{\partial S^\Im_I(\Gamma_I)}{\partial \Gamma_I} = \frac{\partial S^\Im_{II}(\Gamma_{II})}{\partial \Gamma_{II}}. \quad (9)
\]

The first relation leads the usual temperature but the second one produce a new quantity which must be same for the two systems in the equilibriums. The canonical distribution for energy \( \mathcal{E}_{lm} = E_l - i \Gamma_m \) is written by

\[
P(\mathcal{E}_{lm}) = Z^{-1} \exp(-\beta^R E_l - \beta^\Im \Gamma_m), \quad (10)
\]

where \( \beta^R \) should be chosen as the usual factor \( \beta = (k_B T)^{-1} \) of canonical distribution, \( \beta^\Im \) denotes the new physical quantity in the equilibriums and the canonical partition function \( Z \) is given by

\[
Z = \sum_l \sum_m \exp(-\beta E_l - \beta^\Im \Gamma_m).
\]
Note that we can not derive the canonical distribution (10) by replacing a real energy $E$ with a complex energy $E$ in the usual canonical distribution $P(E) = Z^{-1} \exp(-\beta E)$.

What is the new quantity $\beta^3$? In independent particle systems wave functions are written by the product of all constituents such that

$$\Psi(t, r_1, ..., r_N|\mathcal{E}) = \prod_{n=1}^{N} \psi(t, r_n|\varepsilon_n), \quad (11)$$

where the wave function for one constituent with $\varepsilon_n = \epsilon_n - i\gamma_n$ is generally given by

$$\psi(t, r_n|\varepsilon_n) = e^{-i\varepsilon_n t/\hbar} \phi(r_n). \quad (12)$$

The probability density for $\Psi$ at $t$, which is normalized at $t = 0$, is evaluated as

$$\rho(t, r_1, ..., r_N|\mathcal{E}) = |\Psi(t, r_1, ..., r_N|\mathcal{E})|^2 = \prod_{n} e^{-2\gamma_n t/\hbar} |\phi(r_n)|^2 = e^{-2\Gamma t/\hbar} \prod_{n} |\phi(r_n)|^2. \quad (13)$$

We see that all the states with the same total imaginary energy $\Gamma$ have the same time-dependence $e^{-2\Gamma t/\hbar}$. Since the states with complex energy eigenvalues are unstable, the canonical distribution $P(\mathcal{E})$ must depend on time. It is natural that the time-dependence of $P(\mathcal{E})$ is same as that of the probability density, which is determined by the imaginary part $\Gamma$ of the total energy $\mathcal{E}$ of the system. We can specify

$$\beta^3 = 2t/\hbar. \quad (14)$$

Thus we can introduce a common time scale $t$ for two systems being in equilibriums.

Remember that the imaginary parts $\gamma_j$ are expressed by pairs of conjugates, that is, $\pm|\gamma_j|$ ($\forall j \in \mathbb{Z}_+$) as noted in §1. This fact means that the total imaginary part $\Gamma$ can possibly be in microscopic order (quantum size), even if the total real part $E$ is in macroscopic order. In fact such situations can be realized, when most of the constituents are in pairs of $\pm|\gamma_j|$ and number of non-pairing particles are very small in comparison with the macroscopic number $N$. In special cases $\Gamma = 0$ can happen. These systems
have real energies and then there is no reason for the systems to be unstable in time. Remembering that the states with positive imaginary parts and those with negative ones, respectively, represent growing- and decaying-resonance states [1,2], we see that in such systems two processes, that is, growing- and decaying- resonance processes occur with the same probability. It is also noticeable that such systems with real energies are in infinite degrees of degeneracy, because the combinations of the pairing with zero imaginary energy are infinity. We will definitely see this situation in parabolic-potential-barrier models in the next section.

3. Stable and quasi-stable systems connected by quantum stationary flows

In the previous section the existence of stable many resonance systems have been pointed out. How can we understand such systems? Let us start from studying an explicit example in the 2-dimensional parabolic potential case discussed in the paper [4]. Before discussing on the imaginary energies, we note that the real energy eigenvalue is always represented by a fixed constant in parabolic potentials [2,3] and then there is no freedom arising from the real energy eigenvalue. Imaginary eigenvalues $\gamma_j$ for the potential are given by the sum of two eigenvalues for two independent 1-dimensional parabolic potentials ($V(x, y) = -\frac{1}{2} m \gamma^2 (x^2 + y^2)$) such that

$$\gamma_{j_1, j_2} = j \hbar \gamma,$$

where $j = j_1 + j_2$ with $j_1 = \pm (n_1 + \frac{1}{2})$ and $j_2 = \pm (n_2 + \frac{1}{2})$ for $n_1, n_2 \in \mathbb{Z}_+$. It is interesting that we have $\gamma_{j_1, j_2} = 0$ for the cases with $j_1 = -j_2 = \pm(n + \frac{1}{2})$ ($\forall n \in \mathbb{Z}_+$). Note that the zero imaginary eigenvalues are infinitely degenerate. As discussed in ref. 4, such zero imaginary states are well interpreted by the figure in fig. 1, where they are described by the wave function ($\psi_{n_1 n_2}(t, r)$) with equal incoming- and outgoing-stationary flows which are defined by the probability current

$$j(t, r) = \Re [\psi_{n_1 n_2}(t, r)^* (-i \hbar \nabla) \psi_{n_1 n_2}(t, r)]/m.$$
with \( m \) = the mass of particle [4,5].

We see that the stationary flow incoming toward the center of the potential is expressed by the positive eigenvalue and that outgoing from the center done by the negative one. (In details, see ref. 4.)

Let us here consider \( N \) pairs of a particle and a parabolic potential arranged on a line. Since the magnitudes of the two flows are equal at the same distance from the center, we can connect the flow outgoing from a potential to that incoming toward the next potential at the middle point of the two potentials. Such a situation is expressed in fig. 2.

Now we can easily construct 2-dimensional lattices in which all lattice points are connected by stationary flows as figured in fig. 3. It is remarkable that we can have stable systems composed of unstable constituents such as resonances. Note also that every square made up from four lattice points is connected by a circular flow, that is, the total lattice system seems to be composed of small circular flows trapped in the squares. The fact that these lattices are not connected by wave functions but by stationary flows means that they can have some classical properties, because the flows are basically observable in quantum mechanics. Therefore we can call the lattices semiclassical systems. Note here
Fig. 2: 1-dimensional lattice connected by stationary flows.

Fig. 3: 2-dimensional lattice connected by stationary flows.
that length between two neighboring lattice points are arbitrary and then structures of lattices are not rigid but rather flexible.

The following point should be noticed that at the edge of the system incoming- and outgoing-flows can generally not be connected, that is, the system have absorbing points and sending-out points of the stationary flows in environments (heat baths) like breathing of living matters. This fact implies that those systems can generally be unstable and decay at the edge in the 2-dimensions when they are put in unsuitable environments, where the absorbing flows and the sending-out flows are not arranged with an equal weight. Such quasi-stable systems, however, seems to be quite interesting to describe realistic systems slowly decaying from their edges, which can be seen quite often in our daily life. Of course, we can have stable systems on closed surfaces like soccer balls and torus.

In 3-dimensional isotropic parabolic potentials we have no stable states with zero imaginary energy eigenvalue, because energies induced from zero-point energy eigenvalues \( \pm \frac{1}{2} \hbar \gamma \) do not cancel each other in odd dimensions. Provided that the product of the curvature of potential \( \gamma \) and the number of constituents \( N \) is so small that the time scale given by \( \tau = (\frac{1}{2} \gamma N)^{-1} \) is enough large in comparison with the time scale realizing thermal equilibriums, we can observe metastable systems which decay not only on the edges but in the inside of the systems as well.

Even in odd dimensions we find out two possibility that real eigenvalues appear from the compositions of complex eigenvalues in 3-dimensional spaces. One is the case where three coupling constants \( (\gamma_1, \gamma_2, \gamma_3) \) representing the curvatures in 3-dimensions are different from each other but satisfied by some relation, for instance, \( \gamma_1 + \gamma_2 = \gamma_3 \) and three eigenvalues \( \pm i(n_1 + \frac{1}{2}) \hbar \gamma_1, \pm i(n_2 + \frac{1}{2}) \hbar \gamma_2, \mp i(n_3 + \frac{1}{2}) \hbar \gamma_3 \) fulfill the relations \( n_1 \gamma_1 + n_2 \gamma_2 = n_3 \gamma_3 \). States satisfying these two relations can have zero imaginary eigenvalues. Note that at least one state specified by \( n_1 = n_2 = n_3 = 0 \) satisfies the relations. These relations means that all flows incoming from two directions go out from one direction and vice versa. Another possibility for zero imaginary eigenvalues is seen in the case that potentials is described by 2-dimensional parabolic potential and 1-dimensional harmonic
one. Imaginary energy-eigenvalues of total systems can be zero. In these cases we can find very rich and complicated structures in quasi-stable systems. In both cases the decays of those systems can occur only on their surfaces including edges.

4. Remarks

We see that statistical mechanics based on principle of equal \textit{a priori} probability can be applicable to systems composed of many unstable states. To complete statistical mechanics, we still have a lot of problems to investigate, for instance, how to define and interpret thermal quantities corresponding to free energy, pressure, heat capacity and so forth. Ergodic theorem have also to be discussed in the present scheme. We have, however, found out two remarkable results. One is the introduction of a common time scale, which will possibly have some connection with the common time of our universe. The other is the existence of stable and quasi-stable systems which seem to be interesting candidates to describe realistic systems having long life-times. It should be stressed that the structure of those systems can be very much flexible because the distances between any neighboring constituents are arbitrary.

A toy model can represented by systems for gases of which constituents have parabolic potential barriers in each other. Such systems can completely be separable into center of mass motions and relative motions written by the same parabolic potential. The procedure for the statistical mechanics performed in §2 can directly be applicable to this model and reproduce usual temperature from the center of mass motions and time scale from relative motions. In this model growing- and decaying- resonance states, respectively, describe two constituents approaching and leaving each other. Actually 2-dimensional models seems to be applicable to the investigation of problems with respect to surfaces of materials.

It is noticeable that many body systems can possibly be quasi-stable even under such repulsive potentials. Systems composed of many bodies having repulsive forces between any pairs of constituents will be realized electron gases, that is, electron plasma. We have to solve complex eigenvalue problem for the repulsive Coulomb potential. In order to say
whether such quasi-stable systems exist or not, it is enough to show whether there exist
complex eigenvalue solutions or not. We need not understand any details of the complex
eigenvalues, because the existence of complex conjugate pairs is guaranteed in the theory.
We shall study this problem in more detail.

Up to now we have discussed on repulsive potentials. As studied in textbooks [6], it is
known that attractive potentials such as shown in fig. 4 have complex eigenvalue solutions.
For instance, electric potentials of atoms for incoming electrons will be approximated by

\[ V(x) \]

**Fig. 4:** An example of attractive potential with complex energy eigenvalues.

such potentials. Namely there is an attractive force near the center arising from the
positive charge of nucleus, which is surrounded by the repulsive force induced from the
electrons trapped in the atom. There will be a possibility for interpreting chemical bonds
in this scheme.

It is also pointed out that these quasi-stable states are connected by flows which are
generally observable in quantum mechanics. This property indicates that those states can
have some classical properties. It seems to be very attractive to describe phenomena being
in borders between quantum processes and classical ones such as mesoscopic processes in terms of the present scheme. We should notice that the idea of the connection by flows are applicable to real energy eigenvalues states contained in usual Hilbert spaces.

Finally we would like to comment on cases where imaginary eigenvalues are not independent of real ones. In general there may be some relations between real and imaginary energy eigenvalues ($\epsilon_j$ and $\gamma_j$). In such cases the formula (4) for the number of combinations should be written as

$$W(\mathcal{E}) = \sum_{\epsilon_1} \cdots \sum_{\epsilon_N} \delta_{\sum_j \epsilon_j, E} \ W^3(\Gamma : \epsilon_1, \ldots, \epsilon_N),$$

where $\delta_{\sum_j \epsilon_j, E}$ is the Kronecker delta symbol representing the relation $\sum_j \epsilon_j = E$ and $W^3(\Gamma : \epsilon_1, \ldots, \epsilon_N)$ stands for the sum over states with respect to the freedom of the imaginary energies when the real energy eigenvalues of all constituents are fixed. It is obvious that the above formula turns to that of (4), when $W^3(\Gamma : \epsilon_1, \ldots, \epsilon_N)$ does not depend on the real energy eigenvalues. We can follow the same procedure in deriving the entropy. It is, however, very hard to obtain a general formula for the entropy, because the situations so much depend on the relations between the real and imaginary eigenvalues. We have to investigate very carefully and precisely the relation for each interaction, that is, we have to solve Gel’fand-triplet problems for the interaction. It is, however, stressed that the existence of quasi-stable states composed of complex energy eigenstates is guaranteed because of pairings of complex energy eigenvalues, when states having non-zero imaginary-energies are involved in Gel’fand-triplet solutions. We should also investigate the possibility of entropy transfer between two entropies $S^R$ and $S^\mathcal{I}$ given in (5).
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