PERTURBATION THEORY OF A DISSIPATIVE QUANTUM SUBSYSTEM

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It is shown how a nondegenerate quantum perturbation of a dissipative quantum subsystem, part of a larger conservative system, may be carried out. Under a certain condition, an approximately conservative system may result from adding the perturbation, or equivalently the interactions with the full system. For large systems, the condition leads to nonlinear integral equations and induced gap behaviour in the spectrum. Conditions under which the equations may be satisfied are discussed.

Keywords: Perturbation theory, quantum theory.

1. Introduction

There is by now an immense literature which concerns dissipative subsystems of larger conservative systems. Some works generalize the Schrödinger theory [1–3], some adopt a quantum-classical theory [4–6], some study the masters equations and calculate a reduced density matrix [7, 8]. Very general analysis has been made on the effect of adding both dynamics (time) and thermal properties (temperature) [9–11]. Sometimes perturbation theory has been used, but usually on the quantum master equation. It is common to assume a quantum system immersed in a heat bath.

Physical examples readily abound, as in the case of a system of electrons, phonons and the interactions, all making up part of a larger but conservative system of electrons plus phonons. In this example phonons are continually being absorbed, sending electrons from one state to a higher energy one, or are being emitted with electrons dropping to a lower energy level. It is clear in the example that there is no absolute conservation of the number of particles for any given energy level. However, equilibrium does mean that there is an overall conservation of the number of particles for each open subsystem.

We study only the equilibrium situation. In mathematical terms, it is only necessary to show that interactions alone suffice, that is that the subsystem plus interactions is conservative. The actual presence of the second subsystem is in fact immaterial, because without interactions the two subsystems would not see each other. This in turn justifies the use of time independent theory for subsystem plus

interaction. However, the interactions themselves would have to be shaped by the requirement that they, plus the second subsystem, should be considered conservative as well. As such, we only address the first part of the problem.

Here we adopt the conventional fully microscopic and zero temperature approach for nondegenerate levels. This task has already been initiated in [12, 13], in which the possibility of reduction of decay rate due to a complex part of the nondegenerate initial spectrum is noted, and we also find it here. Long-lived unusual (non Gamow) decay states are also noted in [14]. Our purpose is to analyze such situations in more detail, but in general terms, focusing specifically on the construction of states with infinite lifetime within second-order perturbation theory. We show that this surprising solution, apparently previously missed, is possible in systems with a large number of levels. This approach stresses what we think is the simplest possible rigorous one, dealing with both perturbed levels and final lifetimes. Our conclusion is that when interactions are added to a quantum dissipative subsystem, which makes the full system conservative, then the subsystem itself can, to a certain extent, be treated in time independent formulation. Clearly such approach does not immediately consider fluctuation dynamics about a mean, and certainly does not address the interesting case of irreversible quantum dynamics, but in general terms, it should be adequate for average quantities. For example, in the electron–phonon problem, we expect that as time passes, there is an overall equilibrium between the two subsystems.

Typically quantum theory can deal with an increase or decrease of the state probability density in time, by adding imaginary parts to the energy levels. However, traditional methods of quantum theory shun this option, in favour of Hermitian Hamiltonians, which only yield real eigenvalues. While it is true that the full Hamiltonian is expected to be Hermitian, subsystems can clearly violate this requirement. In our example the subsystem does not have real eigenvalues, but addition of interaction turns it into an overall number conserving system. The interaction is added in nondegenerate perturbation theory, adequate for zero temperature. The coupling of the subsystem with the rest of the system is here considered through the interactions U.

2. Model calculations

Time independent nondegenerate perturbation theory yields, to second order, the approximate eigenvalues [13]

$$E_n = E_n^0 + U_{nn} + \sum_{k \neq n} \frac{|U_{nk}|^2}{E_n^0 - E_k^0}. \tag{1}$$

Here E_n are the approximate eigenvalues of the total Hamiltonian H, while E_n^0 are the energy levels of the system represented by H_0 prior to adding the perturbation. The total Hamiltonian has the form $H = H_0 + U$ and $U_{nk} = \langle n|U|k\rangle$ are the matrix elements of U evaluated between the unperturbed eigenstates of H_0. Now imagine

that the eigenvalues of H_0 are not real, but given by the eigenenergies $E_n^0 + iV_n$. The reason for doing this is that the subsystem alone is not conservative. Then, what we should do is to recalculate expression (1) using the new eigenvalues. What we get is a real part, which remains similar to (1), becoming expression (1) when all V_n are zero, plus an imaginary part equal to

$$i\left[V_n - \sum_{k\neq n} \frac{|U_{nk}|^2(V_n - V_k)}{(E_n^0 - E_k^0)^2 + (V_n - V_k)^2}\right]. \tag{2}$$

It should not escape now one's attention that the complex part (2) can be made to vanish, so that the eigenvalues of H become real, at least in perturbation theory. This gives us our nonlinear equation involving the complex part of the subsystem eigenenergies. There are in essence now two expressions (not one) to consider. Clearly our interest lies in those possible solutions of Eq. (4) below, which are not merely trivial, that is the V_n are not all zero. The possibility of setting expression (2) to zero is of interest in analyzing long-lived quasi-particle excitations. Otherwise, in the general case, these expressions give us an idea about the energy and the lifetime of the perturbed levels. Setting expression (2) to zero, means physically that the full system is conservative, at least within second-order perturbation theory. This motivates the following:

ASSUMPTION 1. The following system of two equations is taken as the fundamental set:

$$E_n = E_n^0 + U_{nn} + \mathrm{Re}\left(\sum_{k\neq n} \frac{|U_{nk}|^2}{E_n^0 + iV_n - E_k^0 - iV_k}\right), \tag{3}$$

$$V_n = \sum_{k\neq n} \frac{|U_{nk}|^2(V_n - V_k)}{(E_n^0 - E_k^0)^2 + (V_n - V_k)^2}. \tag{4}$$

Eq. (4) reminds one of the nonlinear equation for the gap function in wave vector space which one obtains for zero temperature superconductivity. As such it is subject to different possible approximations for solution, according to the problem. We will initially make an unnecessarily strong assumption, to get a self-consistent solution, and then relax it to see how solutions should be handled. However, we first note

COROLLARY 1

$$\sum_n V_n = 0. \tag{5}$$

Proof: The terms on the right-hand side of Eq. (4) of Assumption I cancel in pairs. □

This condition means that overall there is no net gain or loss of subsystem particles, when all levels are considered, a conclusion which may also be drawn by looking at the time dependent quantum mechanical version. Let us return now to our assumption. This reads

ASSUMPTION 2. The expression

$$\Delta = \text{Cons} = \frac{|U_{nk}|^2}{(E_n^0 - E_k^0)^2 + (V_n - V_k)^2} = F_{kn} \tag{6}$$

is constant for all n and k.

THEOREM 1. *For an N-level system Assumption 2 leads to the conclusion that $\Delta = 1/N$ fulfills the requirement of a fully consistent system of equations.*

Proof: It is sufficient to write out the equations in detail to check this, for any N. □

This being the case we see that for large N, our assumption is quite consistent with the additional requirement that the level separation is large compared with matrix elements, a requirement for the validity of second order nondegenerate perturbation theory. Using this result, one recalculates the final perturbed spectrum with real eigenvalues, and finds that it spreads out compared with the original real part of the unperturbed eigenvalues. One also finds

LEMMA 1.

$$\sum_n E_n = \sum_n U_{nn} + \sum_n E_n^0 . \tag{7}$$

Proof: It can be checked for any number of levels. □

This constitutes conservation of energy in this model.

However, Assumption 2 is probably too restrictive, in that there is no reason that all matrix elements and energy levels should follow such strict relationship. Therefore our nonlinear set may also be solvable under the looser assumption:

ASSUMPTION 3.

$$1 = \sum_{k \neq n} F_{kn}. \tag{8}$$

This is adequate for a large system. For a dense set of levels such sums can be transformed into integrals. Additional solving assumptions might include the constancy of the matrix elements over a reduced interval of energies, and so on.

When we analyze conditions for the final spectrum to be real, it is clear that we cannot consider just one level as possessing an original complex part, but must consider at least a two-level system as having original complex parts. This has to be of opposite sign for the two levels, as $(V, -V)$. Let U be the original matrix element connecting the two levels, and ΔE the original separation. In this case the solution which must follow is $\Delta = F_{ab} = \frac{1}{2}$, so that the nontrivial solution for $V = \frac{1}{2}\sqrt{2U^2 - (\Delta E)^2}$ is possible as long as $2U^2 > (\Delta E)^2$. Clearly the separation of levels cannot be too great, for the nontrivial solution to be operative. Otherwise the trivial solution will hold, V is zero, and the original eigenvalues taken as real. For a two-level system this is the only possible strategy, but this could vary in a many-level system. Note also that the resonances do not necessarily arise here only

in pairs (as in the Gamow case), N could be odd, as long as it is greater than 2. However, the fully paired solution with N even is always an option.

3. Discussion

In this two-level system, it appears we do not have that much leeway, because we could already plausibly be in the region in which the perturbation theory is invalid. However, take now a system with $N = 10\,000$ levels. Then we must meet the condition $100U > \Delta E$, when we have $10U = \Delta E$, denoting now by U and ΔE the magnitudes of the respective quantities, on the average. Since $100 > 10$, we meet both this condition and the condition for second-order perturbation theory, that energy separations be much larger than matrix elements. Therefore this seemingly exceptional case can well arise within the conditions of second order perturbation theory. In fact, it almost must arise, except for the possibility of the trivial solution.

We have however shown that certain interactions, added to a dissipative quantum subsystem, are able to convert the problem to the one with real eigenvalues. The nature of the perturbed spectrum is that the large eigenvalues are raised by the perturbation, while the small ones are lowered, so we tend to have more gap space in the spectrum. However, as noted previously [12], this increase in gap space is attenuated by the presence of the complex part of the original spectrum. Strategies for solutions would depend on the particular problem, but have much in common with approximations adopted in the theory of zero temperature superconductivity, which yields a similar set of equations [15]. In any particular problem, energy considerations should determine viability of the nontrivial solution.

In usual approaches to the problem of an open subsystem in contact with the rest of the system, two effects arise at the same time. One is the energy shifting effect on the energy levels due to the interactions with the environment, while the other is the effect of dissipation, because the subsystem alone is not conservative. The complete system is conservative. Here we have not tried to correlate the two separate effects at the outset, which should properly arise together. Our initial treatment of the effect of dissipation is phenomenological, as the separately introduced terms V_n. We have only argued a final equilibrium situation which should not have dissipation, and which does give a condition for the interrelation of the two separate effects, because the formulae contain the V_n, E_n and U_n. Because the final equilibrium situation has no assumed dissipation, usual equilibrium treatment of the fluctuations in occupation numbers should be applicable, in the case that everything is immersed in a heat bath. Out of equilibrium fluctuations are perhaps a challenging topic for the future.

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