A toy model of a macroscopic quantum coherent system

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Abstract
This paper deals with macroscopic quantum coherence while using only basic quantum mechanics. A square double well is used to illustrate Leggett–Caldeira oscillations. The effect of thermal radiation on two-level systems is discussed. The concept of decoherence is introduced at an elementary level. Reference values are deduced for the energy, temperature and time scales involved in macroscopic quantum coherence.

1. Introduction

Triggered by a seminal paper [1] by A J Leggett in 1980, macroscopic quantum coherence (MQC) research has yielded impressive experimental [2–5], theoretical [6–9] and technological achievements [10–12]. The ideas developed by Leggett and his collaborators in the last 30 years have changed the way we understand the relations between quantum and classical behaviours, and are now crucial in the development of quantum computing. This paper aims to explain the basic phenomenology of MQC, employing only undergraduate-level quantum mechanics. Thus, we believe it may be of interest to any student who has attended at least a one-year course in quantum physics. It may also be useful for faculty members committed to introducing students to contemporary research.

In order to explain briefly what MQC is, let us consider a particle in a symmetric double well potential (SDWP). Figure 1 depicts an example of such a potential. In freshmen courses we have been told what to expect when the particle is in a high-lying energy level in a nice, analytical potential such as this: for states for which the change in potential energy within a de Broglie wavelength is much smaller than the mean kinetic energy, the specifically quantum
features of the behaviour are negligible and the classical description is adequate [13]. In that sense, classical mechanics can be considered as a limiting case of quantum mechanics [14].

Suppose, nonetheless, the central barrier in the SDWP of figure 1 to be of macroscopic width. In this case quantum and classical predictions certainly clash. A classical viewpoint demands two distinct localized states of stable equilibrium, situated at \(-x_0\) and \(x_0\); while quantum mechanics predicts an even probability distribution for the (non-degenerate) ground state (which is, of course, the more stable stationary state). Figure 2 illustrates the typical profile of the ground state of an SDWP.

Indeed, all the stationary solutions of an SDWP have necessarily even probability distributions, as exemplified by the (odd) first excited eigenfunction of figure 3.

What Leggett predicted more than 30 years ago, and what actually happens in experiments carried out in SDWPs of micrometric and nanometric typical lengths, is the appearance of a twofold degenerate ground level \(E'\), with the system oscillating in harmonic fashion between the localized eigenstates \(|L\rangle\) (figure 4) and \(|R\rangle\) (figure 5). At ground level, the position expectancy value oscillates in the accordance with:

\[
\langle x \rangle_0(t) = \langle x \rangle_0(0) \cos \omega t.
\]

This phenomenon, so-called Leggett–Caldeira oscillations, is closely related to the Rabi oscillations of atomic physics. It is explained as the result of the purported ground level \(E'\) resolving into a true ground level

\[
E_+ = E' - \hbar \omega / 2,
\]

endowed with an even non-localized eigensolution \(|+\rangle\), and a first excited level

\[
E_- = E' + \hbar \omega / 2,
\]

endowed with an odd non-localized eigensolution \(|-\rangle\). When a quantum system tunnels periodically through a macroscopic barrier in an SDWP, we have MQC.

\footnote{Chapter I, section 6.}
\footnote{Chapter III, section 21.}
The states $|R\rangle$ and $|L\rangle$ have, each one on its own, a definite value of a macroscopic property (namely, the property of being localized at the left or the right of the barrier). At the same time, $|R\rangle$ and $|L\rangle$ are linear combinations of the states $|+\rangle$ and $|-\rangle$, which cannot be said to be localized. In order to understand Leggett’s original motivation, notice the analogy between macroscopic SDWPs and Schrödinger’s cat: the celebrated pet can be in any of two different *macroscopically distinguishable* states (let us say, $\Psi_1$ for a live cat and $\Psi_0$ for a dead one), just as a particle in an SDWP. If any of these macroscopic systems is to obey the laws of quantum
mechanics, then it could be prepared in linear combinations that lack a sharp, well-defined value of the macroscopic property. Examples of these linear combinations are the $|\pm\rangle$ states of the SDWPs and the ‘neither dead nor alive’ states

$$\Psi_\pm = \frac{1}{\sqrt{2}} (\Psi_0 \pm \Psi_1)$$  \hspace{1cm} (4)
of the cat. Thus, MQC can more generally be defined as the quantum superposition of distinct macroscopic states. Long before 1980, macroscopic quantum phenomena had been discovered: superconductivity in 1911, and superfluidity in 1937. Yet it remained for Leggett to identify the necessary conditions for the appearance of macroscopically distinguishable states in a quantum system [1].

Some twenty years elapsed between Leggett’s proposal and credible experimental confirmation [4, 5] of MQC. One of the main reasons for this delay lies in the fact that the phase coherence of the $|\pm\rangle$ states is rapidly lost due to the interaction of the system with its surroundings, so that the system collapses into one of the localized states before a period of the Leggett–Caldeira oscillation can be completed [1, 8].

MQC is not only relevant from the purely theoretical point of view. A physical qubit is nothing but a two-level system when considered as a piece of hardware. And as we shall see, at least some SDWPs can behave as effective two-level systems when brought to low enough temperatures. Quantum computing (an area with impressive software development, but with little hardware to show) requires qubits to interact with one another without loss of coherence, for fairly long times, even at fairly high temperatures. Thus, two-level dissipative systems (an area in which Leggett and collaborators made far-reaching contributions while probing the foundations of quantum physics) have revealed themselves as crucial for future technological development [3, 5].

The rest of this paper is structured as follows. In section 2 we discuss the spectra of a family of symmetric double square well potentials, and the conditions under which a member of this family can be considered an effective two-level system. Next, the properties of two-state systems arising from SDWPs are discussed in section 3. We then go on to examine in section 4 how thermal radiation can render the two-level model inapplicable by throwing the system into high-lying energy levels. In section 5 decoherence is introduced in elementary terms, and its relation with dissipation is discussed briefly. Reference values for the time, energy and temperature scales involved in MQC are derived from our toy model in section 6. Finally, conclusions are laid out in section 7.

2. Symmetric double square wells

Leggett resorted to quasi-classical considerations when stating his original proposal [1]. Also, the Wentzel–Kramers–Brillouin (WKB) approximation was applied to double well potentials by Landau and Lifshitz [14]6, and more recently, in this journal by others [15]. Here we take a different perspective, avoiding altogether quasi-classical approximations, by considering a particular family of double infinite square well potentials as approximations to actual, analytic SDWPs. Our procedure will later allow us to obtain some reference values for the energies, temperatures and times involved in MQC. The following family of piece-wise-constant potentials will be considered:

$$U_b(x) = \begin{cases} 
\infty & \text{if } x \leq -a - b, \\
0 & \text{if } -b > x > -a - b, \\
k & \text{if } b \geq x \geq -b, \\
0 & \text{if } b + a > x > b, \\
\infty & \text{if } x \geq b + a.
\end{cases}$$  \hspace{1cm} (5)

A typical member of this family of potentials is depicted in figure 6.

Potentials of this kind have previously been studied in a different context, and it has been shown [16] that, if all other parameters are held fixed, levels $E_{2n+1}$ and $E_{2n}$ coalesce as $k \to \infty$. Here we shall consider the barrier height $k > 0$ as a fixed number, although ‘big’ in a sense

6 Chapter VII, section 50, solved example 3.
that will be readily clarified. This is to keep the gap between the ground and first excited levels sufficiently small. We shall also take the width of each one of the lateral valleys, \(a > 0\), as a fixed value unless otherwise stated, leaving free the only other parameter, that is, the barrier half-width \(b > 0\).

One of the two main objectives of this section is to obtain a global lower bound for the gap between the first and second excited energy levels in the \(U_b\) potentials. Just as important for our purpose, we will learn here that there is a ‘running’ upper bound, (i.e. a bound that depends on the value of \(b\)) for the gap between the ground and first excited levels. The consequences of these two facts, which are vital for the rest of the paper, are explored in sections 3, 4 and 6.

None of the \(U_b\) is continuous, yet they share the most prominent features of an SDWP, namely, they are even potentials with completely bounded, non-degenerate, spectra, as can be shown from boundary conditions. If instead of two minima, the \(U_b\) have two non-overlapping regions of minima namely \((-a - b, -b)\) and \((b, a + b)\), this distinction will prove to be quite unimportant.

Also from boundary conditions (or from more abstract symmetry considerations) it is readily seen that the levels in the spectrum of any of the \(U_b\) are classified according to parity, just as happens for a continuous even potential:

\[
\psi_{2n, b}(-x) = \psi_{2n, b}(x), \quad n = 0, 1, \ldots, b \in (0, \infty) \tag{6}
\]

and

\[
\psi_{2n+1, b}(-x) = -\psi_{2n+1, b}(x), \quad n = 0, 1, \ldots, b \in (0, \infty). \tag{7}
\]

Let us focus on the discretization conditions below the level of the central barrier (\(E < k\)). From the boundary conditions we get, for even states:

\[
-\sqrt{E_{2n}} \cot a \frac{\sqrt{2mE_{2n}}}{h} = \sqrt{k - E_{2n}} \tanh b \frac{\sqrt{2m(k - E_{2n})}}{h}, \tag{8}
\]

while odd levels below the barrier level have to comply with

\[
-\sqrt{E_{2n+1}} \cot a \frac{\sqrt{2mE_{2n+1}}}{h} = \sqrt{k - E_{2n+1}} \coth b \frac{\sqrt{2m(k - E_{2n+1})}}{h}. \tag{9}
\]
Figure 7. Graphical solutions of transcendental equations (8) and (9). Depicted, functions $g(E)$ (solid), $h_b(E)$ (squares) and $j_b(E)$ (crosses). In all cases $k = 40B$ and $b = 0.8a$. In this example only the ground level and the three first excited levels are below the barrier height $k$.

Note how the first of these two conditions can be written in the form:

$$g(E_{2n}) = h_b(E_{2n}),$$

and the second can be rendered as

$$g(E_{2n+1}) = j_b(E_{2n+1}),$$

with the meaning of $g$, $h_b$ and $j_b$ being obvious from the context.

Both of these two last equations are depicted in figure 7, from which it can be seen that there exists an upper bound $B$, given by

$$B = \frac{\pi^2 \hbar^2}{2ma^2},$$

such that the ground and first excited states have to comply with

$$\frac{B}{4} < E_0 < E_1 < B,$$

no matter the value of $b$. Obviously, there can be no levels below the barrier unless $k > B/4$. We shall only consider potentials for which the condition:

$$k \gg B$$

is met, so that we will always have at least two levels below the barrier. Indeed, the number of levels below the barrier increases with increasing quotient $k/B$ and, more importantly, as $B$ is independent of $k$, condition (14) warrants that the gap between the first two levels is always small. It is not difficult to generalize (13) starting from (8) and (9) and definition (12). The result is that

$$(n + \frac{1}{2})^2 B < E_{2n,k} < E_{2n+1,k} < (n + 1)^2 B, \quad n = 0, 1, 2, \ldots, N,$$

if the level $2N + 1$ is still below the barrier.
Doubling the barrier width produces a dramatic decrease in the gap between the ground and first excited levels. Shown: function $h_b$ for $b = 0.8a$ (squares) and $b = 1.6a$ (circles), and function $j_b$ for $b = 0.8a$ (crosses) and $b = 1.6a$ (asterisks). In all cases $k = 40B$.

From inequality (15) it follows that

$$E_{2n+2} - E_{2n+1} > (n + 5/4)B, \quad n = 0, 1, 2, \ldots, N,$$

(16)

if level $2N + 1$ is below the barrier. We then have that the gap between the ground and first excited levels will always be less than the gap between the first and second excited levels:

$$E_2 - E_1 > \frac{5}{4}B > \frac{3}{4}B > E_1 - E_0.$$

(17)

But we can do much more better than that. Indeed, in the appendix it is formally proven that for any given number $\delta > 0$ there exists a value $b(\delta) > 0$ such the gap between the ground and the first excited level of a $U_b$ potential will be less than $\delta$, that is

$$E_1 - E_0 < \delta,$$

(18)

if $b \geq b(\delta)$. In other words, if we choose the barrier length large enough, then we can make $E_0$ and $E_1$ as proximate as we want, while there is a lower bound for the gap between $E_1$ and $E_1$ which is independent of the value of this length. This will allow us to find examples of $U_b$ that will work as effective two-state systems for the lowest-lying energy levels, as illustrated in figure 8.

Finally, there is one more inequality that can be derived from (15) and that will prove useful in section 4. This inequality is

$$E_2 - E_1 < \frac{15}{4}B.$$

(19)

Let us stress that relations (13), (17) and (19) are verified for each $U_b$ regardless of the value of $b$.

3. Two-level systems with reflection symmetry

In the preceding section we proved that there are $U_b$ potentials for which the gap between the ground and first excited energy levels is much narrower than that between the first and
second excited levels. Consequently, for low energy expectancy values, a particle in one of these potentials acts as an effective two-level system [17, 18].

In the rest of this section we shall consider a fixed $U_b$ that behaves as a two-level system, and drop the $b$.

Consider now the non-stationary solutions $\psi_L$ and $\psi_R$ that one obtains from the linear combinations

$$\psi_L(x, t) = \frac{1}{\sqrt{2}} \left[ \exp \left( -i \frac{E_0 t}{\hbar} \right) \psi_0(x) + \exp \left( -i \frac{E_1 t}{\hbar} \right) \psi_1(x) \right]$$

(20)

and

$$\psi_R(x, t) = \frac{1}{\sqrt{2}} \left[ \exp \left( -i \frac{E_0 t}{\hbar} \right) \psi_0(x) - \exp \left( -i \frac{E_1 t}{\hbar} \right) \psi_1(x) \right].$$

(21)

These states have no definite parity, but are instead specular images of one another:

$$\psi_L(-x, t) = \psi_R(x, t),$$

(22)

as can be seen from equations (6), (7), (20) and (21). Figures 9 and 10 show, respectively, the ground (even) and first excited (odd) eigenfunctions for a rectangular double well, while the parity-breaking 50–50 combinations are depicted in figures 11 and 12.

The position expectation value for these states is calculated from (6) in a straightforward manner:

$$\langle x \rangle_L(t) = - \langle x \rangle_R(t) = \langle \psi_0 | x | \psi_1 \rangle \cos \frac{E_1 - E_0}{\hbar} t,$$

(23)

as is the energy expectation value:

$$\langle H \rangle_L = \langle H \rangle_R = \frac{E_0 + E_1}{2}.$$

(24)
Comparing (23) with (1) and (24) with (2) one may be tempted to make the identifications

\[ E' = \langle H \rangle_L \quad \text{and} \quad \omega = \frac{E_1 - E_2}{\hbar}, \]

(25)
from which (3) would follow, so that the states of (20) and (21) could be interpreted as the localized states observed in the experiments, and \( \psi_0 \) and \( \psi_1 \) would correspond to the true ground level \( E_+ \) and the first excited state \( E_- \). That is, it would be cogent that

\[
\langle x | L \rangle = \psi_L(x), \quad \langle x | R \rangle = \psi_R(x), \quad \langle x | + \rangle = \psi_0(x), \quad \langle x | - \rangle = \psi_1(x).
\] 

In this interpretation, however, there is no room for transitions. Indeed, the complete Schrödinger equation for a \( U \) potential, which reads

\[
-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2}(x, t) + U(x)\psi(x, t) = i\hbar \frac{\partial \psi}{\partial t}(x, t),
\] 

predicts that if the system is initially prepared in the state \( \psi_L(x, t = 0) \) at time \( t = 0 \), then it will remain in the \( \psi_L(x, t) \) state for \( t \in [0, \infty) \) (which is a sophisticated way to say: forever). This is a consequence of partial differential equation theory.

Instead of periodic transitions between two different states, our equations predict the existence of a unique ‘oscillating’ state, because \( \psi_R(x, t) \) is a time-displaced replica of \( \psi_L(x, t) \):

\[
\psi_L(x, t + \frac{\pi}{\omega}) = i \exp \left( -\frac{i \pi \Omega}{\omega} \right) \psi_R(x, t),
\] 

where \( \Omega \) stands for

\[
\Omega = (E_1 + E_2)/2\hbar
\]

and \( \omega \) is as in (25). One arrives at this result directly from (20) and (21) after some algebra.

### 3.1. Flip-flops and Leggett–Caldeira oscillations

Let us start from what we know happens in actual experiments (i.e. the existence of an observable degenerate ground level) and proceed to deduce from there the perturbation needed to achieve such degeneracy. The SDWP Hamiltonian \( H \) is represented by the matrix

\[
\begin{pmatrix}
0 & E_0 \\
E_0 & 0
\end{pmatrix}
\] 

(30)
in the symmetry-respecting basis formed by the eigenfunctions \( \psi_0 \) and \( \psi_1 \). Let us consider another Hamiltonian, \( H' \), represented by the matrix

\[
\tilde{H}' = \mathcal{O}H\mathcal{O}^{-1} = \begin{pmatrix} E' & 0 \\ 0 & E' \end{pmatrix}
\]

in the symmetry-violating basis spanned by \( \psi_L \) and \( \psi_R \). Here, \( \mathcal{O} \) stands for the unitary operator which transforms \( \psi_0 \) into \( \psi_L \) and \( \psi_1 \) into \( \psi_R \), thus:

\[
\mathcal{O} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad \text{and} \quad \mathcal{O} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}.
\]

Thus, the perturbation is represented by

\[
\tilde{W} = \tilde{H}' - H = \begin{pmatrix} \hbar\omega/2 & 0 \\ 0 & -\hbar\omega/2 \end{pmatrix}.
\]

Now, in the basis spanned by \( \psi_L \) and \( \psi_R \) things look quite different. Indeed, we have that

\[
\tilde{H} = \mathcal{O}H\mathcal{O}^{-1} = \begin{pmatrix} E' - \hbar\omega/2 & -\hbar\omega/2 \\ -\hbar\omega/2 & E' \end{pmatrix}
\]

and most importantly

\[
\tilde{W} = \mathcal{O}W\mathcal{O}^{-1} = \begin{pmatrix} 0 & \hbar\omega/2 \\ \hbar\omega/2 & 0 \end{pmatrix}.
\]

Note that in this representation the perturbation has no diagonal elements. This means that zeroth order corrections introduced by the perturbation are strictly null. Furthermore, the off-diagonal elements are equal.

To be very clear, let us write the eigenequations for each one of these distinct systems. For \( H \) we have

\[
H\psi(x, t) = i\hbar \frac{\partial \psi_0}{\partial t}(x, t) = E_0 \psi_0(x, t), \quad H\psi_1(x, t) = i\hbar \frac{\partial \psi_1}{\partial t}(x, t) = E_1 \psi_1(x, t),
\]

while \( H' \) responds to

\[
H'\psi_L(x, t) = i\hbar \frac{\partial \psi_L}{\partial t}(x, t) = E' \psi_L(x, t), \quad H'\psi_R(x, t) = i\hbar \frac{\partial \psi_R}{\partial t}(x, t) = E' \psi_R(x, t).
\]

Now, let us consider \( \tilde{H}' \) as the initial, unperturbed, Hamiltonian matrix, and

\[
-\tilde{W} = -\mathcal{O}W\mathcal{O}^{-1}
\]

as the perturbation, so that \( \tilde{H} \) is the final, perturbed, Hamiltonian matrix. Then we can show that the \( \psi_L(x, t) \) and \( \psi_R(x, t) \) states transit from one another in Rabi style. Indeed, resorting to the time-dependent perturbation formalism [14], [19] we write, for a general state \( \psi(x, t) \) of \( \tilde{H} \),

\[
\psi(x, t) = c_L(t)\psi_L(x, t) + c_R(t)\psi_R(x, t),
\]

in order to obtain the equation

\[
i\hbar \frac{d}{dt} \begin{pmatrix} c_0 \\ c_1 \end{pmatrix}(t) = \tilde{W} \begin{pmatrix} c_0 \\ c_1 \end{pmatrix}(t).
\]

\[7\] Chapter VI section 40.
\[8\] Chapter V, section 9
which is equivalent to the $2 \times 2$ system of coupled linear equations:

$$i\hbar \frac{d c_L}{dt} = -\frac{\hbar \omega}{2} c_R,$$
$$i\hbar \frac{d c_R}{dt} = -\frac{\hbar \omega}{2} c_L. \tag{42}$$

By uncoupling this system we get the harmonic oscillator equation

$$\frac{d^2 c_L}{dt^2} = -\frac{\omega^2}{4} c_L \tag{43}$$

and a similar equation for $c_R$, so that

$$c_L(t) = \sin(\omega t/2 + \phi), \quad c_R(t) = \cos(\omega t/2 + \phi), \tag{44}$$

where $\phi$ is a constant that can be deduced from initial conditions. The probability of finding the particle in the state $\psi_L$ is given, according to these last equations, by

$$P_L(t) = \sin^2(\omega t/2 + \phi), \tag{45}$$

and the probability of finding the particle in the $\psi_R$ state is

$$P_R(t) = 1 - P_L(t). \tag{46}$$

This is a particular instance of Rabi oscillation, and this case is resonant due to the degeneracy of the ‘initial’ Hamiltonian $\tilde{H}$. But the ‘perturbed’ Hamiltonian $H$ is nothing other than the SDWP Hamiltonian of equation (27).

Now, equations (45) and (46) predict the ‘flip-flop’ between the stationary states $\psi_R(x)$ and $\psi_L(x)$, so that, if the system is initially prepared in the state

$$\psi(x, t = 0) = \psi_L(x), \tag{47}$$

then we will have a 100% certainty of finding it in state $\psi_R(x)$ at times $t = \frac{\pi}{\omega}, \frac{3\pi}{\omega}, \frac{5\pi}{\omega}, \ldots$ and a 100% certainty of finding it in state $\psi_L(x)$ at times $t = \frac{2\pi}{\omega}, \frac{4\pi}{\omega}, \frac{6\pi}{\omega}, \ldots$. And this last result is consistent with equation (28). Thus, we are in the presence of two different (yet not contradictory) descriptions of one and the same phenomenon: if $H$ is considered an unperturbed Hamiltonian, with complete stationary solutions $\psi_0(x, t)$ and $\psi_1(x, t)$, then we have an ‘oscillating’ non-stationary solution $\psi_L(x, t)$. If, on the other hand, $H$ is considered to be the result of a perturbation acting on the degenerate Hamiltonian $\tilde{H}$, then we get flip-flops between the complete stationary solutions of $\tilde{H}$, that is: periodic transitions between the $\psi_L(x, t)$ and $\psi_R(x, t)$ states.

In this manner, we obtain the periodic transitions (the zero point Leggett–Caldeira oscillations) observed in so many experiments. Note that these transition occur in the absence of external fields, thus without emission or absorption.

## 4. Thermal radiation

Due to the fact that no quantum system can be completely isolated from its environment, in any realistic description the Schrödinger equation must be supplemented with terms that describe the interaction between the system and its surroundings. But there are very different ways to describe this interaction and its results, depending on the time and energy scales involved, and the complexity of the analysis. Here we shall discuss the absorption-induced transitions by which the system is thrown into high-lying energy levels, rendering the two-level model inapplicable. The main result from this discussion will be a limit on the temperature at which Caldeira–Leggett oscillations can be observed.
4.1. Oscillations near resonance

Now, oscillatory behaviour is to be expected not only for the resonant, exactly degenerate, Hamiltonian matrix $H'$. Indeed, it would not be realistic to expect Leggett–Caldeira oscillations only in perfectly isolated systems. Consider a harmonic perturbation of the SDWP matrix Hamiltonian $H$ of equation (30), that is, a perturbative term of the general form

$$\mathcal{V} = A \exp(i\omega' t) + A^\dagger \exp(-i\omega' t),$$

and let us focus on the particularly simple case for which

$$A = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix},$$

so that the perturbative term can be written as

$$\mathcal{V} = A \begin{pmatrix} 0 & \exp(i\omega' t) \\ \exp(-i\omega' t) & 0 \end{pmatrix}.$$  

We then again resort to the time-dependent perturbation formalism, and write

$$\psi(x, t) = c_0(t)\psi_0(x, t) + c_1(t)\psi_1(x, t)$$

in order to obtain the equation

$$i\hbar \frac{dc_0}{dt}(t) = \mathfrak{M}(t) \begin{pmatrix} 0 \\ c_1 \end{pmatrix}(t),$$

where $\mathfrak{M}$, defined by

$$\mathfrak{M}(t) = \exp(i\mathfrak{H} t/\hbar)\mathcal{V}(t)\exp(-i\mathfrak{H} t/\hbar)$$

represents the perturbation in the interaction picture, and in our particularly simple case reduces to

$$\mathfrak{M}(t) = A \begin{pmatrix} 0 & \exp(i(\omega' - \omega) t) \\ \exp(-i(\omega' - \omega) t) & 0 \end{pmatrix},$$

so that equation (52) is equivalent to the $2 \times 2$ system of coupled ordinary differential equations

$$i\hbar \frac{dc_0}{dt} = A \exp[i(\omega' - \omega)t] c_1, \quad i\hbar \frac{dc_1}{dt} = A \exp[-i(\omega' - \omega)t] c_0.$$  

It can be checked by hand that

$$c_0(t) = \exp(i\Omega' t/2) \left\{ \cos(R_0 t) - \frac{i\Omega'}{2R_0} \sin(R_0 t) \right\}$$

and

$$c_1(t) = -\frac{iR_1}{R_0} \exp(-i\Omega' t/2) \sin(R_0 t)$$

provide a solution for the initial conditions $c_0(t = 0) = 1$, $c_1(t = 0) = 0$. Here we have used the following shorthand

$$R_0 = \sqrt{(\lambda/\hbar)^2 + \left(\frac{\omega' - \omega}{2}\right)^2}, \quad \Omega' = \omega' - \omega \quad \text{and} \quad R_1 = \lambda/\hbar,$$

which lead to what is known as Rabi’s formula [19], namely

$$P_1(t) = \left(\frac{R_1}{R_0}\right)^2 \sin^2(R_0 t),$$  

9 Chapter V, section 10.
\begin{equation}
P_0(t) = 1 - P_1(t).
\end{equation}

It is not difficult to find the expressions for $P_R(t)$ and $P_L(t)$ for this particular choice of $\hat{A}$. We omit these, as they are not particularly illuminating. Let us just point out that in all instances $P_R$ and $P_L$ are oscillating functions of time, although they are generally not periodic. If one wishes to describe periodic Rabi oscillations in the $R$ and $L$ states, one should take, instead of (59),

\begin{equation}
\hat{A} = \frac{1}{2} \begin{pmatrix} 1 & -1 \\ 1 & -1 \end{pmatrix}
\end{equation}
as the natural choice for $\hat{A}$. By doing this one obtains expressions completely analogous to (59) and (60) for $P_L$ and $P_R$:

\begin{equation}
P_L(t) = \left( \frac{R_1}{R_0} \right)^2 \sin^2(R_0 t)
\end{equation}

\begin{equation}
P_R(t) = 1 - P_L(t),
\end{equation}

where the new frequency of the oscillation is now given by

\begin{equation}
R_0' = \sqrt{(A/\hbar)^2 + (\omega' / 2)^2}.
\end{equation}

The main conclusion of this subsection is thus that the Leggett–Caldeira can survive the influence of an environment on the particle in an SDWP under certain circumstances.

### 4.2. A limit on temperature

An important result from perturbation theory tells us that for harmonic perturbations the time-dependent transition amplitude, $c_{n \rightarrow m}(t)$, between two given eigenstates of the complete Hamiltonian $H$ is given by [20]:

\begin{equation}
c_{n \rightarrow m}(t) = \langle \psi_m | A | \psi_n \rangle \frac{1 - \exp \left( \frac{E_m - E_n}{\hbar} - \omega' t \right)}{E_m - E_n - \hbar \omega'} + \langle \psi_m | A^* | \psi_n \rangle \frac{1 - \exp \left( \frac{E_m - E_n}{\hbar} + \omega' t \right)}{E_m - E_n + \hbar \omega'}.
\end{equation}

As a consequence we get that, if the system is to stay in the two lowest lying levels, then the perturbation must meet the condition:

\begin{equation}
\omega' < \frac{E_2 - E_1}{\hbar}.
\end{equation}

Otherwise, the perturbation would excite the system to higher levels with non-negligible probability. This gives a limit on the temperature at which the system behaves like a low-lying two-level system. Indeed, recalling Wien’s law for black body radiation, we get that thermal radiation at a temperature $T$ will have a maximal contribution of frequency $\omega'$ when condition

\begin{equation}
\omega' = \frac{2 \pi c}{b_W T}
\end{equation}
is met. (Here, $T$ stands for the temperature of the radiation, $b_W$ is Wien’s constant, and $c$ the velocity of light.) Thus, if $V(x, t)$ is somehow to represent thermal radiation, and if the perturbed Hamiltonian $H'$ is to be described as a low-lying two-level system, then we must have

\begin{equation}
T < \frac{b_W}{2 \pi c} \frac{E_2 - E_1}{\hbar}.
\end{equation}
In other words: for each system there is a limit temperature above which the two-level system description is inapplicable, and zero-point Leggett–Caldeira oscillations become overshadowed by other transitions. Moreover, from inequalities (17) and (19) we get

\[ T_B(a, m) < \frac{b_w}{2\pi c} \frac{E_2 - E_1}{\hbar} < 3T_B(a, m) \]  

with this global bound given by

\[ T_B(a, m) = \frac{5\pi \hbar b_w}{16mc^2}. \]  

The meaning of expressions (69) and (70) is the following: consider a family of double rectangular barriers, with a fixed \( m, a \) and \( k \), but free barrier width. When exposed to thermal radiation, there is a temperature \( T_B \) for the radiation above which the Leggett–Caldeira oscillations are overshadowed by other transitions in at least some of the systems, and at temperature \( 3T_B \) the Caldeira–Leggett oscillations are surpassed by other transitions in all of the systems.

5. Decoherence and dissipation

We begin this section with a simplified exposition of the density matrix formalism as found in Landau and Lifshitz [14]10. After that an also simplified rendering of some of Leggett’s original argumentation is presented. Finally, the rest of this section is dedicated to a brief discussion of decoherence and its relation with dissipation.

The interaction of a system (\( S \)) with its surroundings (\( E \)) can be taken into account by considering an isolated system (\( \mathcal{U} \)) encompassing both \( S \) and \( E \) (that is: \( \mathcal{U} = S \cup E \)). The state of this new, wholly inclusive system, \( \mathcal{U} \) is described by a state function \( \Psi_1(j, \xi) \) that depends on both the coordinates of \( S \) (the \( j \)) and the coordinates of its environment (the \( \xi \)).

The total Hamiltonian \( H_T \) for the system \( \mathcal{U} \) can always be written in the form

\[ H_T = H + H_e + \lambda H_I \]  

where \( H \) depends only on the \( j \) and their generalized momenta, \( H_e \) depends only on the \( \xi \) and its momenta, and \( H_I \) depends on both types of coordinate. We shall take the approximation that \( H \) is the Hamiltonian of \( S \) when isolated, and that \( H_I \) alone models the interaction between \( S \) and \( E \).

In principle, there can be instances in which \( \Psi(j, \xi) \) is the product of two states functions:

\[ \Psi(\xi) = \psi(j)\phi(\xi) \]  

but this does not need to be the case. States that can be written in the form (72) are called pure states. States that are not pure are said to be mixed.

In order to illustrate this let us consider the case in which both the original system and its surroundings can be represented as two-level systems. If the isolated Hamiltonian \( H \) has eigenfunctions \( \psi_+ \) and \( \psi_- \):

\[ H\psi_\pm = E_\pm \psi_\pm \]  

and if \( \phi_\alpha \) and \( \phi_\beta \) are the eigenfunctions of \( H_e \), i.e.

\[ H_e\phi_\alpha = E_\alpha\phi_\alpha, \quad H_e\phi_\beta = E_\beta\phi_\beta, \]  

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then some examples of pure states are
\[
\frac{1}{\sqrt{2}}(\psi_+ + \psi_- + \phi_\beta) = \frac{1}{\sqrt{2}}(\psi_+ + \phi_\beta) + \frac{1}{2}\psi_- + \frac{\sqrt{3}}{2}\psi_- = \psi_+ = \left(\frac{1}{2}\phi_\beta + \frac{\sqrt{3}}{2}\phi_\alpha\right)
\]
and
\[
\frac{1}{4}\psi_- - \frac{3}{4}\psi_- = \left(\frac{1}{2}\psi_- - \psi_+\right)\left(\frac{1}{2}\phi_\beta + \frac{\sqrt{3}}{2}\phi_\alpha\right).
\]
and the following are instances of mixed states:
\[
\frac{1}{\sqrt{2}}(\psi_- + \psi_+ + \phi_\beta), \quad \frac{1}{\sqrt{2}}(\psi_- + \psi_+ + \phi_\beta)
\]
and
\[
\frac{1}{\sqrt{3}}(\psi_- + \psi_+ + \phi_\alpha + \psi_- + \phi_\beta).
\]

The density matrix formalism was developed to treat systems that (like \(\Psi \)) can present mixed states. The density matrix \(\rho\) allows us to calculate the expected value \(\langle f \rangle\) of any observable \(f(x, p_x)\) that depends only on the coordinates and momenta of \(\Psi\), as the trace of a matrix product:
\[
\langle f \rangle = \text{Tr}(f\rho).
\]

The elements of the density matrix \(\rho\) of a state \(\Psi(j, \xi)\) of are defined as
\[
\rho_{j', j} = S\xi \Psi^*(j, \xi)\Psi(j', \xi),
\]
where \(S\xi\) stands for the sum over the discrete \(\xi\) (if any) plus an integral over the continuous \(\xi\) (if any). In the case of our 2 \(\times\) 2-level system, expression (77) reduces to
\[
\rho_{j', j} = \Psi^*_j\Psi_{j'} + \Psi^*_j\Psi_{j'} = \Psi_{j'}\Psi_j.
\]

The diagonal elements of density matrix, of the form \(\rho_{j, j}\) are called populations, while the off-diagonal elements (i.e. the elements with \(j \neq j'\)) are known as coherences.

Suppose now that the 50–50 linear combinations
\[
\psi_L = \frac{1}{\sqrt{2}}(\psi_+ + \psi_-), \quad \psi_R = \frac{1}{\sqrt{2}}(\psi_+ - \psi_-)
\]
are eigenfunctions of a macroscopic observable \(M\), let us say
\[
M\psi_{L,R} = \mu_{L,R}\psi_{L,R},
\]
and take then the mixed state given by
\[
\Psi = c_L\psi_L + c_R\psi_R.
\]

The density matrix associated with (81) is written as
\[
\rho = \begin{pmatrix} |c_L|^2 & 0 \\ 0 & |c_R|^2 \end{pmatrix}
\]
in the \{\psi_L, \psi_R\} basis, as can be seen from (77), so that according to (76) the expected value of any observable \(f\) pertaining to \(\Psi\) yields the value
\[
\langle f \rangle = |c_L|^2 f_L + |c_R|^2 f_R,
\]
where \(f_L\) and \(f_R\) are the expected values of \(f\) in the pure states
\[
\psi_L = \psi_L\phi_\alpha \quad \text{and} \quad \psi_R = \psi_R\phi_\beta.
\]

The point of this discussion is that result (83) would be obtained from both measurements made on an ensemble of \(\Psi\) systems all in states \(\psi_L\) and measurements made on an ensemble consisting of a combination of systems in the pure states \(\psi_L\) and \(\psi_R\), in proportions \(|c_L|^2\) and \(|c_R|^2\). If a \(\Psi\) system could only be prepared in states of the form (81), then it could be argued that property \(M\) has a sharp value for each element of a given ensemble, and that a measurement
made on a particular element of the ensemble only removes our ignorance on the value of \( M \) for that particular system. Clearly, this opens the door to hidden variable theories. To put it succinctly: in an ensemble made of Schrödinger’s cats, each feline would be either dead or alive, and never in superpositions composed of both dead and alive states. Only the behaviour of the ensemble would be quantal, its individual elements being essentially classical.

It is obvious, on the other hand, that the pure state

\[
\Psi_+ = \psi_+ \phi_0
\]  

(85)
cannot be written as a mixed state of the form (81) and that its corresponding density matrix cannot be diagonal in the \((L, R)\) basis, unlike (82). The impossibility of the simultaneous diagonalization of the density matrices of all possible states of a system \( \mathcal{S} \) is then powerful evidence of the true quantal behaviour of such system, as opposed to the behaviour required by hidden variable theories. Thus, for a system \( \mathcal{S} \) to be classical in any sense of the word, the coherences, i.e. the off-diagonal elements, must be absent from the density matrix for each one of its possible states. This conclusion is generally valid, even if we resort to the most trivial case in order to illustrate it [1].

Decoherence can be defined as the decay of the off-diagonal elements in the density matrix as a result of the interaction of the system with its environment. Therefore decoherence allows a system to behave as quantal when isolated and as classical when the coupling with its environment is ‘sufficiently effective’. This is now considered a plausible mechanism for the emergence of classical reality from a quantal substratum.

In most practical applications, the environment (or bath) \( \mathcal{E} \) has a very large number of degrees of freedom (say of the order of the Avogadro number) and not just one, as in the example we have used. In other words, \( \mathcal{U} \) is usually a thermodynamic system, and quantum statistical mechanics must be applied to describe its behaviour. In this case the interaction between \( \mathcal{E} \) and \( \mathcal{E} \) (interaction known as quantum dissipation in this context) involves the relaxation of the thermodynamical variables of \( \mathcal{U} \) towards thermal equilibrium, and not only decoherence.

Various models have been proposed over the years for this dissipative two-level systems, but one of the first and most successful is the spin-boson Hamiltonian, in which \( \mathcal{E} \) is taken to be a collection of harmonic oscillators with various frequencies and the interaction term \( H_I \) is linear in both the \( j \) and the \( \xi \) coordinates. One important result from this approach is that a two-level system \( \mathcal{S} \) will describe damped oscillations between the localized states \(|R\rangle \) and \(|L\rangle \). Depending on the frequency distribution of the environment, \( \mathcal{S} \) may be localized at \( T = 0'K \) (the overdamped case, known as ‘sub-Ohmic’), it may present critical damping (the ‘Ohmic case’) or it may undergo underdamped coherent oscillations (the ‘super-Ohmic case’). The last one of these three instances is the most interesting for the present discussion, as it allows the observation of MQC before the complete relaxation of the system. The possibility of experimental MQC in the super-Ohmic case depends in the interplay between a coherence time depending only on the bath parameters, and the period of the Leggett–Caldeira oscillation for system \( \mathcal{S} \).

\section*{6. The scales of MQC}

Let us start by fixing the width of the lateral wells at:

\[ a = 1 \mu m, \]  

(86)
a value typical of contemporary lithographic circuitry, and take \( m \) to be the rest mass of an electron:

\[ m = m_e = 9.1 \times 10^{-31} \text{kg}. \]  

(87)
Table 1. Period $\tau$ increases exponentially as the barrier width is augmented. $a = 1.0 \ \mu m$, $k = 2 \times 10^{-20} J$. This table, as well as all the figures, was generated using Matlab® R2012a.

| $b$ (nm) | $E_0$ ($\times 10^{-26} J$) | $E_1$ ($\times 10^{-26} J$) | $\Delta E$ ($\times 10^{-28} J$) | $\tau$ (µs) |
|---------|-----------------|-----------------|-----------------|-----------|
| 100.000 00 | 5.375 3895 | 5.438 2093 | 6.3 | 1.0 |
| 116.652 90 | 5.389 9569 | 5.424 6062 | 3.5 | 2.9 |
| 136.079 00 | 5.398 7829 | 5.416 0961 | 1.7 | 3.8 |
| 158.740 11 | 5.403 6276 | 5.411 3353 | 0.77 | 8.6 |
| 185.174 94 | 5.405 9909 | 5.408 9897 | 0.30 | 22.0 |
| 216.011 95 | 5.406 9931 | 5.407 9902 | 0.10 | 66.0 |
| 251.984 21 | 5.407 3539 | 5.407 6298 | $2.7 \times 10^{-2}$ | 240.0 |

With this, $B$ takes the value

$$B = 0.6 \times 10^{-25} J = 0.36 \ \mu eV,$$

and $T_B$ is fixed at

$$T_B \approx 1.1 \ \text{mK}.$$

From equation (25), which gives the fundamental frequency of the Caldeira–Leggett oscillations, we get the corresponding period

$$\tau = \frac{2\pi \hbar}{E_1 - E_0}.$$

A global lower bound for this period is found from expressions (12) and (13):

$$\tau > \frac{2\pi \hbar}{B} = \frac{4ma^2}{\pi \hbar}.$$

For values (86) and (87) this gives

$$\tau > 11 \text{ns}.$$

From table 1 (obtained through computer assisted numerical analysis) we get that as we sweep the barrier width from 0.2 to 0.5 $\mu m$ the period of the Leggett–Caldeira oscillations for our square double well increases from 1.0 to 240 $\mu s$. Based on general considerations it has been estimated [1] that, for all practical purposes, MQC is lost if the period of the Leggett–Caldeira oscillation is of the order $\tau \gtrsim 100 \ \mu s$. Thus, the last row of the table corresponds to a localized system. All the other tabulated values could in principle correspond to observable MQC.

6.1. Some of the many things we have left out

MQC experiments are carried out in superconducting quantum interference devices (SQUIDs) with low capacitance tunnelling Josephson junctions [1, 4] and the relevant coordinate (i.e. the analogous of coordinate $x$) is not of a geometric character (like a position) but is in most cases the phase difference between the states functions of the electrons in a Cooper pair (so that $m$ is not really the mass of the electron). Thus our toy model is in reality a simplification of a mechanical analogy used to discuss experimental MQC.
7. Conclusion

Contemporary quantum mechanics, both experimental and theoretical, provides examples of basic concepts and techniques such as tunnelling, stationary states, two-level systems, perturbation theory, the density matrix and the WKB approximation. Classroom presentations of current areas of research, such as MQC, help to improve understanding of quantum physics at university level, as they connect simplified textbook models with the actual state of the field, and thus with students’ future professional activity. Moreover, MQC illustrates in a beautiful way the interplay between theory and experiment, and between concepts and techniques arising in different areas of quantum physics.

We believe we have achieved in this paper a level of exposition that makes the subject both clear and interesting for senior university students and recent graduates. To do so, we had to glide over the more technical aspects of experimental MQC and the intricate relation between MQC and the epistemology and philosophy of physics. We hope that the paper will encourage the interested reader to delve further into these facets of contemporary research.

Appendix

Consider condition (8) for the ground level \((n = 0)\), that is
\[
E_0 \cot^2 a \frac{\sqrt{2mE_0}}{\hbar} = \frac{(k - E_0) \tan^2 b \sqrt{2m(k - E_0)}}{\hbar}. \tag{A.1}
\]

We will now establish a lower bound for \(E_0\) starting from (A.1), but we have to take some precautions in doing so because \(E_0\) depends implicitly on \(b\). In order to proceed, note that
\[
\forall b \in (0, \infty), \quad \frac{\sqrt{2m(k - E_0)}}{\hbar} < \frac{\sqrt{2m(k - B/4)}}{\hbar}, \tag{A.2}
\]
so that
\[
\forall b \in (0, \infty), \quad \tanh^2 b \frac{\sqrt{2m(k - E_0)}}{\hbar} > \tanh^2 b \frac{\sqrt{2m(k - B/4)}}{\hbar}. \tag{A.3}
\]

The dependence of the rhs of inequality (A.3) is explicit, so that the usual procedures of calculus can be applied. In particular, as we now from elementary theorems that the limit
\[
\lim_{b \to \infty} \tanh^2 b \frac{\sqrt{2m(k - B/4)}}{\hbar} = 1 \tag{A.4}
\]
holds true, we can affirm that: for given \(\delta > 0\) there exists a \(b_0(\delta)\) such that any \(b > b_0(\delta)\)
\[
\tanh^2 b \frac{\sqrt{2m(k - B/4)}}{\hbar} > 1 - \frac{\delta}{2k}. \tag{A.5}
\]

From (A.1), (A.3) and (A.5) we deduce that for any \(b\) above a certain value \(b_0(\delta)\), the ground energy of \(U_b\) satisfies
\[
E_0 \cot^2 a \frac{\sqrt{2mE_0}}{\hbar} > (k - E_0) \left(1 - \frac{\delta}{2k}\right), \tag{A.6}
\]

Turning our attention to the condition for \(E_1\), i.e.
\[
E_1 \cot^2 a \frac{\sqrt{2mE_1}}{\hbar} = \frac{(k - E_1) \coth^2 b \sqrt{2m(k - E_1)}}{\hbar}, \tag{A.7}
\]
we now find an upper bound for \(E_1\), by noting that, because of (A.2) and the known properties of the hyperbolic functions, the inequality
\[
\coth^2 b \frac{\sqrt{2m(k - E_1)}}{\hbar} < \coth^2 b \frac{\sqrt{2m(k - B/4)}}{\hbar} \tag{A.8}
\]
is verified for all strictly positive $b$. Furthermore,
\[
\lim_{b \to \infty} \text{coth}^2 b \sqrt{2m(k - B/4)} = 1
\]  
so that for every $\delta > 0$ there exists a $b_1(\delta)$ such that, if $b > b_1(\delta)$, then inequality
\[
\text{coth}^2 b \sqrt{2m(k - B/4)} < 1 + \frac{\delta}{2k}
\]  
is satisfied for all strictly positive $b$. And from (A.7) and (A.10) we get that, for all $b$ above a certain threshold value $b_1(\delta)$, the inequality
\[
E_1 \cot^2 a \sqrt{2mE_1} < (k - E_1) \left(1 + \frac{\delta}{2k}\right)
\]  
is satisfied. Taking both (A.6) and (A.11) into consideration, we have that for every $\delta > 0$ there exists a number $b'(\delta) = \max\{b_0(\delta), b_1(\delta)\}$ such that for any $b > b'(\delta)$ the inequality
\[
0 < E_1 \cot^2 a \sqrt{2mE_1} - E_0 \cot^2 a \sqrt{2mE_0} < (E_0 - E_1) + \delta \left(1 - \frac{E_0 + E_1}{2k}\right)
\]  
is satisfied. Finally, we note that, as
\[
v(E) = \cot^2 a \sqrt{2mE}
\]  
is a monotonically increasing function of $E$ in the range $B/4 < E < B$, so that
\[
0 < E_1 \cot^2 a \sqrt{2mE_1} - E_0 \cot^2 a \sqrt{2mE_0}
\]  
and in the other hand, as $0 < E_0 < E_1$, it is true that
\[
(E_0 - E_1) + \delta \left(1 - \frac{E_0 + E_1}{2k}\right) < \left(1 - \frac{E_0 + E_1}{2k}\right) \delta < \delta.
\]  
From (A.12), (A.14) and (A.15) we get
\[
0 < E_1 \cot^2 a \sqrt{2mE_1} - E_0 \cot^2 a \sqrt{2mE_0} < \delta
\]  
Finally, we note that, as
\[
v(E) = \cot^2 a \sqrt{2mE}
\]  
is a monotonically increasing function of $E$ in the range $B/4 < E < B$, then inequality
\[
(E_1 - E_0) \cot^2 a \sqrt{2mE_1} < \delta
\]  
follows from (A.16).

As $v(E)$ is monotonically increasing in the region of interest, then (A.19) implies the inequality
\[
(E_1 - E_0) \cot^2 a \sqrt{2mB/4} < \delta.
\]  
Let us stress that $B$ is independent of $b$. In this manner, we have arrived at the following lemma.

For each strictly positive real number $\delta$ there exists a $b(\delta)$ given by
\[
b(\delta) = b' \left(\delta \cot^2 a \sqrt{2mB/4}\right)
\]  
such that for any $b > b(\delta)$ the gap between the ground and first excited levels of $U_b$ is less than $\delta$, that is, such that
\[
E_1 - E_0 < \delta.
\]  
And this is what we set out to prove in this appendix.
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