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Amir O. Caldeira
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Introduction

Since its very beginning, quantum mechanics has been developed to deal with systems on the atomic or sub-atomic scale. For many decades, there has been no reason to think about its application to macroscopic systems. Actually, macroscopic objects have even been used to show how bizarre quantum effects would appear if quantum mechanics were applied beyond its original realm. This is, for example, the essence of the so-called *Schrödinger cat paradox* (Schrödinger, 1935). However, due to recent advances in the design of systems on the meso- and nanoscopic scales, as well as in cryogenic techniques, this situation has changed drastically. It is now quite natural to ask whether a specific quantum effect, collectively involving a macroscopic number of particles, could occur in these systems.

In this book it is our intention to address the quantum mechanical effects that take place in properly chosen or built "macroscopic" systems. Starting from a very naïve point of view, we could always ask what happens to systems whose classical dynamics can be described by equations of motion equivalent to those of particles (or fields) in a given potential (or potential energy density). These can be represented by a generalized "coordinate" $\varphi(\mathbf{r}, t)$ which could either describe a field variable or a "point particle" if it is not position dependent, $\varphi(\mathbf{r}, t) = \varphi(t)$. If not for the presence of dissipative terms which, as we will discuss later, cause problems in the canonical quantization procedure, these equations of motion can, in general, be derived from a Hamiltonian which allows us, through canonical methods, to immediately write down their quantum mechanical versions. Now, depending on the structure of the potential energy of the problem, we can boldly explore any effect there would be if we were dealing with an ordinary quantum mechanical particle.

Everything we have said so far is perfectly acceptable, at least operationally, if two specific requirements are met. Firstly, the parameters present in our problem must be such that any combination thereof, leading to a quantity with dimensions of angular momentum (or action), is of the order of $\hbar$. Secondly, we must be sure that

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the inclusion of dissipative terms, no matter how it is done at this stage, does not interfere greatly with the quantum effects resulting from the former requirement.

Needless to say, following this prescription, we are implicitly assuming that there is no natural limitation for the application of quantum mechanics to any physical system. Although it does pose several conceptual questions, we would have to propose alternative theories if we wanted to think otherwise. So, we have chosen to rely on this hypothesis and explore it as far as we can, not bothering, at least openly, about questions concerning the foundations of quantum mechanics, a promise that is obviously hard to keep fully in such a subtle application of the quantum theory.

In a sense, we will be looking for situations where the microscopic parameters involved in the description of a given phenomenon only appear in particular combinations which rule the dynamics of a few collective macroscopic variables. Moreover, these resulting combinations are such that their numerical values are comparable to those compatible with the application of quantum mechanics to these systems. The remaining degrees of freedom constitute what we shall call the environment, and the signature of their existence is the presence of dissipative terms in the classical equations of motion of the variables of interest. Therefore, it is mandatory to learn how to include dissipative effects in quantum mechanics if we want to understand its application to our target systems. In other words, quantum dissipation is a natural consequence of the study of macroscopic quantum phenomena.

There are many systems that fulfill our requirements to display quantum effects at the macroscopic level. Unfortunately, they are not tiny marbles tunneling across a wall but rather a somewhat more subtle variation thereof. Usually they are magnetic or superconducting samples of reduced dimensions subject to very low temperatures. Although these are not the only examples we could mention, they will be the ones elected as our favorite throughout this book. Magnetic systems provide us with quantum effects that, on top of being experimentally realizable, are easier to interpret whereas superconductors (in particular, superconducting devices) are those systems where the search for quantum effects at the macroscopic level really started and also present the most reliable tests of their existence.

Regarding superconducting devices, we have chosen to deal with current-biased Josephson junctions (CBJJs), superconducting quantum interference devices (SQUIDs), and Cooper pair boxes (CPBs), and investigate the quantum mechanics of the corresponding dynamical variables of interest. We realize that their behavior may also be viewed as a manifestation of genuine quantum mechanical effects as applied to macroscopic bodies. Accordingly, the difficulty of perfect isolation of our tiny (but still macroscopic) devices brings dissipative effects into play which forces us to search for a systematic treatment of the influence of damping on many different quantum mechanical phenomena. It will be shown that this environmental

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influence tends to inhibit the occurrence of quantum effects on the macroscopic level in the great majority of cases.

However, it is not only this fundamental aspect of the subject that attracts the attention of the scientific community to these systems. Since under specific conditions the behavior of some of these devices is well mimicked by a two-state system dynamics, they can be regarded as *qubits*. Therefore, the hope of controlling the destructive influence of dissipation on complex networks using our devices as their basic elements raises expectations toward the fabrication of quantum computers where the new qubits could be accessed by ordinary electronic circuitry.

We have organized the chapters in the following way. We start by introducing some basic concepts on the phenomenology of magnetism and superconductivity in Chapters 2 and 3, respectively, in order to give the reader some background material to understand the specific physical situations where macroscopic quantum phenomena can take place in each of these areas. Nucleation problems, vortex and wall dynamics, and device physics are all analyzed within the quantum mechanical context.

In Chapter 4 we review the classical theory of Brownian motion in order to show the reader how the physics of those systems can be understood if they obey classical mechanics. Then, we develop the general approach for the quantum mechanics of non-isolated systems, the *system-plus-reservoir approach*, and establish the general program to be followed from then onwards.

Once this has been done, we argue, in Chapters 5 and 6, in favor of semi-empirical approaches for treating the so-called dissipative quantum systems and introduce a few models for the reservoir coupled to the system of interest. In particular, we introduce what we call the *minimal model*, where the system of interest is coupled to a set of non-interacting harmonic oscillators through a coordinate–coordinate interaction Hamiltonian. We impose the conditions under which the specific coupling we have chosen allows us to reproduce the expected dynamics of the system in the classical limit and study the quantum mechanics of this composite system. From this study we are able to describe the influence of the environment on the quantum dynamics of the system of interest solely in terms of the phenomenological constants present in the classical dynamics of that system. The way to deal with the same effect with regard to the equilibrium state of the system of interest is also addressed in Chapter 6 for the specific case of the minimal model. We should stress here that although the treatment is broad enough to cope with many different kinds of dissipative systems, we will be focusing on the so-called *ohmic dissipation*, since it is ubiquitous in most systems of interest to us.

Chapters 7, 8, and 9 are devoted to the application of our methods to the dynamics of wave packets in the classically accessible region of the phase space of the system (where a thorough analysis of decoherence is also presented), the decay

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of “massive” particles and field configurations from metastable states by quantum tunneling and coherent tunneling between bistable states, respectively.

Finally, in Chapter 10 we apply some of these results to the superconducting devices presented in this book, aiming at the possibility of using them as reliable qubits. Further applications and experimental results are briefly analyzed in this section.

Functional methods – path integrals in particular – are at the heart of the mathematical techniques employed throughout most of the chapters of this book, and a review of some of them is presented in the appendices.

2

Elements of magnetism

Magnetic phenomena have been observed for a very long time, and by many ancient civilizations. The very fact that a piece of *magnetite*, the so-called *lodestone*, has the ability to attract some particular materials has been reported many times over the centuries. Even the use of this sort of material for building instruments – such as compasses – to orient navigators has been the subject of about three millennia of uncertainty (Mattis, 1988).

However, only recently have more profound and systematic studies been performed on materials which present that kind of property, and a very rich collection of phenomena has appeared related to them. Paramagnetism, diamagnetism, and the ordered ferromagnetic or anti-ferromagnetic phases of some materials are examples we could mention (Mattis, 1988; White, 2007). The lodestone itself is an example of a ferromagnetic substance which provides us with a permanent magnetic field at room temperature.

It is an experimental fact, first observed by Pierre Curie, that many of those materials attracted by the lodestone, which we call *magnetic materials*, do not present any magnetic property if isolated from the external influence of the latter. Actually, their static magnetic susceptibilities, which are a measure of the response of the material to the external stimulus (see below), behave, at sufficiently high temperatures, in the following way:

$$\chi_M \equiv \lim_{H\to 0} \frac{M}{H} = \frac{C}{T}. \tag{2.1}$$

In this expression, C is a positive constant that depends on the material under investigation, M is the magnetization, and H is the external magnetic field, whose definitions will be given shortly. Materials presenting this sort of behavior are called *paramagnetic*.

On the contrary, there are materials whose behavior contrasts with that presented above. Instead of being attracted by the external magnetic field, they are repelled

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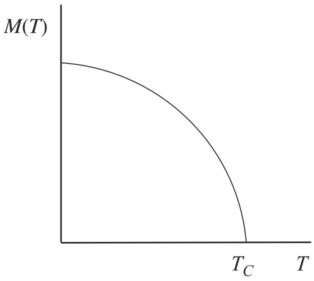

Figure 2.1 Magnetization as a function of temperature

by its presence. In this case, the magnetic susceptibility is negative and varies very slowly with temperature. This is the so-called *diamagnetism*.

Finally, there is a third kind of magnetic material; those materials which present a spontaneous magnetization even in the absence of an externally applied field, the *ferromagnetic materials*. Although there can be paramagnetic substances which keep their magnetic properties as given by (2.1) down to zero temperature, it may happen that the magnetic susceptibility of some materials diverges at a critical temperature, T_C, the so-called Curie temperature. Below that, the material develops a spontaneous magnetization, $M(T)$, which has temperature dependence as shown in Fig. 2.1.

2.1 Macroscopic Maxwell equations: The magnetic moment

In order to explain these three basic phenomena, the natural starting point would be to analyze the macroscopic Maxwell equations (White, 2007) in a given material medium. They read:

$$\begin{aligned}\nabla\cdot\mathbf{D} &= 4\pi\rho,\\ \nabla\cdot\mathbf{B} &= 0,\\ \nabla\times\mathbf{E} &= -\frac{1}{c}\frac{\partial\mathbf{B}}{\partial t},\\ \nabla\times\mathbf{H} &= \frac{4\pi}{c}\mathbf{J}+\frac{1}{c}\frac{\partial\mathbf{D}}{\partial t},\end{aligned}\tag{2.2}$$

where $\mathbf{E}\equiv\mathbf{E}(\mathbf{r},t)$ and $\mathbf{B}\equiv\mathbf{B}(\mathbf{r},t)$ refer, respectively, to averages of the microscopic fields $\langle\mathbf{e}(\mathbf{r}',t)\rangle_{\mathbf{r}}$ and $\langle\mathbf{h}(\mathbf{r}',t)\rangle_{\mathbf{r}}$ over a macroscopic volume ΔV about the position $\mathbf{r}$. $\rho\equiv\rho(\mathbf{r},t)$ and $\mathbf{J}\equiv\mathbf{J}(\mathbf{r},t)$ represent, respectively, the same sort of average of the free charge and free current densities and the fields $\mathbf{D}\equiv\mathbf{D}(\mathbf{r},t)$ and $\mathbf{H}\equiv\mathbf{H}(\mathbf{r},t)$ are defined as usual:

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$$\mathbf{D} = \mathbf{E} + 4\pi\mathbf{P},$$
$$\mathbf{H} = \mathbf{B} - 4\pi\mathbf{M}, \tag{2.3}$$

where $\mathbf{P} \equiv \mathbf{P}(\mathbf{r}, t)$ and $\mathbf{M} \equiv \mathbf{M}(\mathbf{r}, t)$ are, respectively, the polarization and magnetization fields of the material being considered. As we are interested in magnetic phenomena we shall mostly be discussing the role played by $\mathbf{H}$ and, particularly, $\mathbf{M}$.

From the above equations (White, 2007) we conclude that the magnetization is actually due to the existence of the microscopic current density $\mathbf{J}_{\text{mol}}(\mathbf{r}, t)$, which ultimately results from the stationary atomic motion of the electrons. Attributing a local current density $\mathbf{J}^{(i)}_{\text{mol}}(\mathbf{r}, t)$ to the electronic motion about a given molecular or ionic position $\mathbf{r}_i$, we can associate a magnetic moment

$$\boldsymbol{\mu}_i(t) \equiv \boldsymbol{\mu}(\mathbf{r}_i, t) = \frac{1}{2c}\int d\mathbf{r}'(\mathbf{r}' - \mathbf{r}_i) \times \mathbf{J}^{(i)}_{\text{mol}}(\mathbf{r}', t) \tag{2.4}$$

with that position. From this expression and a general representation of $\mathbf{J}^{(i)}_{\text{mol}}(\mathbf{r}', t)$ in terms of $\boldsymbol{\mu}_i(t)$ itself it can be shown (White, 2007) that the magnetization is written

$$\mathbf{M}(\mathbf{r}, t) = \left\langle \sum_i \Delta(\mathbf{r}' - \mathbf{r}_i)\boldsymbol{\mu}_i(t) \right\rangle_{\mathbf{r}}, \tag{2.5}$$

where $\Delta(\mathbf{r}' - \mathbf{r}_i)$ is a function normalized to unity and strongly peaked about $\mathbf{r}_i$. Integrating the latter expression over the whole volume of the sample, we easily see that $\mathbf{M}(\mathbf{r}, t)$ is the total magnetic moment per unit volume.

If we consider the presence of N_e point electrons per ion (or molecule) at positions $\mathbf{r}^{(i)}_k$ relative to $\mathbf{r}_i$ with velocities $\mathbf{v}^{(i)}_k$, the local current density reads

$$\mathbf{J}^{(i)}_{\text{mol}}(\mathbf{r}) = \sum_{k=1}^{N_e} e\mathbf{v}^{(i)}_k \delta(\mathbf{r} - \mathbf{r}_i - \mathbf{r}^{(i)}_k), \tag{2.6}$$

which we can use in (2.4) to show that

$$\boldsymbol{\mu}_i = \frac{e}{2mc}\sum_{k=1}^{N_e} \mathbf{r}^{(i)}_k \times \mathbf{p}^{(i)}_k = \frac{e}{2mc}\mathbf{L}_i, \tag{2.7}$$

where $\mathbf{p}^{(i)}_k = m\mathbf{v}^{(i)}_k$ is, in the absence of an external field, the canonical momentum of the kth electron at $\mathbf{r}_i$ and $\mathbf{L}_i \equiv \sum_{k=1}^{N_e} \mathbf{r}^{(i)}_k \times \mathbf{p}^{(i)}_k$ is the total electronic angular momentum at the same site.

Now, it is a standard example of statistical mechanics textbooks to compute the total magnetization of a set of non-interacting magnetic moments at a finite

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temperature (see, for example, Reif (1965)) using as a starting point its energy when acted on by an external field **H**, which reads

$$E = -\sum_i \boldsymbol{\mu}_i \cdot \mathbf{H}. \tag{2.8}$$

As a result we find that the magnetization so obtained agrees with the empirical form suggested by Langevin, which stated that

$$M = f\left(\frac{H}{T}\right), \tag{2.9}$$

where f is an odd function of its argument.[1] We see that for sufficiently high temperatures, the argument of the above function is small, allowing us to replace it by the lowest-order term of its Taylor expansion. Then, evaluating the paramagnetic static susceptibility with this expression, we see that it obeys the Curie expression (2.1) for a material in its paramagnetic phase and, therefore, classical physics can explain paramagnetism without any problem.

The same does not hold if we try to explain, for example, diamagnetism by the same token. For this, suppose we apply a constant external field **H** to our sample. In this case, the expression for the magnetic moment in terms of the angular momentum must be modified by replacing

$$\mathbf{p}_k \rightarrow \mathbf{p}_k - \frac{e}{c}\mathbf{A}(\mathbf{r}_k) \tag{2.10}$$

in (2.7), where $\mathbf{A}(\mathbf{r})$ is the vector potential which, in the symmetric gauge, reads

$$\mathbf{A}(\mathbf{r}) = \frac{1}{2}\mathbf{H} \times \mathbf{r}. \tag{2.11}$$

Accordingly, the Hamiltonian of the electronic system must also be replaced by

$$\mathcal{H}(\ldots \mathbf{p}_k, \mathbf{r}_k \ldots) = \sum_k \frac{1}{2m}\left(\mathbf{p}_k - \frac{e}{c}\mathbf{A}(\mathbf{r}_k)\right)^2 + U(\ldots \mathbf{r}_k \ldots), \tag{2.12}$$

where $U(\ldots \mathbf{r}_k \ldots)$ represents any possible interaction regarding the electronic system.

Now we can use (2.12) in the classical Boltzmann factor to compute the magnetization of the system at finite temperatures, as we have done for paramagnetic materials. However, in this case, the Bohr–van Leeuwen theorem (Ashcroft and Mermin, 1976) states that the phase space integral which determines this quantity must vanish. In other words, there is no classical explanation for diamagnetism and this is the first situation where we do need quantum mechanics to deal with magnetic materials.

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[1] For a classical magnetic moment this function is $n\mu\left(\coth\theta - \frac{1}{\theta}\right)$, where $\theta = \frac{\mu H}{k_B T}$ and n is the density of magnetic moments.

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2.2 Quantum effects and the order parameter

Let us start the analysis of quantum mechanics applied to magnetic systems by writing the quantum mechanical form of (2.7). In order to do that we must remember the results of the quantization of angular momentum (Merzbacher, 1998), which tell us that the orbital angular momentum eigenstates of the electronic motion are given by $|\,\ell, m_\ell\rangle$ such that

$$\begin{aligned} L^2|\,\ell, m_\ell\rangle &= \ell(\ell+1)\,\hbar^2|\,\ell, m_\ell\rangle\,; \qquad && \ell = 0, 1, 2\ldots \\ L_z|\,\ell, m_\ell\rangle &= m_\ell\,\hbar|\,\ell, m_\ell\rangle\,; && m_\ell = 0, \pm1, \pm2, \ldots, \pm\ell \end{aligned} \tag{2.13}$$

where the conventional notation $\mathbf{L} = \mathbf{r} \times \mathbf{p}$ has been used and all the dynamical variables are now regarded as operators. Then, if we are interested in one of the components of the magnetic moment operator, say μ_z, we can rewrite the z component of (2.7) applied on $|\,\ell, m_\ell\rangle$ as

$$\mu_z|\,\ell, m_\ell\rangle = -m_\ell\,\mu_B|\,\ell, m_\ell\rangle, \tag{2.14}$$

where we have used the fact that $e = -|\,e|$ and

$$\mu_B \equiv \frac{\hbar|\,e|}{2mc} = 9.27 \times 10^{-21}\,\mathrm{erg}\cdot\mathrm{G}^{-1}\;\;(\mathrm{or}\;\;\times 10^{-24}\,\mathrm{J}\cdot\mathrm{T}^{-1}) \tag{2.15}$$

is the *Bohr magneton.*

However, this is not the whole story. The Zeeman effect and the Stern–Gerlach experiment (Merzbacher, 1998) indicate that the electron itself must carry an intrinsic magnetic moment which is related to the generator of rotations in a two-dimensional Hilbert space spanned by the states $|\,s, m_s\,\rangle$. The eigenvalue problem associated with these generators is

$$\begin{aligned} S^2|\,s, m_s\rangle &= s(s+1)\,\hbar^2|\,s, m_s\rangle\,; \qquad && s = \frac{1}{2} \\ S_z|\,s, m_s\rangle &= m_s\,\hbar|\,s, m_s\rangle\,; && m_s = \pm\frac{1}{2} \end{aligned} \tag{2.16}$$

and the relation equivalent to (2.7) now reads

$$\boldsymbol{\mu} = -g_s\frac{\mu_B}{\hbar}\mathbf{S} \equiv \gamma_g\mathbf{S}, \tag{2.17}$$

where $\mathbf{S} = \hbar\boldsymbol{\sigma}/2$, $\boldsymbol{\sigma}$ is a vector whose components are the well-known 2×2 Pauli matrices and $g_s \approx 2$ and γ_g are the electron gyromagnetic factor and ratio, respectively. Notice that γ_g has the same sign as the particle's charge.

Consequently, assuming that the electron is subject to a localized potential and an external field along the $\mathbf{z}$ direction, strong enough so that the energy eigenstates can be considered as $|\ell, s, m_\ell, m_s\rangle = |\ell, m_\ell\rangle \otimes |s, m_s\rangle$, its energy eigenvalues now read

$$E_{m_\ell m_s} = (m_\ell + 2m_s)\,\mu_B H. \tag{2.18}$$

For weak fields, it is more appropriate to characterize the magnetic state by the eigenstates of the total angular momentum $\mathbf{J} = \mathbf{L} + \mathbf{S}$, $|j, \ell, s, m\rangle$, from which we can write (Ashcroft and Mermin, 1976; Merzbacher, 1998)

$$\boldsymbol{\mu} = -g(j, l, s)\frac{\mu_B}{\hbar}\mathbf{J} \equiv \gamma_j \mathbf{J}, \tag{2.19}$$

where $g(j, l, s)$ is the well-known Landé g-factor.

Now we can compute the statistical Boltzmann factor corresponding to the interaction $-\boldsymbol{\mu}\cdot\mathbf{H}$ and reproduce again expression (2.1) for the paramagnetic susceptibility (see, for example, Ashcroft and Mermin (1976)) where the constant C is determined in terms of the total angular momentum quantum number j and the Bohr magneton.

2.2.1 Diamagnetism

Let us turn now to the diamagnetic phenomenon and suppose we start by taking the quantum mechanical version of (2.12). So, if we consider the system under the influence of an external field $\mathbf{H}$ we can write

$$\mathcal{H}(\ldots \mathbf{p}_k, \mathbf{r}_k \ldots) = \sum_k \frac{p_k^2}{2m} + U(\ldots \mathbf{r}_k \ldots) + \Delta\mathcal{H}, \tag{2.20}$$

where the full magnetic correction $\Delta\mathcal{H}$ in the symmetric gauge (2.11) reads

$$\Delta\mathcal{H} = \mu_B(\mathbf{L} + 2\mathbf{S})\cdot\mathbf{H} + \frac{e^2}{8mc^2}H^2\sum_k \left(x_k^2 + y_k^2\right), \tag{2.21}$$

with $\mathbf{L} + 2\mathbf{S} = \sum_k \mathbf{L}_k + 2\mathbf{S}_k$. Notice that the total angular momentum is not given by this expression but by $\mathbf{J} = \mathbf{L} + \mathbf{S}$ instead. It should be stressed that in (2.21) we are neglecting spin–orbit terms (see below).

If the full Hamiltonian (2.20) has eigenstates $|\,n\rangle$ and the external field can be treated perturbatively, we find corrections of the order of H^2 to the energy eigenvalue E_n (Ashcroft and Mermin, 1976):

$$\Delta E_n = \mu_B\langle\, n\,|\,(\mathbf{L} + \mathbf{2S})\cdot\mathbf{H}\,|\,n\,\rangle + \sum_{n'\neq n}\frac{|\,\mu_B\langle\, n\,|\,(\mathbf{L} + \mathbf{2S})\cdot\mathbf{H}\,|\,n'\,\rangle\,|^2}{E_n - E_{n'}}$$
$$+\frac{e^2}{8mc^2}H^2\sum_k\langle\, n\,|\,x_k^2 + y_k^2\,|\,n\,\rangle, \tag{2.22}$$

from which we see that the paramagnetic effects are dominant for small fields whenever $\langle\,\mathbf{L}\,\rangle$ or $\langle\,\mathbf{S}\,\rangle \neq 0$. However, for a system with filled atomic