Coherence versus decoherence – a few illustrative examples

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The interplay of coherence and decoherence is a vexing issue in contemporary condensed matter physics, quantum optics and quantum information theory. We present an overview of this important topical subject, in terms of three different paradigms, in which the 'noisy' effect of the environment on small quantum subsystems is analysed.

Keywords: Coherence, decoherence, dissipative diamagnetism, qubit.

Introduction

QUANTUM coherence is the consequence of a phase of a wave function[1]. The phase has two components – spatial and temporal, leading to spatial coherence and temporal coherence respectively. Spatial coherence is best illustrated by the double slit experiment (Figure 1) in which a parallel electron beam, say, is envisaged to traverse through two holes, a distance d apart, and is collected on a screen, kept at a sufficiently large distance.

The interference pattern, observed on the screen, is characterized by an intensity – sometimes called the structure factor – $S(\underline{k})$ that has two components

$$S(\underline{k}) = S_1(\underline{k}) + S_2(\underline{k}), \tag{1}$$

where

$$S_1(\underline{k}) = 2|A(\underline{k})|^2, \tag{2}$$

and

$$S_2(\underline{k}) = 2|A(\underline{k})|^2 \cos((\underline{k}) \cdot (\underline{d})). \tag{3}$$

In the above, the wave vector ($\underline{k}$) is the difference between the final and incident wave vectors of the beam, and $A(\underline{k})$ is the amplitude. The first term $S_1(\underline{k})$ is the so called 'classical' component while the second term, arising out of the phase of the final beam: $\exp(i\underline{k}\cdot\underline{d})$, is responsible for interference, yielding alternate maxima and minima of the interference pattern, because of the oscillatory nature of the cosine function. The regular occurrence of the interference fringes and their separation would naturally depend on the 'size' of the phase factor $|\underline{k}\cdot\underline{d}|$, and hence the name, spatial coherence.

Temporal coherence, on the other hand, can be attributed once again to a similar cosine function, but now in the time-domain, as can be exemplified by quantum tunnelling of, say, an electron moving in a one-dimensional symmetric double well[2] (Figure 2).

The potential for the latter can be written as

$$V(x) = \frac{1}{2}k(|x| - a)^2, \tag{4}$$

where x is the coordinate and $2a$ is the distance between the minima of the two wells. An electron, initially localized in, say, the left well, would keep oscillating back and forth, coherently, characterized by the so-called tunnel frequency Δ. The latter, in the WKB approximation[3], is given by

$$\Delta = \sqrt{\frac{8\hbar\omega_0 V_0}{\pi}} \exp\left(-\frac{2V_0}{\hbar\omega_0}\right), \tag{5}$$

where $\hbar$ is the Planck constant, ω_0 the small oscillation frequency in each of the two wells, governed by the curvature of the potential at the two minima, and V_0 is the energy barrier separating the two wells. Temporal

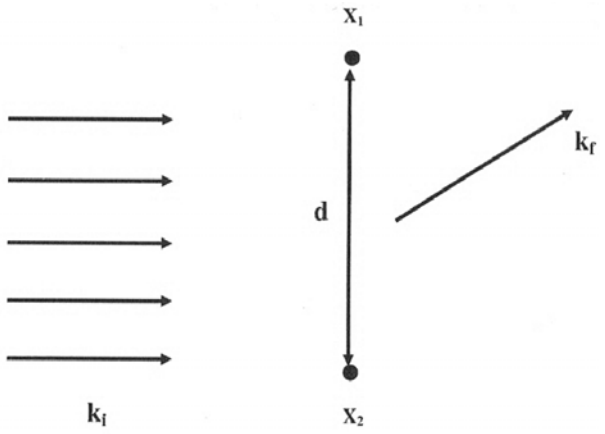

Figure 1. Interference from a double slit.

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coherence is manifested by the mean, instantaneous position of the electron, expressed by

$$\langle x(t)\rangle = a\cos(\Delta t). \tag{6}$$

Thus the mean position of the electron keeps oscillating between the two extreme values of $-a$ and a.

Decoherence – tunnelling in a double well

The spatial and temporal coherence, illustrated by the physical situation depicted in Figures 1 and 2, are attributes of an isolated physical system, e.g. an individual electron. But, in reality, the electron or the subsystem would inevitably be in interaction with the external world. One common occurrence of such a coupling in solid-state physics is the presence of lattice vibrations, or phonons, in their quantized versions. Such a coupling would lead to decoherence in the tunnelling behaviour of the electron, as described below.

If the wells shown in Figure 2 are sufficiently deep and the temperature of the system is sufficiently low, only the two lowest wave functions would be accessible[2]. These two wave functions ψ_0 and ψ_1 are schematically shown in Figure 3.

However, ψ_0 and ψ_1 are not the physical wave functions which are associated with the electron being localized either in the left or the right well. A glance at Figure 3 would make it amply clear that the physical wave functions are the symmetric and antisymmetric combinations of ψ_0 and ψ_1, given by

$$\psi_s = \frac{1}{\sqrt{2}}(\psi_0 + \psi_1), \tag{7}$$

$$\psi_a = \frac{1}{\sqrt{2}}(\psi_0 - \psi_1). \tag{8}$$

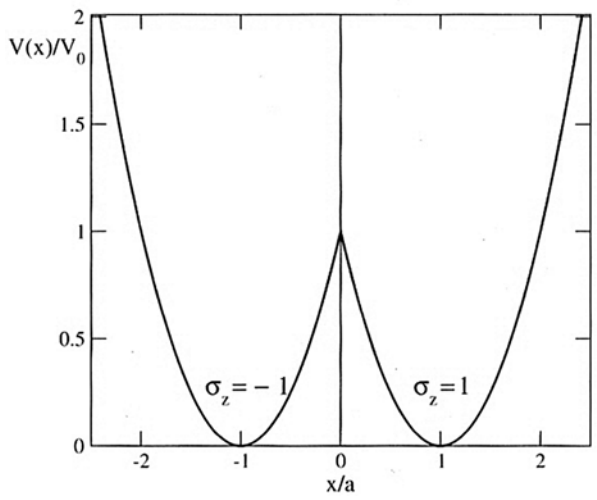

Figure 2. Symmetric double well.

Evidently, ψ_s is peaked at the right well associated with the electron being localized in the right well, whereas ψ_a is peaked at the left well associated with the electron being localized in the left well. Thus, the quantum mechanics of the electron is restricted to a two-dimensional Hilbert space. It is natural then to associate ψ_s and ψ_a with the eigenfunctions $|+\rangle$ and $|-\rangle$ of the Pauli spin operator $\hat{\sigma}_z$. Suffice it to say however that $|\pm\rangle$ are *not* the eigenstates of the system Hamiltonian $\mathcal{H}_S$ which must account for the tunnelling of the electron between the two localized states $|+\rangle$ and $|-\rangle$. Appropriately, $\mathcal{H}_S$ can be constructed as

$$\mathcal{H}_S = \Delta\hat{\sigma}_x, \tag{9}$$

where $\hat{\sigma}_x$, the x-component of the Pauli spin, is entirely off-diagonal in the representation in which $\hat{\sigma}_z$ is diagonal. (It may be remarked parenthetically that ψ_0 and ψ_1 are indeed the eigenstates of $\hat{\sigma}_x$.) Given the form of $\mathcal{H}_S$ as in eq. (9), coupling with the phonons (in the linear approximation) can be described by the so-called spin-boson Hamiltonian[4]

$$\mathcal{H} = \mathcal{H}_S + \hat{\sigma}_z \sum_k g_k (b_k + b_k^\dagger) + \sum_k \hbar\omega_k b_k b_k^\dagger. \tag{10}$$

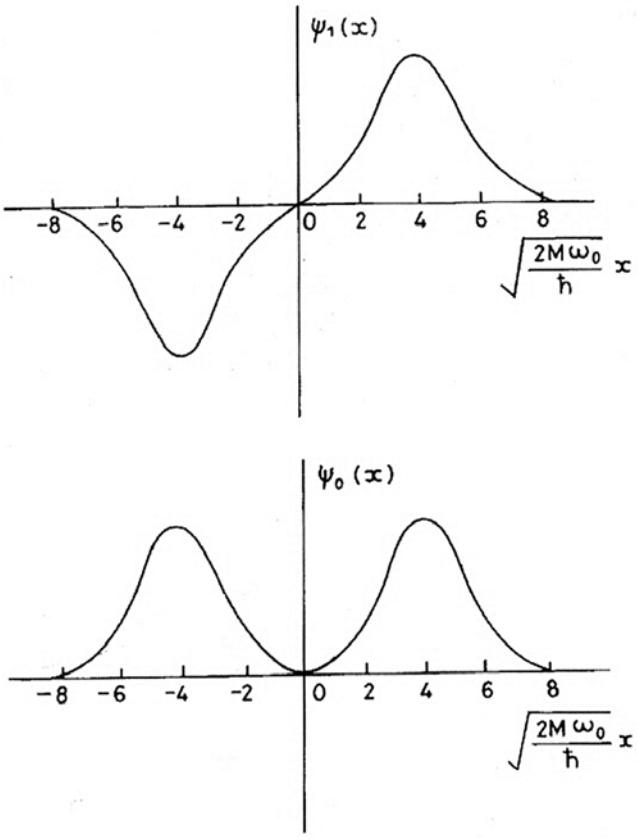

Figure 3. Ground state and first excited state wave functions.

In eq. (10), b_k and $b_k^\dagger$ are the annihilation and creation bosonic operators representing the kth phononic mode, g_k is the coupling constant and ω_k is the 'free' phononic frequency. The physics of the spin-boson Hamiltonian can be summarized thus: because $\hat{\sigma}_z$ is off-diagonal in the representation in which $\hat{\sigma}_x$ is diagonal, the second term in eq. (10) would cause transitions between the eigenstates of $\hat{\sigma}_x$. These transitions are however quantum-incoherent because of the bosonic fields b_k and $b_k^\dagger$, which themselves are jiggled by the free bosons, represented by the third term in eq. (10). Thus tunnelling, which is characterized by the cosine term in eq. (6), is now impeded by repeated interventions from the 'phonon bath' leading to dephasing/decoherence. Decoherence can be quantified by the so called 'stay-put' probability $P(t)$. The latter measures the probability that the electron continues to stay at the right well, say, given that it was localized there at time $t = 0$. It is defined by

$$P(t) = \langle + | \hat{\sigma}_z | + \rangle, \tag{11}$$

where $\hat{\sigma}_z(t)$ is the Heisenberg representation of $\hat{\sigma}_z$

$$\hat{\sigma}_z(t) = \exp(\mathrm{i}\mathcal{H}t)\, \hat{\sigma}_z(0) \exp(-\mathrm{i}\mathcal{H}t). \tag{12}$$

Evidently, when $\mathcal{H}$ is governed only by the free Hamiltonian $\mathcal{H}_S$ in eq. (9), $P(t)$ would have the form

$$P(t) = \cos(2\Delta t). \tag{13}$$

But, the phonon coupling changes the behaviour of $P(t)$ to incoherent oscillations, as depicted in Figure 4.

Transition from coherent to decoherent diamagnetism

Diamagnetism arises from the induced orbital magnetic moment of a collection of mobile electrons by an external magnetic field. Because a moving electron under the Lorentz force due to the external magnetic field would yield an electric current, the latter generates a magnetic moment opposing the direction of the field, in accordance with the Faraday–Lenz law. A many-body system of such electrons is therefore expected to lead to a macroscopic moment and hence, a susceptibility which, for diamagnetism, has a negative sign. It is however an intriguing feature of diamagnetism that the concomitant susceptibility, when calculated from rules of classical statistical mechanics, has an answer that is perplexingly zero. This result is the celebrated Bohr–van Leeuwen theorem[5]. Apart from the technical reasons of the magnetic field being 'gauged away' from the partition function, there is a deeper cause for null diamagnetism in classical statistical mechanics. It turns out that the diamagnetic contribution of those electrons which collide on the boundary and get reflected back into the enclosure exactly cancels that of the bulk electrons. This cancellation is however incomplete in quantum mechanics, as was shown by Landau[6]. Diamagnetism is therefore an intrinsic quantum attribute. It is also a coherent phenomenon because phase of the electron remains intact as it Larmor-precesses around the magnetic field.

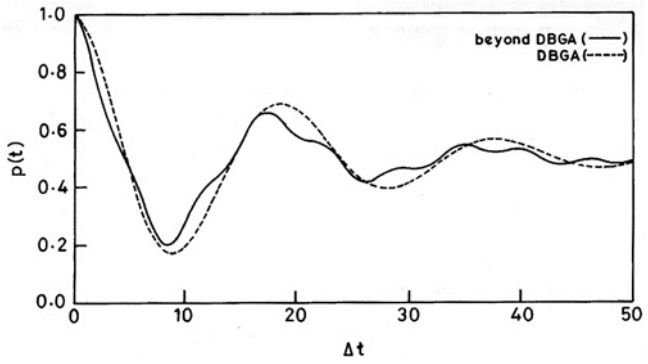

Figure 4. Stay-put probability $P(t)$ as a function of time t.

How does one run into the issue of docoherence in Landau diamagnetism? Well, much like in the problem of Drude electrical conductivity, the moving electrons are interrupted by the lattice vibrations or phonons. The coupling to the phonons, again assumed linear as in eq. (10), can occur through the position vector of the electron. Such a coupling has been widely studied in the context of a free particle, a harmonic oscillator or more generally in the so-called Caldeira–Leggett model[7], in which the partition function has been computed in a functional integral approach[8–10].

We will follow a different method, that due to Ford *et al.*[11], in which a quantum Langevin equation (QLE) is formulated. The latter has the same structure as for the classical Langevin equation, but for the explicit presence of the Lorentz force and the tacit recognition that the position and momentum operators do not commute with each other. The resulting QLE reads[12]

$$m\ddot{\vec{Q}} + m\gamma\dot{\vec{Q}} - \frac{e}{c}(\dot{\vec{Q}} \times \vec{B}) = \hat{\Theta}(t), \tag{14}$$

where m is the mass of the electron, e the electric charge, γ the friction coefficient, $\vec{B}$ the external magnetic field, and $\hat{\Theta}(t)$ is the so called 'noise operator'. Unlike in the classical Langevin description, the correlation of $\hat{\Theta}(t)$ at different times is not a delta function but has separate symmetric and antisymmetric components

$$\langle (\hat{\Theta}_i(t)\hat{\Theta}_j(t') + \hat{\Theta}_j(t')\hat{\Theta}_i(t)) \rangle$$

$$= \delta_{ij} \frac{m\gamma}{\pi} \int_0^\infty \mathrm{d}\omega \hbar\omega \times \coth\left(\frac{\beta\hbar\omega}{2}\right) \cos[\omega(t - t')], \tag{15}$$

and

$$\langle(\hat{\Theta}_i(t)\hat{\Theta}_j(t') - \hat{\Theta}_j(t')\hat{\Theta}_i(t))\rangle$$

$$= \delta_{ij}\frac{2m\gamma}{i\pi}\int_0^\infty \mathrm{d}\omega\hbar\omega \times \sin[\omega(t-t')]. \quad (16)$$

Evidently, in the classical limit $\hbar \to 0$, the antisymmetric correlation in eq. (16) vanishes, whereas eq. (15) reduces to

$$\langle(\hat{\Theta}_i(t)\hat{\Theta}_j(t') + \hat{\Theta}_j(t')\hat{\Theta}_i(t))\rangle = \delta_{ij}2m\gamma k_B T\delta(t-t'). \quad (17)$$

One other crucial difference in the classical case is that the *kinematic* momentum $m\dot{\vec{Q}}$ is not the same as the *canonical* momentum $\vec{p}$, the two being related by

$$m\dot{\vec{Q}} = \left(\vec{p} - \frac{e}{c}\vec{A}\right), \quad (18)$$

where $\vec{A}$ is the vector potential that yields the magnetic field through the relation

$$\vec{B} = \mathrm{curl}\,\vec{A}. \quad (19)$$

Consequently, the three operators: $\vec{Q}$, $\dot{\vec{Q}}$ and $\ddot{\vec{Q}}$ do not commute with each other. In terms of 'scaled' resistances, defined by[13–15]

$$r = \frac{R_D}{R_H},\ R_D = \frac{m\gamma}{ne^2},\ R_H = \frac{B}{nec}, \quad (20)$$

where R_D and R_H are the so-called Drude and Hall resistances respectively, and n is the electron density, the magnetization M per particle can be expressed as

$$M = -\frac{k_B T}{2B}\Omega_c^2\sum_{n=1}^{\infty}\frac{1}{(\gamma+\nu_n)^2 + \Omega_c^2}, \quad (21)$$

where Ω_c is the scaled cyclotron frequency

$$\Omega_c = \frac{\hbar eB}{k_B Tmc}, \quad (22)$$

and

$$\nu_n = \frac{2k_B Tn\pi}{\hbar}. \quad (23)$$

Equation (21) is a remarkably compact answer that manifestly has all the right limits. For instance, because Ω_c is identically zero in the classical case, M vanishes. On the other hand, for zero damping ($\gamma = 0$), we may express M as

$$M = -\frac{2k_B T}{B}\Omega_c^2\left[\sum_{n=0}^{\infty}\frac{1}{\nu_n^2 + \Omega_c^2} - \frac{1}{\Omega_c^2}\right]$$

$$= -\frac{e\hbar}{2mc}\left[\coth(\Omega_c) - \frac{1}{\Omega_c}\right], \quad (24)$$

the Landau answer. Finally, in the limit of infinitely large damping ($\gamma \to \infty$), M vanishes too, suggesting that frequent interactions with the phonon-bath render the system completely incoherent as though the Bohr–van Leeuwen result is resurrected from a fully quantum mechanical expression. This is illustrated in Figure 5, in which the negative of the dimagnetic moment is plotted against a dimensionless resistance indicating the coherent-to-decoherent transition[15].

Dephasing of a qubit

A qubit – a standard paradigm for studying quantum information – is a set of two quantum dots whose states are ordinarily entangled[16]. However, environment-induced decoherence is an impediment for storage of quantum information. The basic qubit Hamiltonian can be written in terms of projection operators as

$$\mathcal{H}_S = \varepsilon(|L\rangle\langle L| - |R\rangle\langle R|) + \Delta(|L\rangle\langle R| + |R\rangle\langle L|), \quad (25)$$

where $|L, R\rangle$ represents the left (right) dot, ε the difference of the two site energies and Δ is the overlap energy. A reasonable model for assessing decoherence process is to expand the Hamiltonian $\mathcal{H}_S$ to

$$\mathcal{H}_0 = (\varepsilon + \hat{\tau}_x\zeta_\varepsilon)(|L\rangle\langle L| - |R\rangle\langle R|)$$

$$+ (\Delta + \hat{\tau}_x\zeta_\Delta)(|L\rangle\langle R| + |R\rangle\langle L|), \quad (26)$$

and introduce an interaction Hamiltonian $\mathcal{H}_I$ as

$$\mathcal{H}_I = \hat{\tau}_z\sum_k g_k(b_k + b_k^\dagger). \quad (27)$$

Here $\hat{\tau}_x$ and $\hat{\tau}_z$ are pseudo Pauli operators. Like in the double-well problem discussed earlier, $\mathcal{H}_0$ can be alternately expressed as

$$\mathcal{H}_0 = \varepsilon\hat{\sigma}_z + \Delta\hat{\sigma}_x + \hat{\tau}_x(\zeta_\varepsilon\hat{\sigma}_z + \zeta_\Delta\hat{\sigma}_x). \quad (28)$$

The total Hamiltonian then is an expanded version of eq. (10)

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1 + \sum_k g_k b_k b_k^\dagger. \tag{29}$$

The physics of eqs (27)–(29) is amply clear. The operator $\hat{\tau}_z$ (in eq. (27)), modulated by the bosonic operators b_k and $b_k^\dagger$, causes random flips of $\hat{\tau}_x$ (in eq. (28)). The consequent effect is to create modulations in ζ_ε and ζ_Δ, thereby causing fluctuations in the site and overlap energies.

While the above formulation is fully quantum mechanical, we will follow a simpler semi-classical analysis in which the operator $\hat{\tau}_x$ (and influence on it by the surrounding phonon fields) is subsumed within a classical stochastic field $f(t)$ that is assumed to be a telegraph process[17]. A formal justification for this scheme can be had in certain high-temperature limits. We will make a further simplification of taking ε to be zero – the so-called symmetric case in which the two site energies are identical. However, a bit of generality is injected by taking the overlap energy Δ to be complex. This can be realized in practice by coupling the dots via two different channels with a phase mismatch, as can be done, for instance, by inserting an Aharonov–Bohm flux on the dots[18]. Hence, our modified Hamiltonian reads

$$\mathcal{H}(t)=\mathcal{H}_S + \hat{V} f(t), \tag{30}$$

where

$$\mathcal{H}_S = \frac{1}{2}(\Delta\sigma_+ + \Delta^*\sigma_-), \tag{31}$$

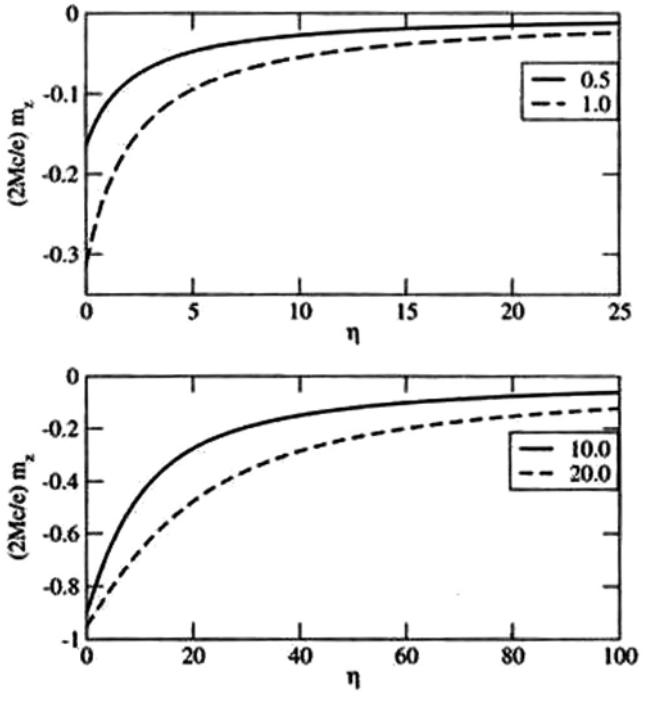

Figure 5. Negative of the diamagnetic moment plotted against a dimensionless resistance r.

and

$$\hat{V} = \frac{1}{2}(\zeta_\Delta\sigma_+ + \zeta_\Delta^*\sigma_-). \tag{32}$$

As $f(t)$ stochastically jumps between the two values ± 1, the overlap energy fluctuates between $(\Delta \pm \zeta_\Delta)$ and $(\Delta^* \pm \zeta_\Delta^*)$, thereby inducing decoherence. Our aim in the following will be to devise a scheme in which initial information, stored in the qubit, can be at least partially retrieved despite decoherence.

Quantum information is usually stored in qubits that can be thought to exist in linear superposition of two basis states

$$|\psi_0\rangle = \cos\alpha \begin{pmatrix} 1 \\ 0 \end{pmatrix} + e^{i\gamma} \sin\alpha \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \tag{33}$$

where α and γ are real parameters.

As is well known, quantum computation has the prerequisite of quantum coherence such that the state stored in each qubit can stay stable. However, the perturbation of the stochastic process $f(t)$ is expected to lead to total decoherence. The resultant loss of information is captured by the asymptotic form of the reduced density operator, which assumes a diagonal form with constant coefficients. Note that the reduced density operator is obtained by tracing the full density operator over the bath quantum states; thus $\rho_{nm}(t=\infty) = (1/2)\delta_{nm}$, in the so-called fully *mixed* state, independent of the particular basis comprising the underlying Hilbert space.

Our stratagem is to contrive a situation in which there is decoherence sans dissipation, i.e. there no energy exchange between the subsystem and the environment[19]. This can be ascertained by finding conditions under which the two operators $\mathcal{H}_S$ and $\hat{V}$, in eqs (31) and (32), commute with each other. Yet, the asymptotic density operator retains off-diagonal terms that carry the signatures of the initial quantum state $|\psi_0\rangle$. The desired scheme is implemented as follows[18].

It is clear that the condition under which $[\mathcal{H}_S, \hat{V}] = 0$ can be achieved, when

$$\Delta\zeta_\Delta^* - \Delta^*\zeta_\Delta = 0, \tag{34}$$

or, equivalently

$$\frac{\zeta_\Delta}{\Delta} = \frac{\zeta_\Delta^*}{\Delta^*} = x, \tag{35}$$

x being a real parameter. The condition given in eq. (35) implies that if Δ is written as $|\Delta|\exp(i\theta)$, the same θ must appear as the phase of ζ_Δ, i.e. $\zeta_\Delta = |\zeta|\exp(i\theta)$. The above condition entails that $\mathcal{H}_S$ and $\hat{V}$ can be simultaneously diagonalized among the basis states that are referred to as

the 'bonding' and 'anti-bonding' states in the chemical physics literature (cf. with ψ_0 and ψ_1 mentioned earlier), given by

$$|\pm\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\end{pmatrix} \mp \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\end{pmatrix}. \tag{36}$$

Evidently, the bonding and anti-bonding states are eigen states of both $\mathcal{H}_S$ and $\hat{V}$

$$\mathcal{H}_S|\pm\rangle = \mp|\Delta|\,|\pm\rangle, \quad \hat{V}\,|\pm\rangle = \mp|\zeta|\,|\pm\rangle, \tag{37}$$

with eigenvalues $\mp|\Delta|$ and $\mp|\zeta|$ respectively.

If the density operator $\hat{\rho}$ is written in the basis of bonding and anti-bonding states, it will clearly be diagonal and remain diagonal at all times. But, like in the problem of tunnelling in a double well, the physical states are the localized ones on the left and right dots, given by $\begin{pmatrix}1\\0\end{pmatrix}$ and $\begin{pmatrix}0\\1\end{pmatrix}$ respectively. A detailed and fully time-dependent analysis of $\hat{\rho}(t)$ following its Liouville evolution under the influence of the underlying telegraph process reveals that asymptotically the off-diagonal elements of the density operator acquire the form[18]

$$\begin{aligned}\rho_{LR}(t=\infty) &= \rho^*_{RL}(t=\infty)\\ &= \exp(i\theta)\Re[\exp(-i\theta)\rho_{LR}(0)],\end{aligned} \tag{38}$$

whereas the diagonal elements remain one-half each. Here

$$\rho_{LR}(0) = \langle L|\psi_0\rangle\langle\psi_0|R\rangle. \tag{39}$$

Employing eq. (31)

$$\rho_{LR}(0) = \frac{1}{2}\sin(2\alpha)\exp(-i\gamma). \tag{40}$$

Thus the asymptotic density operator does not belong to a mixed state, implying that the system retains partial coherence notwithstanding the environmental influence. Hence the initial information on the qubit is at least partially protected – a desired objective of quantum computation.

Concluding remarks

By way of three different examples, taken from condensed matter physics and quantum information theory, we have illustrated the idea of coherence, arising from definite phase relation inherent in the quantum wave function, and decoherence. Decoherence is an inevitable consequence of the environmental influence and is particularly severe for small (nano/mesoscopic) systems which are the very devices appropriate for storing quantum information[20–23]. Coherence-to-decoherence transition is a hallmark of dissipative quantum systems and has been exemplified here in terms of the phenomena of tunnelling in a double well and Landau diamagnetism. Our third example, in the context of a qubit, brings up an interesting twist, viz. how coherence can be partially preserved even in the presence of environmental influences. Throughout our discussion, a system-plus-bath approach has been adopted, in the spirit of path-breaking contributions of Feynman and Vernon Jr.[24]; Caldeira and Leggett[7]; Ford, Kac and Mazur[11], and others.

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