

# Decoherence in nanostructures and quantum systems

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## Abstract

Decoherence phenomena are pervasive in the arena of nanostructures but perhaps even more so in the study of the fundamentals of quantum mechanics and quantum computation. Since there has been little overlap between the studies in both arenas, this is an attempt to bridge the gap. Topics stressed include (a) wave packet spreading in a dissipative environment, a key element in all arenas, (b) the definition of a quantitative measure of decoherence, (c) the near zero and zero temperature limit, and (d) the key role played by initial conditions: system and environment entangled at all times so that one must use the density matrix (or Wigner distribution) for the complete system or initially decoupled system and environment so that use of a reduced density matrix or reduced Wigner distribution is feasible. Our approach utilizes generalized quantum Langevin equations and Wigner distributions.

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## 1. Introduction

Quantum interference effects have become pervasive in two rather disparate areas of physics, (a) mesoscopic systems [1–9] and (b) fundamental quantum physics and quantum computation [10–24]. Whereas, of necessity, there is a certain commonality of approach, in general each area tends to emphasize the use of particular techniques. Since our own emphasis has been in the latter area, we feel that it might be worthwhile to present an overall account of our approach to an audience whose main interests lie in the former area.

The generic problem of interest is the motion of a quantum particle in an environment. This problem has been addressed by a variety of methods such as

the Feynman–Vernon functional integral approach, the use of master equations and various stochastic methods. We have found that the generalized quantum Langevin equation (GLE), supplemented by use of the Wigner distribution function, provides the basis of a powerful and physically transparent approach to all such problems.

In Section 2, we discuss fundamentals. Starting with the Hamiltonian for the whole system, we summarize how the GLE was derived and we discuss its properties. The solution for a non-localized quantum particle in a very general dissipative environment is then presented. Results are also presented for the correlation and commutation of both the coordinate and the fluctuation force operators appearing in the GLE. In Section 3, we derive the mean-square displacement of the quantum particle. The latter result, which is valid for arbitrary temperatures and arbitrary dissipation, is a key ingredient of a very general expression for the

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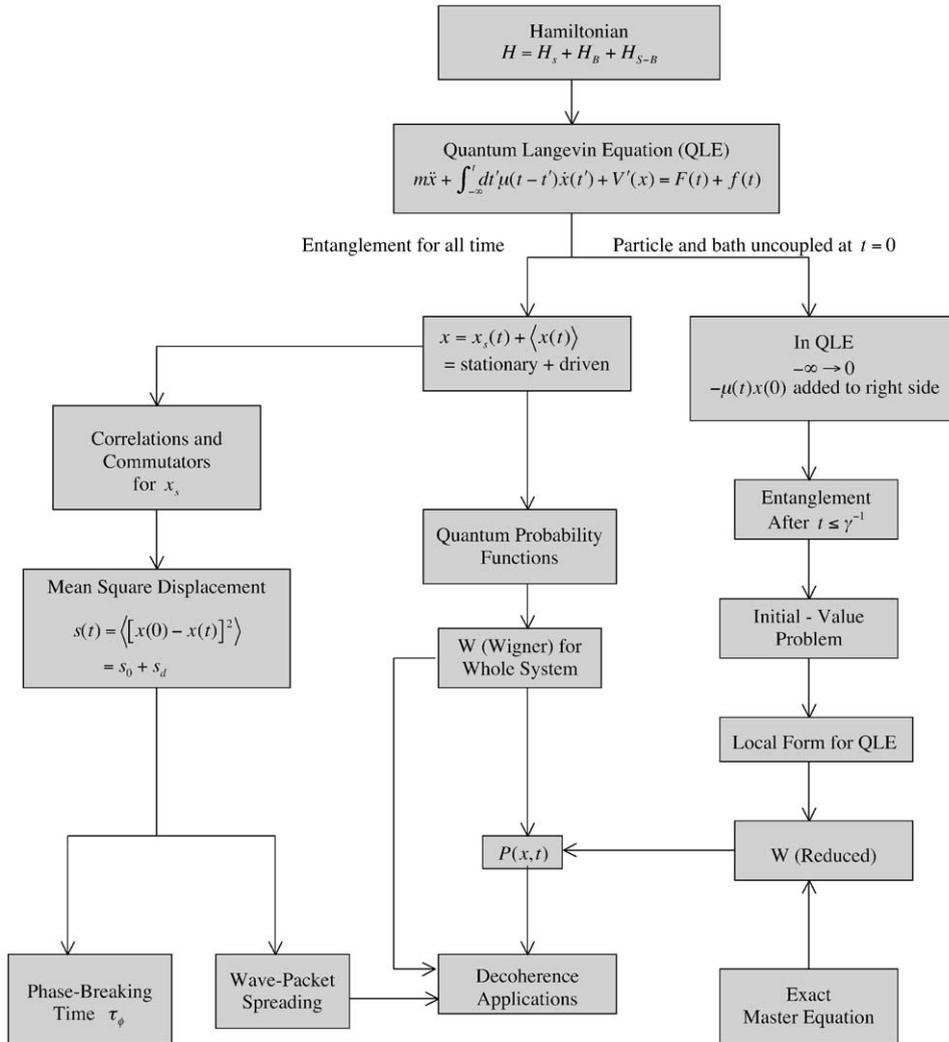


Fig. 1. Calculation of wave-packet spreading and of the decay time of quantum interference.

spreading of the width of the particle's wave packet. It also plays a vital role in quantum transport studies. In addition, it is relevant to a determination of the phase-breaking time  $\tau_\phi$ , of interest for many mesoscopic systems. In Section 4, we apply our results to a calculation of the decoherence of interference terms in a quantum superposition. Section 5 presents a generalization to the case of an external field and, in Section 6, we present our conclusions. Fig. 1 presents a schematic summary of the progression from fundamental theory to applications.

## 2. Fundamentals

In recent years, there has been widespread interest in dissipative problems arising in a variety of areas in physics. As it turns out, solutions of many of these problems are encompassed by a generalization of Langevin's equation to encompass quantum, memory, and non-Markovian effects, as well as arbitrary temperature and the presence of an external potential  $V(x)$ . As in Ref. [25], we refer to this as the generalized quantum Langevin equation

(GLE)

$$m\ddot{x} + \int_{-\infty}^t dt' \mu(t-t') \dot{x}(t') + V'(x) = F(t) + f(t), \quad (2.1)$$

where  $V'(x) = dV(x)/dx$  is the negative of the time-independent external force and  $\mu(t)$  is the so-called memory function.  $F(t)$  is the random (fluctuation or noise) operator force with mean  $\langle F(t) \rangle = 0$  and  $f(t)$  is a  $c$ -number external force (due to an electric field, for instance). In addition, it should be strongly emphasized that “— the description is more general than the language —” [25] in that  $x(t)$  can be a generalized displacement operator (such as the phase difference of the superconducting wave function across a Josephson junction).

A detailed discussion of (2.1) appears in Ref. [25]. In particular, it was pointed out that the GLE, while very general, can be realized with a simple and convenient model, viz., the independent-oscillator (IO) model. The Hamiltonian of the IO system is

$$H = \frac{p^2}{2m} + V(x) + \sum_j \left( \frac{p_j^2}{2m_j} + \frac{1}{2} m_j \omega_j^2 (q_j - x)^2 \right) - x f(t). \quad (2.2)$$

Here  $m$  is the mass of the quantum particle while  $m_j$  and  $\omega_j$  refer to the mass and frequency of heat-bath oscillator  $j$ . In addition,  $x$  and  $p$  are the coordinate and momentum operators for the quantum particle and  $q_j$  and  $p_j$  are the corresponding quantities for the heat-bath oscillators. The infinity of choices for the  $m_j$  and  $\omega_j$  give this model its great generality [25].

Use of the Heisenberg equations of motion leads to the GLE (2.1) describing the time development of the particle motion, where

$$\mu(t) = \sum_j m_j \omega_j^2 \cos(\omega_j t) \theta(t), \quad (2.3)$$

is the memory function, with  $\theta(t)$  the Heaviside step function. Also

$$F(t) = \sum_j m_j \omega_j^2 q_j^h(t), \quad (2.4)$$

is a fluctuating operator force with mean  $\langle F(t) \rangle = 0$ , where  $q^h(t)$  denotes the general solution of the

homogeneous equation for the heat-bath oscillators (corresponding to no interaction). These results were used to obtain the results for the (symmetric) autocorrelation and commutator of  $F(t)$ , viz.,

$$\begin{aligned} & \frac{1}{2} \langle F(t)F(t') + F(t')F(t) \rangle \\ &= \frac{1}{\pi} \int_0^\infty d\omega \operatorname{Re}[\tilde{\mu}(\omega + i0^+)] \hbar \omega \coth(\hbar \omega / 2kT) \\ & \quad \times \cos[\omega(t-t')], \end{aligned} \quad (2.5)$$

$$\begin{aligned} [F(t), F(t')] &= \frac{2\hbar}{i\pi} \int_0^\infty d\omega \operatorname{Re}\{\tilde{\mu}(\omega + i0^+)\} \omega \\ & \quad \times \sin \omega(t-t'). \end{aligned} \quad (2.6)$$

Here  $\tilde{\mu}(z)$  is the Fourier transform of the memory function:

$$\tilde{\mu}(z) = \int_0^\infty dt \mu(t) e^{izt}. \quad (2.7)$$

Eq. (2.5) is often referred to as the second fluctuation–dissipation theorem and we note that it can be written down explicitly once the GLE is obtained. Also, its evaluation requires only knowledge of  $\operatorname{Re} \tilde{\mu}(\omega)$ . On the other hand, the first fluctuation–dissipation theorem is an equation involving the autocorrelation of  $x(t)$  and its explicit evaluation requires a knowledge of the generalized susceptibility  $\alpha(\omega)$  (to be defined below) which is equivalent to knowing the solution to the GLE and also requires knowledge of both  $\operatorname{Re} \tilde{\mu}(\omega)$  and  $\operatorname{Im} \tilde{\mu}(\omega)$ . This solution is readily obtained when  $V(x)=0$ , corresponding to the original Brownian motion problem [26]. As shown in Ref. [25], a solution is also possible in the case of an oscillator. Taking  $V(x) = \frac{1}{2} Kx^2 = \frac{1}{2} m\omega_0^2 x^2$ , these authors obtained the solution of the Langevin equation (2.1) in the form

$$x(t) = \int_{-\infty}^t dt' G(t-t') \{F(t') + f(t')\}, \quad (2.8)$$

where  $G(t)$ , the Green function, is given by

$$G(t) = \frac{1}{2\pi} \int_{-\infty}^\infty d\omega \alpha(\omega + i0^+) e^{-i\omega t} \quad (2.9)$$

with  $\alpha(z)$  the familiar response function

$$\alpha(z) = \frac{1}{-mz^2 - iz\tilde{\mu}(z) + K}. \quad (2.10)$$

It is often convenient to write (2.8) in the form

$$x(t) = x_s(t) + x_d, \quad (2.11)$$

where  $x_d$  is the “driven” contribution [27] due to the external force  $f(t)$  and  $x_s$  is the contribution due to the fluctuation force  $F(t)$ . Here we have introduced a subscript  $s$  to emphasize that  $x_s(t)$  is a stationary operator-process, in the sense that correlations, probability distributions, etc. for this dynamical variable are invariant under time-translation ( $t \rightarrow t + t_0$ ). In particular, the correlation,

$$\begin{aligned} C_0(t - t') &\equiv \frac{1}{2} \langle x_s(t)x_s(t') + x_s(t')x_s(t) \rangle \\ &= \frac{\hbar}{\pi} \int_0^\infty d\omega \operatorname{Im}\{\alpha(\omega + i0^+)\} \\ &\quad \times \coth \frac{\hbar\omega}{2kT} \cos \omega(t - t'), \end{aligned} \quad (2.12)$$

is a function only of the time-difference  $t - t'$ . Furthermore, [27]

$$\begin{aligned} C_d(t, t') &\equiv \frac{1}{2} \langle x(t)x(t') + x(t')x(t) \rangle \\ &= C_0(t - t') + \langle x(t) \rangle \langle x(t') \rangle, \end{aligned} \quad (2.13)$$

where  $\langle x(t) \rangle$  is the steady mean of the driven motion.

Also, taking the Fourier transform of (2.8), we obtain

$$\tilde{x}(\omega) = \alpha(\omega) \{ \tilde{F}(\omega) + \tilde{f}(\omega) \}, \quad (2.14)$$

where the superposed tilde is used to denote the Fourier transform. Thus,  $\tilde{x}(\omega)$  is the Fourier transform of the operator  $x(t)$ :

$$\tilde{x}(\omega) = \int_{-\infty}^{\infty} dt x(t) e^{i\omega t}. \quad (2.15)$$

We have now all the tools we need to calculate observable quantities. It is also useful to note that while the commutator, which is temperature independent, is given by the formula [28]

$$\begin{aligned} [x(t_1), x(t_1 + t)] &= \frac{2i\hbar}{\pi} \int_0^\infty d\omega \operatorname{Im}\{\alpha(\omega + i0^+)\} \\ &\quad \times \sin \omega t. \end{aligned} \quad (2.16)$$

### 3. Mean-square displacement and wave packet spreading

The mean-square displacement of the quantum particle in a dissipative environment,  $s(t)$  say, plays a key

role in all of our subsequent discussions. In particular, it determines the diffusion time through a mesoscopic system of interest. In order to concentrate on the fundamental features, we take  $V = 0$  and  $f(t) = 0$  but we will return to  $f(t) \neq 0$  in Section 5. Then using (2.12), we obtain

$$\begin{aligned} s(t) &\equiv \langle [x_s(t) - x_s(0)]^2 \rangle \\ &= 2 \{ C_0(0) - C_0(t) \} \\ &= \frac{2\hbar}{\pi} \int_0^\infty d\omega \operatorname{Im}\{\alpha(\omega + i0^+)\} \\ &\quad \times \coth \frac{\hbar\omega}{2kT} (1 - \cos \omega t), \end{aligned} \quad (3.1)$$

where now

$$\alpha(z) = \frac{1}{-mz^2 - iz\tilde{\mu}(z)}. \quad (3.2)$$

It is informative to consider some limiting cases. In particular, in the quantum physics/quantum optics literature the Ohmic model (no memory in the GLE), for which

$$\tilde{\mu}(\omega) = m\gamma = \text{constant} \quad (\text{Ohmic}), \quad (3.3)$$

is often considered. Then, in the high temperature limit one obtains [29], with  $t > 0$ ,

$$s(t) = \frac{2kT}{m\gamma^2} \{ e^{-\gamma t} - 1 + \gamma t \}, \quad kT \gg \hbar\gamma. \quad (3.4)$$

For long times

$$s(t) \rightarrow \frac{2kT}{m\gamma} t, \quad \gamma t \gg 1 \quad (3.5)$$

which is the familiar Einstein relation from Brownian motion theory. However, for short times (which are more characteristic of decoherence decay times [16])

$$s(t) \rightarrow \frac{kT}{m} t^2, \quad \gamma t \ll 1, \quad (3.6)$$

independent of  $\gamma$ .

The situation is very different for low temperatures ( $kT \ll \hbar\gamma$ ), in which case the main contribution is from the zero-point ( $T = 0$ ) oscillations of the electromagnetic field. This calculation has recently been carried out [24] and it was found necessary to use a model incorporating memory since the Ohmic model lead to

singular and unphysical results for very short times. In particular, the single relaxation time ( $\tau$ ) model

$$\tilde{\mu}(z) = \frac{m\gamma}{1 - z\tau}, \quad (3.7)$$

leads to the result [24]

$$s(t) = -\frac{\hbar\gamma}{\pi m} t^2 \log(\gamma\tau), \quad \tau \ll t \ll \gamma^{-1}. \quad (3.8)$$

It would be of interest to obtain corresponding results for the actual dissipative models which describe various mesoscopic systems.

Whereas  $s(t)$  is of interest per se, it also plays a key role in the determination of wave packet spread and attenuation of coherence. Recently [16], we obtained a general formula for the spreading of a free particle Gaussian wave packet: if initially the complete system is in equilibrium at temperature  $T$  and the wave packet describing the quantum particle has a width  $\sigma$ , then after a time  $t$  the width is given by

$$w^2(t) = \sigma^2 - \frac{[x(t_1), x(t_1 + t)]^2}{4\sigma^2} + s(t). \quad (3.9)$$

For example, for a free particle in a high temperature environment

$$w^2(t) \rightarrow \sigma^2 + \frac{\hbar^2 t^2}{4m^2 \sigma^2} + \frac{kT}{m} t^2. \quad (3.10)$$

The width  $w(t)$  is a vital ingredient in the determination of decoherence decay times, as we shall see in the following section. For  $T = 0$ , (3.10) reduces to the familiar formula of quantum mechanics [30,31].

#### 4. Decoherence

Decoherence refers to the destruction of a quantum interference pattern and is relevant to the many experiments that depend on achieving and maintaining entangled states. Examples of such efforts are in the areas of quantum teleportation [13], quantum information and computation [10,11], entangled states [12], Schrödinger cats, and the quantum-classical interface. For an overview of many of the interesting experiments involving decoherence, we refer to Refs. [12–15].

Much of the discussion of decoherence [14,16–24] has been in terms of a particle moving in one dimension that is placed in an initial superposition state (Schrödinger “cat” state) corresponding to two

widely separated wave packets, separated by a distance  $d$ . Thus, in an obvious notation we write the wave-function of the two-Gaussian state as

$$\psi(x, t) = N[\psi_1(x, t) + \psi_2(x, t)], \quad (4.1)$$

where

$$N = \frac{1}{\sqrt{2(1 + e^{-d^2/8\sigma^2})}}. \quad (4.2)$$

Hence

$$P(x, t) = N^2(|\psi_1|^2 + |\psi_2|^2 + 2\text{Re}\{\psi_1^* \psi_2\}). \quad (4.3)$$

Thus, the probability distribution consists of three contributions, two of which correspond to the separate packets, whereas the third is an interference term. The first two terms are of the single-Gaussian form while the interference term is characterized by a cosine factor.

In general, the interference term disappears in time due to either temperature or dissipative effects. There are various measures of decoherence, based on decay of diagonal and off-diagonal density matrix elements or probability distributions in phase space, momentum space or coordinate space [20] but we consider the latter to be the most desirable because it is closest to experiment. Thus, we measure the disappearance of the interference term, that is, the loss of coherence (decoherence), by defining an attenuation coefficient  $a(t)$ , which is the ratio of the factor multiplying the cosine in the interference term to twice the geometric mean of the first two terms.

Next, using quantum probability functions [16], we obtained

$$a(t) = \exp\left\{-\frac{s(t)}{8\sigma^2 w^2(t)}\right\}. \quad (4.4)$$

#### 5. Presence of an external field ( $f(t) \neq 0$ )

As we saw in Section 2, in particular (2.11) and (2.13), the effect of an external classical force  $f(t)$  is to replace  $x_s \rightarrow x_s + x_d$  and  $C_0 \rightarrow C_d$ . This leads, with the help of (3.1) to the conclusion that, in the expression for  $a(t)$  given by (4.4), we simply replace  $s(t) \rightarrow s(t) + s_d$ , where

$$s_d(t) = \langle x_d^2(t) \rangle$$

$$= \int_0^t dt' \int_0^{t'} dt'' G(t-t') G(t-t'') \times g(t' - t'') \quad (5.1)$$

with

$$g(t' - t'') = \langle f(t') f(t'') \rangle. \quad (5.2)$$

In order to proceed further, one must, of course, specify the time dependence of the external force. For details, we refer to Ref. [23].

## 6. Conclusion

The material present above is an overview of our work in the arena of quantum physics/quantum optics, where the models we have discussed display great generality: arbitrary temperature and arbitrary heat bath allowing for non-Markovian (memory) effects and with no restriction to initial decoupling of the bath and system. They are relevant not only to fundamental questions but also have implications for quantum computation studies (since decoherence is always a stumbling block to the maintenance of superposition states). Our hope is that they will stimulate new ideas in the study of nanostructures and mesoscopic systems generally since analytic results have been obtained in most cases which facilitate attainment of physical insight into the important facets of the various problems. The next steps should include, in particular, an analysis of more complicated potentials and also heat baths which display memory effects obtained from physical models. The latter, in turn, will have to reflect, in many cases, the actual systems of interest since, for example, the inelastic phase coherence time has very different forms depending on the parameters of the system [8,9].

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