Teaching decoherence and dissipation

Lecture Quantum Information and Theoretical Quantum Optics II – Carsten Henkel[*][§]

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Abstract.

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1.

Dephasing is a process where only the off-diagonal elements of the density matrix decay, while the populations are left unchanged. The Lindblad operator is

$$L_{\rm deph} = \sqrt{\kappa}\,\sigma_3 \tag{1}$$

with a rate κ. By solving the Lindblad master equation (exercise!), we find

$$\rho(t) = \left(\begin{array}{cc} \rho_{\rm ee}(0) & {\rm e}^{-\kappa t}\rho_{\rm eg}(0) \\ {\rm e}^{-\kappa t}\rho_{\rm ge}(0) & \rho_{\rm gg}(0) \end{array} \right) \tag{2}$$

This process can be mimicked in a "classical way" by assuming that a superposition state vector

$$|\psi(t)\rangle = \alpha {\rm e}^{{\rm i}\varphi(t)}|{\rm e}\rangle + \beta {\rm e}^{-{\rm i}\varphi(t)}|{\rm g}\rangle \tag{3}$$

acquires a relative phase $\varphi(t)$ that is "randomly fluctuating". Experimentally, this happens for a two-level system embedded in a solid: the motion of the immediate environment perturbs the form of the electronic orbitals and hence their energy, even if the electron stays in this orbital ("adiabatic perturbation"). Hence only the energy is randomized, but the population is kept constant.

In this context, we can define a quantum-mechanical "average ensemble" by building the density matrix $|\psi(t)\rangle\langle\psi(t)|$ and taking the average over the probability distribution of $\varphi(t)$ (denoted by an overbar):

$$\rho(t) = \overline{|\psi(t)\rangle\langle\psi(t)|} \tag{4}$$

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With the identification

$$\overline{\mathrm{e}^{\mathrm{i}\varphi(t)}} = \mathrm{e}^{-\kappa t} \tag{5}$$

we get the same result as with the Lindblad form. This is true if $\varphi(t)$ is a gaussian random variable with zero average and with variance $\langle\varphi(t)^2\rangle = \kappa t$. This behaviour is similar to Brownian motion (hence the name "phase diffusion"), in the mathematics literature, it is called a "Wiener process".

2. Exactly solvable dephasing model

References: N. G. van Kampen, *J Stat Phys* 1995 and G. Massimo Palma and Kalle-Antti Suominen and Artur K. Ekert, *Proc Roy Soc London A* 1996, in particular Section 4.

We consider a two-level system that couples to a quantized field (in the following: "bath") via

$$H_{\mathrm{int}} = \sigma_3 \sum_k \left(g_k b_k^\dagger + g_k^* b_k \right) \tag{6}$$

with coupling constants g_k that are summarized by the spectral density (ω_k is the frequency of bath mode k)

$$S(\omega) = \sum_k |g_k|^2 \delta(\omega - \omega_k) \tag{7}$$

From the master equation (**??**) in the Heisenberg picture, we see that the inversion σ_3 is conserved. Hence, only the "off-diagonal operator" σ is affected by the bath. Going back to the Schrödinger picture, one can show that the off-diagonal elements of the density matrix behave like

$$\rho_{\mathrm{eg}}(t) = \mathrm{e}^{-\Gamma(t)} \rho_{\mathrm{eg}}(0) \tag{8}$$

where the "decoherence factor" is given by

$$\Gamma(t) = \frac{1}{2} \sum_k |\xi_k(t)|^2 \coth(\beta\omega_k/2) \tag{9}$$

where $\beta = \hbar/k_B T$ is the inverse temperature of the initial bath state (we assume factorized initial conditions) and

$$\xi_k(t) = 2 g_k \frac{1 - \mathrm{e}^{\mathrm{i}\omega_k t}}{\omega_k} \tag{10}$$

A proof of this result is sketched in Sec.2.1 below.

Discussion For short times, we can expand the effective coupling constants $\xi_k(t)$ and get

$$t \to 0: \qquad \Gamma(t) \approx 2t^2 \sum_k |g_k(t)|^2 \coth(\beta\omega_k/2) = 2t^2 \int\limits_0^\infty \mathrm{d}\omega\, S(\omega) \coth(\beta\omega/2) \tag{11}$$

The quadratic dependence on time is characteristic for this initial regime. In fact, from perturbation theory, we see that the probability amplitude for states orthogonal to the initial one must increase linearly in t. The corresponding probability thus starts off proportional to t^2. The integral in Eq.(11) is often dominated by large frequencies, and can be made finite with a "UV cutoff frequency" $\omega_\mathrm{c} = 1/\tau_\mathrm{c}$. (Without this cutoff, the integral actually diverges and the short-time regime may even lead to mathematical inconsistencies.) The quadratic regime then applies only on time scales $t < \tau_\mathrm{c}$ that are typically very short compared to the dissipative dynamics.

At larger times, we can make the approximation that $|\xi_k(t)|^2$ approaches a δ-function:‖

$$t \to \infty: \qquad \left| \frac{1 - \mathrm{e}^{\mathrm{i}\omega_k t}}{\omega_k} \right|^2 \to 2\pi t\, \delta^{(1/t)}(\omega_k) \tag{13}$$

where the width of the δ-function is of the order $1/t$. In this limit, only low-frequency modes contribute to the decoherence factor.

Let us first assume that $1/t$ is larger than $1/\beta$ (intermediate range $\tau_\mathrm{c} \ll t \ll \hbar/k_\mathrm{B}T$). Then we can make the zero-temperature approximation $\coth(\beta\omega/2) \approx 1$ for the relevant modes and get

$$\tau_\mathrm{c} \ll t \ll \beta: \qquad \Gamma(t) \approx 4\pi S(0) t \tag{14}$$

hence an exponential decay with a rate $\kappa = 4\pi S(0)$ that involves the spectral strength at zero frequency (more precisely: at frequencies $T/\hbar \ll \omega \ll \omega_\mathrm{c}$). This behaviour is consistent with a Lindblad master equation because $\mathrm{e}^{-\Gamma t}$ becomes exponential in t. We thus see that the Lindblad form is not valid on the short time scale τ_c that sets the correlation time of the bath fluctuations.

• logarithmic behaviour for Ohmic bath at large times, $T = 0$.

Finally, when $t \gg \hbar/k_\mathrm{B}T$, we have to take into account the thermal occupation of the low-frequency modes. The integral cannot be performed any more without knowledge of the behaviour of the function $S(\omega)$, in particular the limit $\lim_{\omega\to 0} S(\omega)\coth(\beta\omega/2)$. One class of spectral densities gives power laws $\mathrm{e}^{-\Gamma(t)} \propto t^\alpha$ with exponents α that depend on $S(\omega)$ and the temperature. • find an example?

An exponential decay at a T-dependent rate is possible as well, in particular in the so-called "Ohmic case" where the spectrum is linear for small frequencies, $S(\omega) \approx \alpha\omega$ with a dimensionless coefficient α. We then get at large t:

$$\begin{aligned} t \to \infty: \Gamma(t) &\approx 4\pi t \sum_k |g_k(t)|^2 \delta^{(1/t)}(\omega_k) \coth(\beta\omega_k/2) \\ &\approx 4\pi t \int_0^\infty \mathrm{d}\omega\, \alpha\omega\, \delta^{(1/t)}(\omega) \frac{2T}{\hbar\omega} = 4\pi\alpha(T/\hbar)t \end{aligned} \tag{15}$$

The decoherence rate thus becomes $4\pi\alpha T/\hbar$.

‖ This is based on the integral

$$\int_{-\infty}^{\infty} \mathrm{d}x \frac{\sin^2(x/2)}{x^2} = \frac{\pi}{2}. \tag{12}$$

2.1. Calculation of the decoherence factor

For the states $|\mathrm{g}\rangle$ and $|\mathrm{e}\rangle$ of the spin, the action of the full Hamiltonian is easy:

$$H|\mathrm{g}\rangle = |\mathrm{g}\rangle H_{\mathrm{g}}, \qquad H_{\mathrm{g}} = -\frac{\hbar\omega_A}{2} + H_B - \sum_k \hbar(g_k b_k^\dagger + g_k^* b_k) \tag{16}$$

where H_{g} acts on the bath variables only. A similar expression applies to H_{e}, with the opposite sign in the first and last term. We therefore get from the full time evolution operator $U(t)$:

$$\langle\sigma\rangle_t = \mathrm{tr}_{\mathrm{SB}}[U^\dagger(t)|\mathrm{g}\rangle\langle\mathrm{e}|U(t)\rho(0)\otimes\rho_T(B)] \tag{17}$$

$$= \mathrm{tr}_{\mathrm{SB}}[|\mathrm{g}\rangle\langle\mathrm{e}|\rho(0)\otimes U_{\mathrm{g}}^\dagger(t)U_{\mathrm{e}}(t)\rho_T(B)] \tag{18}$$

$$= \langle\sigma\rangle_0 \mathrm{tr}_{\mathrm{B}}[U_{\mathrm{g}}^\dagger(t)U_{\mathrm{e}}(t)\rho_T(B)] \tag{19}$$

The bath trace can be taken for each mode separately since both $U_{\mathrm{g,e}}(t)$ and $\rho_T(B)$ factorize into a product of single-mode operators. For a single mode b with parameters g, ω, we have (dropping the label k for the moment and assuming real g)

$$U_{\mathrm{g}}^\dagger(t) = \exp[\mathrm{i}t(\omega b^\dagger b - gb - gb^\dagger)] = \exp[\mathrm{i}\omega t(b^\dagger - \gamma)(b-\gamma)]\,\mathrm{e}^{-\mathrm{i}tg^2/\omega} \tag{20}$$

$$U_{\mathrm{e}}(t) = \exp[-\mathrm{i}t(\omega b^\dagger b - gb - gb^\dagger)] = \exp[-\mathrm{i}\omega t(b^\dagger + \gamma)(b+\gamma)]\,\mathrm{e}^{-\mathrm{i}tg^2/\omega}$$

with $\gamma = g/\omega$. We now recall the action of the displacement operator $D(\gamma)$ on a function of the operators b, $b^\dagger$:

$$D^\dagger(\gamma)f(b,b^\dagger)D(\gamma) = f(b+\gamma, b^\dagger+\gamma^*) \tag{21}$$

• recap a proof of this relation ('displacement operator').

We can therefore write

$$U_{\mathrm{g}}^\dagger(t)U_{\mathrm{e}}(t)\rho_T(B)$$

$$= D^\dagger(-\gamma)\exp(\mathrm{i}\omega t b^\dagger b)D(-\gamma)D^\dagger(\gamma)\exp(-\mathrm{i}\omega t b^\dagger b)D(\gamma) \tag{22}$$

$$= D^\dagger(-\gamma)\exp(\mathrm{i}\omega t b^\dagger b)D(-2\gamma)\exp(-\mathrm{i}\omega t b^\dagger b)D(\gamma) \tag{23}$$

where in the last step, we have used $D^\dagger(\gamma) = D(-\gamma)$ and the composition law of the displacement operators. (The projective phase in QO I, Eq.(3.37) vanishes in this case.) We now use the identity, similar to Eq.(21)

$$U_0^\dagger(t)f(b,b^\dagger)U_0(t) = f(b\,\mathrm{e}^{-\mathrm{i}\omega t}, b^\dagger\,\mathrm{e}^{\mathrm{i}\omega t}) \tag{24}$$

where $U_0(t) = \exp(-\mathrm{i}\omega t b^\dagger b)$ is the 'free' time evolution operator. • just one sentence to justify.

Applying this to the displacement operator $D(-2\gamma) = \exp(-2\gamma b^\dagger + 2\gamma^* b)$ that is 'sandwiched' in Eq.(23), we have

$$\exp(\mathrm{i}\omega t b^\dagger b)D(-2\gamma)\exp(-\mathrm{i}\omega t b^\dagger b) = D(-2\gamma\,\mathrm{e}^{\mathrm{i}\omega t}) =: D(-2\gamma(t)) \tag{25}$$

We end up with a product of three displacement operators

$$D(\gamma)D(-2\gamma(t))D(\gamma) = \mathrm{e}^{-2\mathrm{i}\,\mathrm{Im}\gamma^*\gamma(t)}D(\gamma - 2\gamma(t))D(\gamma) \tag{26}$$

$$= \mathrm{e}^{-2\mathrm{i}\,\mathrm{Im}\gamma^*\gamma(t)}\mathrm{e}^{-2\mathrm{i}\,\mathrm{Im}\gamma^*(t)\gamma}D(\xi_t) \tag{27}$$

$$\xi_t = 2g\frac{1-\mathrm{e}^{\mathrm{i}\omega t}}{\omega} \tag{28}$$

where the projective phases cancel and we recover the parameter $\xi_k(t)$ of Eq.(10).

We finally have to calculate the average of a displacement operator in a thermal state:

$$\langle D(\xi_t)\rangle_{\mathrm{B}} = \mathrm{tr}\,[D(\xi_t)\rho_T] \tag{29}$$

where Z is the partition function. The calculation of this trace is typically done in the number state basis, but this is quite involved. The fastest way is to remember the P-representation of the thermal state

$$\rho_T = \int \mathrm{d}^2\alpha |\alpha\rangle\langle\alpha| P_T(\alpha), \qquad P_T(\alpha) = \frac{\mathrm{e}^{-|\alpha|^2/\bar{n}}}{\pi\bar{n}} \tag{30}$$

• a paragraph on the P-representation

and to calculate

$$\begin{aligned}\langle D(\xi_t)\rangle_{\mathrm{B}} &= \mathrm{tr}\int \mathrm{d}^2\alpha D(\xi_t)|\alpha\rangle\langle\alpha|P_T(\alpha)\\ &= \mathrm{tr}\int \mathrm{d}^2\alpha\, \mathrm{e}^{\mathrm{i}\,\mathrm{Im}\,\xi_t^*\alpha}|\alpha+\xi_t\rangle\langle\alpha|P_T(\alpha)\\ &= \int \mathrm{d}^2\alpha\, \mathrm{e}^{\mathrm{i}\,\mathrm{Im}\,\xi_t^*\alpha}\langle\alpha|\alpha+\xi_t\rangle P_T(\alpha)\\ &= \int \mathrm{d}^2\alpha\, \mathrm{e}^{2\mathrm{i}\,\mathrm{Im}\,\xi_t^*\alpha}\mathrm{e}^{-|\xi_t|^2/2} P_T(\alpha)\end{aligned}$$

At this point, we can take out the exponential factor $\mathrm{e}^{-|\xi_t|^2/2}$. Note that the projective phases now remain and determine the temperature dependence of the result. The gaussian integral can be performed • recall that $\mathrm{Im}\,\xi_t^*\alpha$ generalizes a scalar product in the phase space

and gives

$$\langle D(\xi_t)\rangle_{\mathrm{B}} = \mathrm{e}^{-|\xi_t|^2/2}\mathrm{e}^{-|\xi_t|^2\bar{n}} = \exp\left(-\tfrac{1}{2}|\xi_t|^2\coth\beta\omega/2\right) \tag{31}$$

Going back to $\langle\sigma\rangle_t$, we restore the factor $\mathrm{e}^{-\mathrm{i}\omega_A t}$ that we forgot in Eqs.(20) and take the product over all modes. This gives a sum in the exponent and hence

$$\langle\sigma\rangle_t = \mathrm{e}^{-\Gamma(t)}\langle\sigma\rangle_0 \tag{32}$$

$$\Gamma(t) = \sum_k \tfrac{1}{2}|\xi_k(t)|^2\coth(\beta\omega_k/2) \tag{33}$$

which is Eq.(34).

2.2. Long-time limit

We evaluate here in more detail the decoherence factor $\mathrm{e}^{-\Gamma(t)}$ in the limit of long times. The spectral density is taken in Ohmic form with a dimensionless prefactor α and a cutoff frequency ω_c:

$$\Gamma(t) = 8\alpha\int_0^\infty \mathrm{d}\omega\frac{\omega\omega_c^2}{\omega^2+\omega_c^2}\coth\frac{\omega}{2T}\frac{\sin^2(\omega t/2)}{\omega^2} \tag{34}$$

• exact upper limit on $\Gamma(t)$ by bounding the $\sin^2$.

Observe that the integrand is even in ω, extend the integration from $-\infty$ to ∞ and write $\sin^2(\omega t/2) = \mathrm{Re}\frac{1}{2}(1-\mathrm{e}^{\mathrm{i}\omega t})$. When we shift the integration path from the real axis to a large semi-circle at infinity, we encounter simple poles in the $\coth(\omega/2T)$ at $\omega = \mathrm{i}\xi_n = 2\pi n T$, the so-called Matsubara frequencies. Since

$$\coth\frac{\omega}{2T} = 2T\frac{\mathrm{d}}{\mathrm{d}\omega}\log\sinh\frac{\omega}{2T} \tag{35}$$

these poles arise from the zeros of $\sinh\frac{\omega}{2T}$ and have a residue $2T$. There is also a simple pole at $\omega = \mathrm{i}\omega_c$, from the cutoff of the mode density. Finally, we have to take into account half the residue of the singularity at $\omega = 0$. • a few words and a sketch of the path to justify.

Because $\coth(\omega/2T) \approx 2T/\omega$ for small ω, we have a singularity $1/\omega^2$ (a double pole) at the origin. Hence, the residue is the first derivative of the rest of the integrand:

$$4\alpha T\,\mathrm{Re}\,\pi\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}\omega}\frac{\omega_c^2}{\omega^2+\omega_c^2}(1-\mathrm{e}^{\mathrm{i}\omega t}) = 4\alpha T\,\mathrm{Re}\,\pi\mathrm{i}(-\mathrm{i}t) = 4\pi\alpha T t \tag{36}$$

This coincides with the term linear in t that we found with the approximation $\delta^{(t)}(\omega)$ to the $\sin^2$ function, Eq.(15). The contributions from the other poles give the sum

$$\Gamma(t) = \gamma t + 4\alpha\,\mathrm{Re}2\pi\mathrm{i}(\sum_{n=1}^{\infty}\frac{\omega_c^2}{\omega_c^2-\xi_n^2}\frac{T(1-\mathrm{e}^{-\xi_n t})}{\mathrm{i}\xi_n} + \frac{\omega_c^2}{2\mathrm{i}\omega_c}\coth\frac{\mathrm{i}\omega_c}{2T}\frac{1-\mathrm{e}^{-\omega_c t}}{\mathrm{i}\omega_c}) \tag{37}$$

For $t \gg \tau_c$, we can set $\mathrm{e}^{-\omega_c t} = 0$. If we further assume $\xi_1 t = 2\pi T t \gg 1$, then also the sum becomes time-independent, and we have an expression for the offset K (or "initial slip") between $\Gamma(t)$ and the linear approximation γt. Putting $N_c = \omega_c/2\pi T$,

$$K = 4\alpha(-\cot\pi N_c + \sum_{n=1}^{\infty}\frac{N_c^2}{n(N_c^2-n^2)}) \tag{38}$$

Note that N_c is not an integer if ω_c does not coincide with any of the Matsubara frequencies ξ_n. A typical limiting case is a large cutoff, $N_c \gg 1$. The apparent divergence at $n \approx N_c$ is cancelled by the first term. We cannot take the limit $N_c \to \infty$ because the sum would not converge. Instead, we can take N_c to a half-integer so that the cotangent vanishes, split the sum into $n = 1 \ldots \lfloor N_c \rfloor$ and $n = \lceil N_c \rceil \ldots \infty$ and approximate the cutoff function of the mode density by simple limiting forms:

$$K \approx 4\alpha(\sum_{n=1}^{\lfloor N_c \rfloor}\frac{1}{n} - N_c^2\sum_{n=\lceil N_c \rceil}^{\infty}\frac{1}{n^3}) \tag{39}$$

Replacing the summations by integrations, we get

$$K \approx 4\alpha(\log N_c - N_c^2\frac{-3}{N_c^2}) = 4\alpha(\log\frac{\omega_c}{2\pi T} + 3) \tag{40}$$

up to corrections of order unity in the parenthesis. • check in a plot.

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