Coupling of Quantum Systems to the Environment: 
Functional Differential Treatment

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Abstract

A functional differential treatment, via the quantum dynamical principle, is given for the coupling of quantum systems to the environment. As one is involved in taking the trace over the dynamical variables of the environment, the analysis necessarily deals with transition probabilities rather than with amplitudes. It is shown that the functional differential treatment is quite suitable for such a study as it involves in carrying out functional differentiations, with respect to classical sources, on functionals describing decoupled physical systems from the environment.

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1 Introduction

The functional differential treatment [2–9,11–13], via the quantum dynamical principle, has been a very powerful tool for investigating properties of quantum systems and for carrying out explicit computations. In this regard, it has been quite successful in gauge theories and of the generation of essential modifications [2–6] needed for their proper quantization with no much effort. For a pedagogical treatment of the theory and for several applications of the functional differential method, via the quantum dynamical principle, in quantum mechanics, the reader may wish to refer to [7, Ch. 11]. The purpose of this work is to carry out an analysis, using the functional differential approach, of the coupling of quantum mechanical systems to the environment, understood

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to be surrounding a physical system, as the former systems, in the real world, are never in isolation from the latter. The incorporation of the environment in quantum mechanical systems has led to much physical insights into such fundamental problems as quantum decoherence, Schrödinger’s cat and in measurement theory, in general [7, §8.7, §8.9, §12.7], [1,10,14,15]. We will see, that the functional differential approach is quite suitable for studying the coupling of quantum mechanical systems to the environment. It involves in carrying out functional differentiations, with respect to classical sources, of a functional describing “decoupled” systems from the environment. As one is involved in taking the trace over the dynamical variables of the environment in studying the response of physical systems to it, the analysis necessarily involves in dealing directly with transition probabilities rather than amplitudes. This is a basic departure from the far simpler case of studying quantum mechanical systems in isolation. In dealing with probabilities and in taking traces, it turns out that two different sets of classical sources, coupled to the dynamical variables of the theory, should, a priori, be introduced. The physically relevant probabilities are then recovered in the limit as the two sets of sources coincide and are eventually set equal to zero. The general expression for transition probabilities of quantum mechanical systems, coupled to the environment, is given in Eq.(5) involving functional differentiations with respect to these two sets of classical sources. The method used in this work generalizes to quantum field theory and will be studied in a forthcoming report.

2 Transition Probabilities and the Role of the Environment

Typically a quantum mechanical system may be described by a Hamiltonian

$$H_1(t) = H(q,p,t) - qF(t) + pS(t)$$  \hspace{1cm} (1)

written in terms of dynamical variables in the \((q,p)\) language, where \(F(t)\) and \(S(t)\) are classical source functions introduced to generate functions of \(q\) and \(p\), respectively. For simplicity of the notation, we have in Eq.(1), suppressed indices in \(q\) and \(p\) reflecting the dimensionality of space and of the number of particles involved in the theory. In most applications, the classical sources \(F(t)\), \(S(t)\) are set equal to zero after all relevant functional differentiations in the theory, with respect to them, are carried out, with \(H(q,p;t)\) finally emerging as the Hamiltonian describing the actual physical system into consideration.

The quantum dynamical principle states [cf. 7, Ch. 11], that a transition amplitude \(\langle at_2 | bt_1 \rangle\) for the system governed by (1), from time \(t_1\) to time \(t_2\), is
given by

$$\langle at_2 | bt_1 \rangle = \exp \left( -\frac{i}{\hbar} \int_{t_1}^{t_2} d\tau H \left[ -i\hbar \frac{\delta}{\delta F(\tau)}, i\hbar \frac{\delta}{\delta S(\tau)} \right] \right) \langle at_2 | bt_1 \rangle_0$$

(2)

where $H$ in (2) is obtained from $H(q, p, \tau)$ by simply replacing $q$ and $p$ in the latter by the operators of functional differentiations $-i\hbar \delta F(\tau)/\delta F(\tau)$, $i\hbar \delta S(\tau)/\delta S(\tau)$, respectively, and $\langle at_2 | bt_1 \rangle_0$ denotes the transition amplitude governed by the simple “Hamiltonian” $[-qF(t) + pS(t)]$ only.

To investigate the role of the environment on the quantum mechanical system, governed initially by the Hamiltonian $H(t)$ in (1), one modifies the latter Hamiltonian by including, in the Hamiltonian, the contribution of the environment and of its interaction with the physical system at hand. Of particular interest is in the response of the physical system to the environment. Accordingly, one takes a trace over the dynamical variables of the environment in the manner to be spelled out below. The Hamiltonian of the combined system is taken to be of the form

$$H(t) = H_1(q_1, p_1, t) - q_1 F_1(t) + p_1 S_1(t) + H_2(q_2, p_2, t) - q_2 F_2(t) + p_2 S_2(t) + H_I(q_1, p_1, q_2, p_2, t),$$

(3)

where the indices 1, 2 correspond, respectively, to the physical system and the environment, and $H_I$ specifies the interaction term between them.

The transition amplitude for the combined system to evolve from a state, say, $|a, A; 0\rangle$, initially at time $t = 0$, to a state, say, $|b, B; t\rangle$, at time $t > 0$, is then given by

$$\langle b, B; t | a, A; 0 \rangle = \exp \left( -\frac{i}{\hbar} \int_0^t d\tau H_I \left( -i\hbar \frac{\delta}{\delta F_1(\tau)}, i\hbar \frac{\delta}{\delta S_1(\tau)} \right), \right.$$

$$\left. -i\hbar \frac{\delta}{\delta F_2(\tau)}, i\hbar \frac{\delta}{\delta S_2(\tau)} \right) \langle b; t | a; 0 \rangle^{F_1, S_1} \langle B; t | A; 0 \rangle^{F_2, S_2}$$

(4)

as in (2), where $\langle b; t | a; 0 \rangle^{F_1, S_1}$, $\langle B; t | A; 0 \rangle^{F_2, S_2}$ are the transition amplitudes of the decoupled subsystems in the presence of their respective classical sources.

To find the response of the physical system, described by the Hamiltonian $H_1(q_1, p_1, t)$ in (3), to the environment, it is necessary to work with transition probabilities, corresponding to the process associated with the expression in (4), rather than with amplitudes as done in the latter equation, and “trace out” over the environment. To this end, let $\{B_n; t\}$ denote a complete set of states pertaining to the environment, then the probability for the physical system to make a transition from an initial state $|a; 0\rangle$ to a state $|b; t\rangle$ in time $t$, responding in the process to the environment, emerges as

$$\text{Prob}[|a; 0 \rightarrow (b; t)| ]_E = \mathcal{O}(\mathcal{O}^* \langle b; t | a; 0 \rangle^{F_1, S_1} \langle b; t | a; 0 \rangle^{F_1, S_1} \rangle^*)$$

$$\mathcal{F}[F_2, S_2; F'_2, S'_2]$$

(5)
where
\[ O = \exp \left( -\frac{i}{\hbar} \int_0^t d\tau H_1 ( -i\hbar \frac{\delta}{\delta F_1(\tau)} ; i\hbar \frac{\delta}{\delta S_1(\tau)} , -i\hbar \frac{\delta}{\delta F_2(\tau)} ; i\hbar \frac{\delta}{\delta S_2(\tau)} , \tau ) \right) \] (6)

with \( O' \) defined similarly with \( F_1, S_1, F_2, S_2 \) replaced by \( F'_1, S'_1, F'_2, S'_2 \), respectively, and the presence of the letter \( E \) attached to the probability on the left-hand side of (6) is to emphasize the coupling of the environment to the physical system as the latter evolves in time. The functional \( F \) is given by
\[ F[F_2, S_2; F'_2, S'_2] = \sum_n \langle B_n; t | A; 0 \rangle^{F_2, S_2} \left( \langle B_n; t | A; 0 \rangle^{F'_2, S'_2} \right)^* . \] (7)

We note that (7) reduces to the trace over the environment in the special case for which \( F'_2 = F_2 \), and \( S'_2 = S_2 \). One cannot, \textit{a priori}, set such equalities until the functional differentiations, with respect to these sources, as accomplished by the operators \( O, (O')^* \), are independently carried out. The bar sign on the right-hand side of (5) refers to the fact that finally one is to set \( F = F' = 0, S = S' = 0 \), after all the operations of functional differentiations have been done.

Eq. (5) gives the general expression for the transition probability of a physical system, as it evolves in time, in response to the environment.

Of significance importance is for systems written in terms of creation and annihilation operators, which most conveniently describe processes of transitions between their allowed states. Such a typical example is given by the Hamiltonian
\[ H(t) = H_1(t) + H_2(t) + H_{12}(t) \] (8)

with
\[ H_1(t) = \hbar \omega a^\dagger a - a^\dagger F(t) - F^*(t)a \] (9)
\[ H_2(t) = \sum_k \hbar \omega_k b_k^\dagger b_k - \sum_k \left( K_k(t)b_k^\dagger + b_k K_k^*(t) \right) \] (10)
\[ H_{12}(t) = a^\dagger \sum_k \lambda_k b_k + a \sum_k \lambda_k^* b_k^\dagger \] (11)

and \( (a, a^\dagger), (b_k, b_k^\dagger) \), pertaining to the physical system in consideration and the environment, respectively, \( [a, a^\dagger] = 1, [b_k, b_k^\dagger] = \delta_{kk'} \) for the corresponding commutators.
Suppose that the environment is initially in the ground-state $|0; 0\rangle_2$. Let $U_2(t)$ denote the time evolution unitary operator describing the time evolution of the environment in the absence of the physical system. The so-called Heisenberg operator $b_k(t)$ associated with $b_k$ is given by

$$b_k(t) = U_2^\dagger(t)b_k U_2(t)$$

which works out to be

$$b_k(t) = b_k e^{-i\omega_k t} + \frac{i}{\hbar} \int_0^t d\tau K_k(\tau)e^{-i\omega_k(t-\tau)}$$

The quantum dynamical principle \[2–9, 11–13\] for the vacuum-to-vacuum transition amplitude $\langle 0; t | 0; 0 \rangle_2^K$ gives

$$-i\hbar \left\langle 0; t | 0; 0 \right\rangle_2^K = \left\langle 0; t | b_k(t') | 0; 0 \right\rangle_2^K$$

for $0 < t' < t$. From the expression in (13), Eq.(14) simplifies to

$$-i\hbar \frac{\delta}{\delta K_k^*(t')} \left\langle 0; t | 0; 0 \right\rangle_2^K = \frac{i}{\hbar} \left\langle 0; t | 0; 0 \right\rangle_2^K \int_0^{t'} d\tau K_k(\tau)e^{-i\omega_k(t'-\tau)}$$

which integrates out to

$$\left\langle 0; t | 0; 0 \right\rangle_2^K = \exp \left(-\frac{1}{\hbar^2} \sum_k \int_0^t d\tau \int_0^{t'} d\tau' e^{-i\omega_k(\tau-\tau')} K_k^*(\tau) \Theta(\tau - \tau') K_k(\tau') \right)$$

where $\Theta(\tau - \tau')$ is the step function.

The functional $\mathcal{F}[K, K']$, corresponding to the one in (7), may be worked out in closed form. To this end, set $K(t) = K_1(t) + K_2(t)$, with $K_1(t), K_2(t)$ localized in time between $(0, t)$, such that $K_2(t)$ is “switched on” after the source $K_1(t)$ is “switched off”. That is, in particular, $K_2(t)$ and $K_1(t)$ do not overlap in time.

From (16) we may then write

$$\left\langle 0; t | 0; 0 \right\rangle_2^{K_1+K_2} = \left\langle 0; t | 0; 0 \right\rangle_2^{K_2} \exp \left[ \sum_k \left( \int_{-\infty}^{\infty} d\tau e^{-i\omega_k \tau} \frac{i}{\hbar} K_k^*(\tau) \right) \times \left( \int_{-\infty}^{\infty} d\tau' e^{i\omega_k \tau} \frac{i}{\hbar} K_1(\tau') \right) \right] \left\langle 0; t | 0; 0 \right\rangle_2^{K_1}$$

where due to the fact that $K_1(\tau), K_2(\tau')$ are localized in time, we have extended the time integrations in the middle exponential from $-\infty$ to $\infty$. 
Let $|n; n_{k_1}, n_{k_2}, \ldots\rangle_2$ denote a state of $n$ excitations, $n_{k_1}$ of which in the state $k_1$, $n_{k_2}$ of which in state $k_2$, and so on, i.e., such that $n = n_{k_1} + n_{k_2} + \ldots$. Then upon introducing the unitarity completeness property

$$\langle 0; t | 0; 0 \rangle_{K_1 + K_2} = \sum_{n=0}^{\infty} \sum_{(n_{k_1} + n_{k_2} + \ldots = n)} \langle 0; t | n; n_{k_1}, n_{k_2}, \ldots \rangle_2^K_1 \langle n; n_{k_1}, n_{k_2}, \ldots | 0 \rangle_2^K_2$$

(18)

where the intermediate states are evaluated at any time after the switching off of source $K_1$ and before the switching on of source $K_2$, and the Fourier transform

$$K_k(t) = \int_{-\infty}^{\infty} \frac{d\omega_k}{2\pi} K_k(\omega) e^{-i\omega_k t}$$

(19)

we obtain by expanding the middle exponential in powers of the source functions $K_{1k}(\omega_k), K_{2k}(\omega_k)$ the expression

$$\langle n; n_{k_1}, n_{k_2}, \ldots; t | 0; 0 \rangle_2^K = \langle 0; t | 0; 0 \rangle_2^K \left( \frac{\left( \frac{i}{\hbar} K_{1k}(\omega_k) \right)^{n_{k_1}}}{\sqrt{n_{k_1}!}} \right) \left( \frac{\left( \frac{i}{\hbar} K_{2k}(\omega_k) \right)^{n_{k_2}}}{\sqrt{n_{k_2}!}} \right) \ldots$$

(20)

for a given source $K(t)$. The functional $\mathcal{F}[K, K']$, corresponding to the one in (7), is then given by

$$\mathcal{F}[K, K'] = \sum_{n=0}^{\infty} \sum_{(n_{k_1} + n_{k_2} + \ldots = n)} \langle n; n_{k_1}, n_{k_2}, \ldots; t | 0; 0 \rangle_2^K \times \left( \langle n; n_{k_1}, n_{k_2}, \ldots; t | 0; 0 \rangle_2^{K'} \right)^*$$

(21)

and may be summed exactly over $n$ giving

$$\mathcal{F}[K, K'] = \langle 0; t | 0; 0 \rangle_2^K \exp \left[ \frac{1}{\hbar^2} \sum_k \left( \int_0^t d\tau e^{i\omega_k \tau} K_k(\tau) \right) \right] \times \left( \int_0^t d\tau' e^{-i\omega_k \tau'} K_k^*(\tau') \right)^*$$

(22)

which cannot be expressed as the product of two functionals one depending on $K$ and the other on $K'$, as expected. Formally one checks the unitarity condition: $\mathcal{F}[K, K] = 1$ directly from (22).

Suppose that the physical system is initially in the ground-state, i.e., the vacuum-state $|0; 0\rangle$. The vacuum persistence amplitude of the physical system,
in isolation from the environment, but in the presence of the external sources $F(t), F^*(t)$ in (9), may be then inferred from (16) to be

$$
\langle 0; t | 0; 0 \rangle^F_{1} = \exp \left( -\frac{1}{\hbar^2} \int_0^t d\tau \int_0^t d\tau' e^{-i\omega(\tau-\tau')} F^*(\tau) \Theta(\tau-\tau') F(\tau') \right) \tag{23}
$$

From our general expression in (5), we then obtain for the vacuum persistence probability of the physical system, in response to the environment,

$$
\text{Prob}[\langle 0; 0 | 0; t \rangle_E] = O(\langle 0; t | 0; 0 \rangle^F_{1})^* O' \left( \langle 0; t | 0; 0 \rangle^F_{1} \right)^* F[K, K'] \tag{24}
$$

where

$$
O = \exp -\frac{i}{\hbar} \sum_k \int_0^t d\tau \left[ \lambda_k \frac{\hbar}{i} \delta F(\tau) \delta F^*(\tau) + \lambda_k^* \frac{\hbar}{i} \delta K_k(\tau) \delta K_k^*(\tau) \right] \tag{25}
$$

and $O'$ similarly defined with $F, F^*, K_k, K_k^*$ replaced, respectively, by $F', F'^*, K'_k, K'^*_k$, and $F[K, K']$ given by the explicit expression in (22).

To evaluate the expression on the right-hand side of (24), we use, in the process, the identity

$$
e^A e^B = \exp \left( e^A e^{-A} \right) e^A \tag{26}
$$

for two operators $A, B$. We note that $\delta / \delta F(\tau), \delta / \delta F^*(\tau)$, in (25), give rise to translation operators, via $O$, to functionals of $F$ and $F^*$ as given, for example, in (23), and similarly for $\delta / \delta K(\tau), \delta / \delta K^*(\tau)$. The functional differentiations operations in (24) are then readily carried for a physical system weakly coupled to the environment, and after setting the classical sources equal to zero, we obtain for the survival probability the expression

$$
\text{Prob}[\langle 0; 0 | 0; t \rangle_E] = \exp \left( -\frac{1}{\hbar^2} \int_0^t d\tau \int_0^t d\tau' \cos [(\omega - \omega_k)(\tau' - \tau)] \right) \tag{27}
$$

For the environment described by an infinite set of degrees of freedom, we replace the sum over $k$ by an integral over the frequency $\omega_k \rightarrow \omega$, and in turn introduce a frequency density $n(\omega')$ to rewrite (27) as

$$
\text{Prob}[\langle 0; 0 | 0; t \rangle_E] = \exp \left( -\frac{1}{\hbar^2} \int_0^\infty d\omega' |\lambda(\omega')|^2 n(\omega') \frac{\sin^2(\omega' - \omega)t}{(\omega' - \omega)^2/4} \right) \tag{28}
$$
Upon introducing the integration variable $x = (\omega' - \omega)t/2$, one may rewrite the integral in (28) as

$$2t \int_{-\infty}^{\infty} dx \left| \lambda(\omega(1 + \frac{x}{\omega t})) \right|^2 n(\omega(1 + \frac{x}{\omega t})) \sin^2 \frac{x}{x^2}$$  \hspace{1cm} (29)$$

If one makes the Markov approximation by assuming that $|\lambda(\omega')|^2 n(\omega')$ is slowly varying around the point $\omega' = \omega$, and hence for $\omega t \gg \pi$, it may be taken outside the integral evaluated at $\omega$, one gets for the integral in (29)

$$2t |\lambda(\omega)|^2 n(\omega) \int_{-\omega t/2}^{\infty} dx \sin^2 \frac{x}{x^2}$$  \hspace{1cm} (30)$$

with increasing accuracy for $\omega t \gg \pi$. And for $\omega t \gg \pi$, we obtain from (28), (30) the familiar exponential law

$$\text{Prob}[(0; 0) \rightarrow (0; t)]_E = e^{-\gamma t}$$  \hspace{1cm} (31)$$

where $\gamma$ is the decay constant $2\pi |\lambda(\omega)|^2 n(\omega) / \hbar^2$. This expression is strictly valid for $\pi/\omega \ll t \ll 1/\gamma$ consistent with the property of the decay of quantum systems and the Paley-Wiener Theorem [cf. 7, §3.5], that the exponential law may be valid for intermediate values of $t$ and not in the truly asymptotic limit $t \rightarrow \infty$.

### 3 Conclusion

A general expression was obtained in (5) for the transition probability of quantum systems when coupled to the environment, and in response to it, involving functional differentiations, with respect to classical sources, using functional calculus techniques. It is important to note that as the functional $F$ in (7) cannot be written as the product of two terms one involving the sources $F_1, S_1, F_2, S_2$, and one involving the sources $F'_1, S'_1, F'_2, S'_2$, one necessarily has to deal directly with transition probabilities of the physical system as it evolves in time in response to the environment rather than amplitudes. In case the amplitudes $\langle b; t | a; 0 \rangle^{F_i, S_i}$ in (5) are not explicitly given for the decoupled physical system from the environment, one may use the integral expression in (2) to carry out various approximations suitable for the system in consideration. The main analysis shows the power of the functional differential treatment, involving functional differentiations with respect to classical, thus commuting, functions. The method developed in this work will be extended to quantum field theories, including gauge theories, in a subsequent report.
References


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