Generalized Feynman-Vernon approach to dissipative quantum systems

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In this paper the so-called Feynman-Vernon influence functional theory has been generalized in order to include the possibility of dealing with initial conditions of the system plus environment other than the factorizable one. It has been shown that the new influence functional can now be written in terms of paths which represent the coupling of quantum-statistical to quantum-dynamical effects. Once the thermal paths are integrated out of this new influence functional, a generalization of the original Feynman-Vernon expression is obtained.

The problem of the quantum dynamics of a dissipative physical system is still an open question in physics.[1] However, among many attempts to settle this issue, there is one which is very satisfactory, namely, the system-plus-reservoir approach. Although this approach does not answer all the fundamental questions related to the main problem it, at least, helps us to solve many practical questions of general interest such as dissipative quantum tunneling[2,3] or dissipative quantum coherence.[4] In particular, the method of applying path integrals to the system-plus-reservoir approach, first proposed by Feynman and Vernon (FV),[5,6] has been very useful in solving the quantum dynamics of a Brownian particle[1] or the dissipative quantum coherence problem.[4]

In the FV approach it is assumed that the system and its environment are decoupled at $t=0$ (factorizable initial condition). This particular choice was modified by Hakim and Ambegaokar[7] when they solved the problem of a free particle coupled to a bath of oscillators. Nevertheless, the method they used exploited the translation invariance of the total Hamiltonian, which cannot be generalized to any system.

Our intention in this short note is to propose a path-integral formulation (in the same spirit as FV) which allows one to use nonfactorizable initial conditions. The model we shall employ is the standard one for dissipative systems (see, for example, Refs. 1 or 4)

$$H = \frac{p^2}{2M} + V(q) + \sum_k C_k q_k q + \sum_k \left(\frac{p_k^2}{2m_k} + \frac{1}{2} m_k \omega_k^2 q_k^2 \right) + \frac{1}{2} \sum_k \frac{C_k^2}{m_k \omega_k^2} q^2 ,$$ (1)

where the set of harmonic oscillators has the spectral function

$$J(\omega) \equiv \frac{\pi}{2} \sum_k \frac{C_k^2}{m_k \omega_k} \delta(\omega - \omega_k) .$$ (2)

Therefore, we can write the reduced density operator of the particle at time t as

$$\tilde{\rho}(x,y,t) = \int d\mathbf{R} \langle x\mathbf{R} | \rho(t) | y\mathbf{R} \rangle = \int \int \int \int \int dx'\,dy'\,d\mathbf{R}'\,d\mathbf{Q}'\,d\mathbf{R}\, K(x,\mathbf{R},t;x',\mathbf{R}',0)$$
$$\times K^*(y,\mathbf{R},t;y',\mathbf{Q}',0) \langle x'\mathbf{R}' | \rho(0) | y'\mathbf{Q}' \rangle ,$$ (3)

where $\mathbf{R}$, $\mathbf{R}'$, and $\mathbf{Q}'$ are general configurations of the bath of oscillators and K is the propagator of the particle-plus-reservoir composite system. In the usual FV approach one takes the last term on the right-hand side of Eq. (3) as $\rho_0^{(S)}(x',y')\rho_{eq}^{(R)}(\mathbf{R}',\mathbf{Q}')$ which results in the traditional FV formalism used in Refs. 1, 5, and 6. We shall consider three different possibilities in this work:

$$\rho_0(x',y';\mathbf{R}',\mathbf{Q}') = \rho_0^{(S)}(x',y')\rho_{eq}^{(RS)}(x',y';\mathbf{R}',\mathbf{Q}') ,$$ (4)

$$\rho_0(x',y';\mathbf{R}',\mathbf{Q}') = \bar{\rho}_{eq}^{(RS)}(x',y';\mathbf{R}',\mathbf{Q}') ,$$ (5)

$$\rho_0(x',y';\mathbf{R}',\mathbf{Q}') = \rho_0^{(S)}(x',y')\bar{\rho}_{eq}^{(RS)}(x',y';\mathbf{R}',\mathbf{Q}') ,$$ (6)

where $\rho_0^{(S)}(x',y')$ is chosen in such a way that $\mathrm{tr}\rho_0 = 1$.

The first initial condition Eq. (4) means that the particle *and* its environment are in equilibrium at $t=0$ and at this same time one performs a position measurement on the particle *only*. The second initial condition represents the particle *and* its environment in equilibrium, but the particle is subject to a potential $V_0(q)$ ($V_0 \neq V$) which is abruptly changed to $V(q)$ at $t=0^+$ (V_0 is the "preparation potential"). Finally, the third initial condition is a combination of Eq. (4) and Eq. (5). Since the latter is the most general of the three cases we shall explicitly deal with it throughout this work (the other two cases can be trivially obtained from the most general result).

From Eq. (3) and Eq. (6) we can write

$$\tilde{\rho}(x,y,t) = \int \int dx'\,dy'\, J(x,y,t;x',y',0) \times \rho_0^{(S)}(x',y') ,$$ (7)

where

$$J = \int\!\!\int_{x'}^{x} \int\!\!\int_{y'}^{y} Dx\, Dy \exp\left[\frac{i}{\hbar} \tilde{S}_A[x] \right] \exp\left[-\frac{i}{\hbar} \tilde{S}_A[y] \right] \times F([x],[y],x',y') ,$$ (8)

$$F = \int\int\int d\mathbf{R}'d\mathbf{Q}'\,d\mathbf{R}\,\bar{\rho}_{eq}^{(RS)}(x',\mathbf{R}';y',\mathbf{Q}')$$
$$\times G([x],[y],\mathbf{R},\mathbf{R}',\mathbf{Q}') \ . \tag{9}$$

and

$$G = \underline{\int\int}_{\mathbf{R}'}^{\mathbf{R}}\,\underline{\int\int}_{\mathbf{Q}'}^{\mathbf{R}}\,D\mathbf{R}\,D\mathbf{Q}\exp\left[\frac{i}{\hbar}(S_I[x,\mathbf{R}]+S_B[\mathbf{R}])\right]$$

$$\times\exp\left[-\frac{i}{\hbar}(S_I[y,\mathbf{Q}]+S_B[\mathbf{Q}])\right] \ . \tag{10}$$

In our notation, variables within brackets are paths connecting the appropriate end points (variables without brackets) and D (variable) is the properly normalized variation of those paths. The functionals $\tilde{S}_A$, S_B, S_I, and $\tilde{S}_0$ are the actions of the particle subject to $V(q)$, the environment, the interaction, and the particle subject to $V_0(q)$, respectively. Notice that we include the counterterm action [the last term in Eq. (1)] into $\tilde{S}_A$ and $\tilde{S}_0$.

As Eq. (10) involves purely Gaussian path integrals it can be easily evaluated (see, for example, Ref. 6) and the result reads

$$G = \prod_{a}\left\{\frac{m_a\omega_a}{2\pi\hbar\sin(\omega_a t)}\exp\left[\frac{i}{\hbar}\frac{m_a\omega_a}{\sin(\omega_a t)}\left[\cos(\omega_a t)\frac{(R_a'^2-Q_a'^2)}{2}-R_a(R_a'-Q_a')\right.\right.\right.$$

$$+\frac{R_a}{m_a\omega_a}\int_0^t C_a[x(t')-y(t')]\sin(\omega_a t')\,dt'$$

$$+\frac{1}{m_a\omega_a}\int_0^t C_a[R_a'x(t')-Q_a'y(t')]\sin[\omega_a(t-t')]\,dt'$$

$$\left.\left.\left.-\frac{C_a^2}{m_a^2\omega_a^2}\int_0^t d\tau\int_0^\tau d\sigma[x(\tau)x(\sigma)-y(\tau)y(\sigma)]\sin[\omega_a(t-\tau)]\sin(\omega_a\sigma)\right]\right]\right\} \ . \tag{11}$$

On the other hand, the equilibrium density operator has the following path integral representation[8]

$$\bar{\rho}_{eq}^{(RS)}(x',\mathbf{R}';y',\mathbf{Q}') = \underline{\int\int}_{y'}^{x'}Dz\exp\left[-\frac{1}{\hbar}\tilde{S}_0^{(E)}[z]\right]\tilde{G}(\mathbf{R}',\mathbf{Q}',[z]) \ , \tag{12}$$

where

$$\tilde{G}(\mathbf{R}',\mathbf{Q}',[z]) = \prod_{a}\underline{\int\int}_{Q_a'}^{R_a'}D\tilde{R}_a\exp\left[-\frac{1}{\hbar}(S_I^{(E)}[z,\tilde{R}_a]+S_B^{(E)}[\tilde{R}_a])\right] \ , \tag{13}$$

and $S^{(E)}$ is the Euclidean version of the corresponding action which means that we must replace all the potentials (including the interaction) by minus its value. $\tilde{G}$ also involves only Gaussian integrals which can be easily evaluated[8] as $(U\equiv\hbar\beta)$

$$\tilde{G} = \prod_{a}\left[\frac{m_a\omega_a}{2\pi\hbar\sinh(\omega_a U)}\exp\left[\frac{C_a^2}{4hm_a\omega_a}\int_0^U\int_0^U\exp(-\omega_a|u-u'|)z(u)z(u')\,du\,du'\right]\right.$$

$$\times\exp\left[-\frac{m_a\omega_a}{2\hbar\sinh(\omega_a U)}[(R_a'^2+Q_a'^2)\cosh(\omega_a U)-2R_a'Q_a'+2B_a(R_a'e^{\omega_a U}-Q_a')\right.$$

$$\left.\left.+2A_a(Q_a'e^{\omega_a U}-R_a')+(A_a^2+B_a^2)e^{\omega_a U}-2A_aB_a]\right]\right] \ , \tag{14}$$

where

$$A_a\equiv\frac{C_a}{2m_a\omega_a}\int_0^U e^{-\omega_a u}z(u)\,du \ , \tag{15}$$

$$B_a\equiv\frac{C_a}{2m_a\omega_a}\int_0^U e^{-\omega_a(U-u)}z(u)\,du \ . \tag{16}$$

Now, substituting Eqs. (14), (12), and (11) into Eq. (9) and integrating over $\mathbf{R}'$, $\mathbf{Q}'$ and $\mathbf{R}$ [integrate first over R_a and then define new variables of integration $\zeta_a'\equiv R_a'-Q_a'$ and $X_a'\equiv(R_a'+Q_a')/2$ to make things simpler] one finally obtains

$$F([x],[y],x',y') = \mathcal{F}[x,y] \int\!\!\!\int_{y'}^{x'} Dz \exp\left[-\frac{1}{\hbar}S_0^{(E)}[z]\right]$$

$$\times \prod_a \left[\frac{\text{csch}(\omega_a U/2)}{2} \exp\left[\frac{C_a}{4m_a\omega_a\hbar}\int_{-\infty}^{\infty}du\int_0^U du'\exp[-\omega_a|u-u'|]z(u)z(u')\right]\right.$$

$$\times \exp\left[-\frac{C_a(A_a-B_a)e^{\omega_a U/2}}{2\hbar\sinh(\omega_a U/2)}\int_0^t [x(t')-y(t')]\sin(\omega_a t')dt'\right.$$

$$\left.\left.+i\frac{C_a(A_a+B_a)e^{\omega_a U/2}}{2\hbar\sinh(\omega_a U/2)}\int_0^t [x(t')-y(t')]\cos(\omega_a t')]dt'\right]\right],$$

(17)

where $\mathcal{F}[x,y]$ is the original influence functional as obtained by FV. Using Eqs. (2), (15), and (16) and completing squares of the exponent involving $z(u)z(u')$, Eq. (17) reduces to

$$F([x],[y],x',y') = \mathcal{F}[x,y] \int\!\!\!\int_{y'}^{x'} Dz \exp\left[-\frac{1}{\hbar}S_0^{(E)}[z]\right]$$

$$\times \exp\left[\frac{1}{4\pi\hbar}\int_0^U du\int_{-\infty}^{\infty}du'\int_0^{\infty} d\omega J(\omega)\exp(-\omega|u-u'|)[z(u)-z(u')]^2\right]$$

$$\times \exp\left[\frac{1}{\pi\hbar}\int_0^U z(u)f(u)du\right],$$

(18)

where

$$f(u) = \int_0^t dt'[x(t')-y(t')]\int_0^{\infty} d\omega J(\omega)\sin(\omega t')[\coth(\omega U/2)\sinh(\omega u)-\cosh(\omega u)]$$

$$+i\int_0^t dt'[x(t')-y(t')]\int_0^{\infty} d\omega J(\omega)\cos(\omega t')[\coth(\omega U/2)\cosh(\omega u)-\sinh(\omega u)],$$

(19)

and $S_0^{(E)}[z]$ contains no contribution due to the counterterm action. Actually there also appear terms in $\mathcal{F}[x,y]$ which naturally cancel the counterterm actions in $\tilde{S}_A[x]$ and $\tilde{S}_A[y]$ in (8) (see, for example, Ref. 1). Notice that since the product $\prod_a \text{csch}(\omega_a U/2)$ is only a multiplicative factor we shall include it in an overall normalization constant for expression (7).

Expression (18) shows us that the generalized FV influence functional can be obtained by multiplying the original one by a functional integral over a thermal path which describes the equilibrium of the particle (subject to the preparation potential), with its environment. As one can easily see, the dynamics of the particle at $t > 0$ is influenced by this equilibrium state through the "force" $f(u)$ which is a functional of $x(t')$ and $y(t')$ and a function of the thermal parameter u.

Notice that expression (18) is solely written in terms of

path integrals, therefore making no use of specific symmetries of the composite system as in Ref. 7.

In conclusion, we have been able to generalize the FV theory for different choices of initial conditions only in terms of functional integrals. Although the evaluation of the integral over paths $z(u)$ [see Eq. (18)] might not be an easy task for general potentials, we believe this form for F is very useful once one decides to solve the dynamical problem within a given approximation, such as the semiclassical limit. A more extensive work containing applications of Eqs. (18) and (19) is in preparation.

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