DENSITY MATRIX : DYNAMICS

When one uses a wave-function or "state vector" formulation of quantum mechanics, it is very useful to formulate the theory in terms of the propagator of the wave-function, the Green function operator $\hat{G}(2,1)$. The dynamics of a quantum system can then be entirely formulated in terms of $G(2,1)$. The propagator is most conveniently defined either (i) as the Green fn. of the Schrodinger eqtn., or (ii) diagrammatically, or (iii) using a path integral.

In the same way one can set up the more general formulation of QM in terms of density matrices, whose dynamics is actually given by a 2-particle propagator. This propagator $K(22',11')$ thus, in a certain sense, contains all possible information about the system dynamics. In the same way one can describe the dynamics of the reduced density matrix by a propagator $\bar{K}(22',11')$.

(1) PROPAGATORS FOR ρ AND $\bar{\rho}$

We briefly recall the propagator formalism for single particle propagation. Consider a quantum system with Hamiltonian $\mathcal{H} = \mathcal{H}_0 + V$, and suppose we know the eigenstates $|n\rangle \equiv |\psi_n\rangle$ of $\mathcal{H}_0$, so that

$$(\mathcal{H}_0 - \epsilon_n^0)\,|n\rangle = 0 \tag{1}$$

and so

$$\psi_n(t_2) = e^{-i/\hbar\,\epsilon_n^0(t_2-t_1)}\,\psi_n(t_1) \tag{2}$$

We define the unperturbed propagator $G_0(\rho_2\rho_1; t_2t_1)$ for the Hamiltonian $\mathcal{H}_0$ in terms of the operator $G_0(t_2t_1)$ by

$$G_0(\rho_2\rho_1; t_2t_1) = \langle \rho_2 |\, G_0(t_2t_1)\,| \rho_1 \rangle \tag{3}$$

where $\hat{G}_0$ is defined by (here $\hat{1}$ is the unit operator):

$$(\hat{\mathcal{H}}_0 - i\hbar\hat{\partial}_t)\,\hat{G}_0(t,t') = -i\hbar\,\delta(t-t')\,\hat{1} \tag{4}$$

so that

$$(\hat{\mathcal{H}}_0 - i\hbar\hat{\partial}_{t_2})\,G_0(\rho_2\rho_1; t_2t_1) = -i\hbar\,\delta(t_2-t_1)\,\delta(\rho_2-\rho_1) \tag{5}$$

In the basis of the eigenstates of $\mathcal{H}_0$, G_0 is diagonal:

$$\hat{G}_0(t_2t_1) = \sum_n |n\rangle\, e^{-i/\hbar\,\epsilon_n^0(t_2-t_1)}\,\langle n| \tag{6}$$

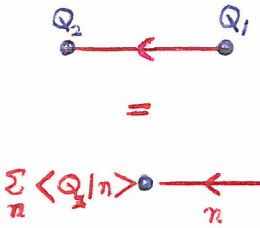
and hence we have

$$G_0(\rho_2\rho_1; t_2t_1) = \sum_n \psi_n^*(\rho_2)\,\psi_n(\rho_1)\,e^{i/\hbar\,\epsilon_n^0(t_2-t_1)} \tag{7}$$

We can Fourier transform these results in time, to get

$$\left.\begin{aligned} \hat{G}_0(\omega) &= \int_0^\infty dt\, \hat{G}_0(t)\, e^{i\omega t} \equiv \int_0^\infty dt\, e^{i(\omega - \hat{H}_0/\hbar)t} \\ &= \frac{i\hbar}{\hbar\omega - \hat{\mathcal{H}}_0} \end{aligned}\right\} \qquad (8)$$

so that we also have



$$\left.\begin{aligned} G_0(Q_2 Q_1; \omega) &= i\hbar \sum_n \frac{\psi_n^*(Q_2)\,\psi_n(Q_1)}{\hbar\omega - \epsilon_n^0} \\ &\equiv \sum_n \langle Q_2|n\rangle\, G^0_{nn}(\omega)\, \langle n|Q_1\rangle \end{aligned}\right\} \qquad (9)$$

shown diagrammatically at left.

We can write similar eqtns for the full operator $\mathcal{H} = \mathcal{H}_0 + V$, in terms of its eigenfunctions; or we can write a perturbative expansion for the Green fn $\mathcal{G}$ of this operator, in terms of the ϕ_n; we do not go into this here.

Finally, we recall that $\hat{G}_0$ and $\hat{\mathcal{G}}$ can be written as path integrals. We have

$$G_0(Q_2 Q_1; t_2 t_1) = \int_{q(t_1)=Q_1}^{q(t_2)=Q_2} \mathcal{D}q(\tau)\; e^{\frac{i}{\hbar} S_0[q,\dot{q}]} \qquad (10)$$

for the free particle, and

$$\mathcal{G}(Q_2 Q_1; t_2 t_1) = \int_{q(t_1)=Q_1}^{q(t_2)=Q_2} \mathcal{D}q(t)\; e^{\frac{i}{\hbar} S[q,\dot{q}]} \qquad (11)$$

where $S_0 = \int_{t_1}^{t} d\tau\, L_0(q\dot{q})$ is the free particle action, and

$$S[q,\dot{q}] = \int_t^t d\tau \left[L_0(q,\dot{q}) - V(q,\dot{q},\tau)\right] \qquad (12)$$

is the full action.

1(a) PROPAGATORS for $\hat{\rho}$

: The density matrix is just a particular kind of 2-particle Green function. We do not develop the full theory of these here. The theory is particularly simple in path integral language.

We recall that for a single quantum system, the density matrix operator is defined by

$$\hat{\rho} = |\alpha\rangle p_\alpha \langle\alpha| \qquad (13)$$

where the basis set $\{|\alpha\rangle\}$ diagonalizes $\hat{\rho}$, and p_α are the probabilities of occupation of states $|\alpha\rangle$. In some arbitrary basis $\{|i\rangle\} \equiv \{|\psi_i\rangle\}$, the density operator $\hat{\rho}$ has matrix elements

$$\rho_{ij} = \langle i|\hat{\rho}|j\rangle = \langle i|\alpha\rangle p_\alpha \langle\alpha|j\rangle \tag{14}$$

where we use from now on the summation convention. For a pure state $|\Psi\rangle$, with $|\Psi\rangle = \sum_j c_j |\psi_j\rangle$, we have

$$\left.\begin{aligned} \hat{\rho} &= |\Psi\rangle\langle\Psi| = \sum_{ij} |i\rangle \rho_{ij} \langle j| \\ \text{with} \quad \rho_{ij} &= c_i c_j^* \end{aligned}\right\} \quad (\text{PURE}) \tag{15}$$

A pure state can always be differentiated from a mixed state, since

$$\left.\begin{aligned} \mathrm{Tr}[\hat{\rho}^2] &= \mathrm{Tr}\,\hat{\rho} = 1 \qquad (\text{PURE}) \\ \mathrm{Tr}[\hat{\rho}^2] &< \mathrm{Tr}\,\hat{\rho} = 1 \qquad (\text{MIXED}) \end{aligned}\right\} \tag{16}$$

(1) FREE PARTICLE PROPAGATOR $\hat{K}_0$: Consider again a Hamiltonian $\mathcal{H}_0$, which we now assume to describe non-interacting particles with some energy dispersion ϵ_i^0 (this could, e.g., describe particles moving in some lattice or even a random potential). Thus we assume eqns (1) - (11) are valid for this system.

The propagator for the density matrix $\hat{\rho}_0$ for this system is then defined by

$$\hat{\rho}_0(t_2) = K_0(t_2, t_1)\,\hat{\rho}_0(t_1) \tag{17}$$

or, taking matrix elements between some set of states $|i\rangle, |j\rangle$ (which are NOT necessarily eigenstates of the system), we have

$$\rho^0_{jj'}(t_2) = K^0_{jj'ii'}(t_2, t_1)\,\rho^0_{ii'}(t_1) \tag{18}$$

In the basis of states $|n\rangle, |m\rangle$ (see (1), (2), (6)) in which the Hamiltonian $\mathcal{H}_0$ and G_0 are diagonal, so is K_0:

$$\hat{K}_0(t_2, t_1) = \sum_{nm} |nm\rangle\, e^{-\frac{i}{\hbar}(\epsilon_n - \epsilon_m)(t_2 - t_1)} \langle nm| \tag{19}$$

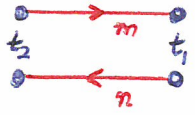
and thus K_0 satisfies a modified Schrodinger eqtn:

$$\left[(\hat{\mathcal{H}}_0 - \hat{\mathcal{H}}_0'^{*}) - i\hbar\partial_{t_2}\hat{\mathbb{1}}\right]\hat{K}_0(t_2, t_1) = -i\hbar\,\delta(t_2 - t_1)\,\hat{\mathbb{1}} \tag{20}$$

where the meaning of this operator eqtn becomes clearer if we turn it into a matrix equation, by sandwiching it between a set of states (PTO):

$$[(\mathcal{H}_0 - \mathcal{H}_0'^{*}) - i\hbar\partial_{t_2}]\, K^0_{JJ',ll'}(t_2-t_1) = -i\hbar\,\delta_{ij}\,\delta_{i'j'}\,\delta(t_2-t_1) \tag{21}$$

It is useful to show these relations diagrammatically, and to also specialize to the real space basis. Consider first the propagator in the eigenstate basis:



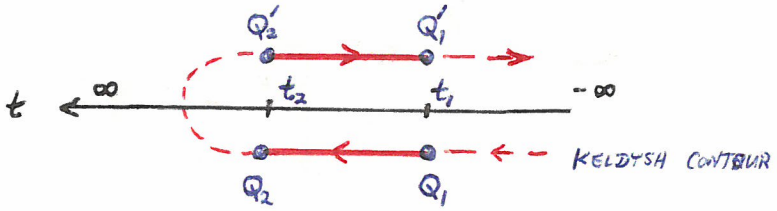
$K^0_{nm,nm}(t_2,t_1)$

$$\langle nm|K^0(t_2-t_1)|n'm'\rangle = \delta_{nn'}\,\delta_{mm'}\,e^{-\frac{i}{\hbar}(\epsilon_n^0-\epsilon_m^0)(t_2-t_1)} \tag{22}$$

which is necessarily diagonal. However in the real state representation, where we go over to states $|Q\rangle$, and to wave functions $\psi_n(Q) = \langle Q|n\rangle$, we have the diagrammatic forms (compare eqtn. (9)):

$$= K^0(Q_2Q_2'Q_1Q_1';t_2t_1) \tag{23}$$

Careful note should be paid to the directions of the arrows here. An alternative representation of this graph is



(24)

where the path is now a continuous single one, which we imagine to be continued out to $t = \infty$ before returning - this is a Keldysh contour.

From these graphs we can read off the expressions

$$K_0(Q_2Q_2';Q_1Q_1';t_2t_1) = \sum_{nm} \psi_n(Q_2)\psi_n^*(Q_1)\psi_m(Q_1')\psi_m^*(Q_2') \times e^{-\frac{i}{\hbar}\epsilon_n^0(t_2-t_1)}\, e^{\frac{i}{\hbar}\epsilon_m^0(t_2-t_1)} \tag{25}$$

or the Fourier transformed version

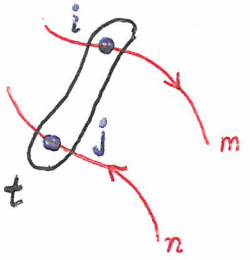
$$K_0(Q_2Q_2';Q_1Q_1';\omega) = i\hbar\sum_{nm} \frac{\psi_n(Q_2)\psi_n^*(Q_1)\psi_m^*(Q_2')\psi_m(Q_1')}{\hbar\omega - \epsilon_n^0 + \epsilon_m^0} \tag{26}$$

where again we notice the relative sign of the 2 energies.

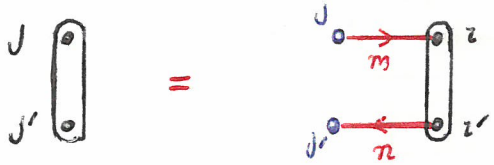
We note that this diagrammatic representation can also be extended to the density matrix itself. Consider that at time t, the density matrix is given by

$$\left.\begin{aligned} \rho^0_{ij}(t) &= \sum_{nm} \langle i|m(t)\rangle \rho_{nm} \langle n(t)|j\rangle \\ &\equiv \sum_{nm} \rho^0_{nm}\ \psi_n(j)\,\psi^*_m(i)\, e^{-\frac{i}{\hbar}(\epsilon^0_n - \epsilon^0_m)t} \end{aligned}\right\} \qquad (27)$$

But in diagrammatic terms, this instantaneous form for ρ_0 is simply a "snapshot" of the propagator K_0 at time t, as shown in the propagator diagram at left (the 2 red lines represent the propagator, and the 2 points on the lines represent the 2 states $|i\rangle$ and $|j\rangle$ upon which the density matrix is projected at time t).



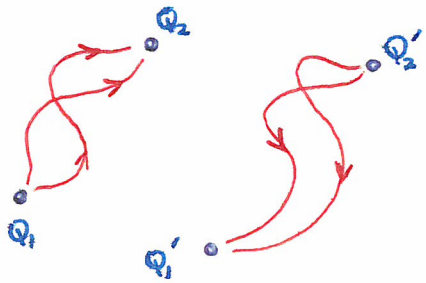
In this representation of the density matrix and propagator, we can represent the eqtn of motion for the density matrix, given in its integral form in eqtns (17) and (18), by the diagrammatic form:



(28)

Finally, we note that the density matrix propagator for the free system can be written in path integral form, using now a real state representation. One simply has

$$K_0(Q_2Q_2'Q_1Q_1';t_2t_1) = \int_{q(t_1)=Q_1}^{q(t_2)=Q_2} Dq(\tau) \int_{q'(t_1)=Q_1'}^{q'(t_2)=Q_2'} Dq'(\tau)\, e^{\frac{i}{\hbar}\{S_0[q,\dot q] - S_0[q',\dot q']\}} \qquad (29)$$



which is represented diagrammatically at left (where we now show Feynman paths in real space). Note the directions of the arrows in this representation. These do NOT show how time propagates in these expressions - instead they show the direction in which phase propagates.

The path integral formalism can be developed starting from (29), to give an alternative derivation of the results (19)-(26). Since the particles are not

interacting, this development is precisely analogous to the way one would find the same expression for the 1-particle propagator - we do not continue this development here.

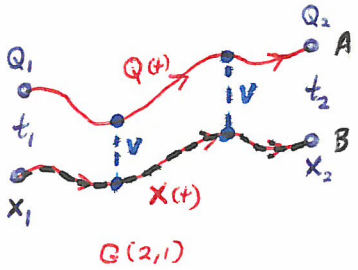
(ii) **PROPAGATOR FOR 2 INTERACTING SYSTEMS**: The case of 2 non-interacting systems is trivial (we just double up the variables, to have new collective coordinates $\underline{R} \equiv (X, Y)$, where X and Y are the coordinates of the individual systems, and consider single paths in $(\underline{R}, \dot{\underline{R}})$ space).

However if there are interactions between the 2 systems, we must be more careful. We consider 2 possible scenarios here:

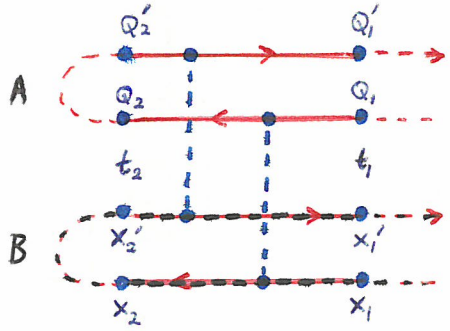
(a) **DIRECT INTERACTION BETWEEN 2 SYSTEMS**: In this scenario, we have 2 systems, with 2 separate coordinates Q and X, and a direct interaction between them - this scenario is encapsulated in the Hamiltonian

$$\mathcal{H}(Q,X) = \mathcal{H}_A(Q) + \mathcal{H}_B(X) + V_{AB}(Q,X) \tag{30}$$

This Hamiltonian is only consistent if it is assumed that the interaction $V(Q,X)$ is instantaneous - any retardation effects would imply that the interaction should be treated as a consequence of the coupling of the 2 systems to a background quantum field (see below).



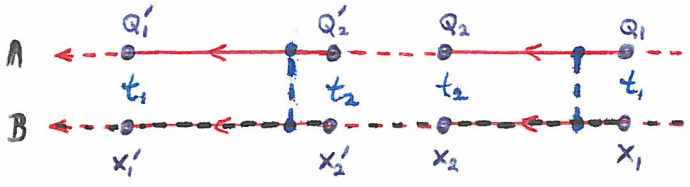
G(2,1)



$K(22', 11')$ (31)

Above left we see a diagram for a Green function $G(2,1)$ for the combined system; and at right a diagram for the propagator $K(22', 11')$ of the density matrix. The interaction lines are vertical because they act instantaneously.

It is actually convenient to display the graph for the density matrix propagator, shown above right, in a slightly different form, in which the Keldysh lines are "unfolded" to form single long lines - this makes the diagram easier to display (see left).



$K(22', 11')$

We can most conveniently write the expressions for this propagator in path integral language. The action for the double system, following a path $(Q(\tau), X(\tau))$, is given by

$$S_T[Q,X] = S_0^A[Q] + S_0^B[X] + S_{int}^{AB}[Q,X] \tag{32}$$

and the density matrix propagator is given by

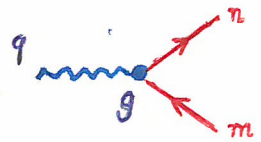
$$K(22',11') = \int_{Q_1}^{Q_1} \mathcal{D}q(\tau) \int_{Q_1'}^{Q_2'} \mathcal{D}q'(\tau) \int_{X_1}^{X_2} \mathcal{D}X(\tau) \int_{X_1'}^{X_2'} \mathcal{D}X'(\tau)\, e^{\frac{i}{\hbar}\left(S_T[q,x] - S_T[q'x']\right)} \tag{33}$$

By expanding the interaction term $(S_{int}^{AB}[q,x] - S_{int}^{AB}[q'x'])$ in the exponential, we recover all possible diagrams for the density matrix propagator, to infinite order in $V_{AB}(q,x)$.

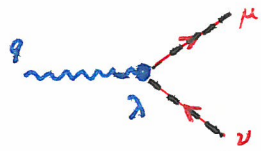
(b) <u>FIELD-MEDIATED INTERACTION BETWEEN 2 SYSTEMS</u> : All interactions are of course mediated by some external field. Thus the true theory underlying the Hamiltonian in (30) will have a Hamiltonian

$$S_T[Q,X;\phi_q] = S_0^A[Q] + S_0^B[X] + S_0^\phi[\phi_q] + S_{int}^T[Q,X;\phi_q] \tag{34}$$

where ϕ_q is the external field (already resolved into its "normal modes", labelled by the index q), and S_{int} describes the interaction between the external field and each of the 2 systems. Typically these interactions will look like:



$$S_{int}^A[Q,\phi_q] = -\int d\tau \sum_q \sum_{nm} \left[g_q(n,m)\, \phi_q\, \psi_n\, \psi_m^\dagger + \text{H.c.} \right] \tag{35}$$



$$S_{int}^B[X,\phi_q] = -\int d\tau \sum_q \sum_{\mu\nu} \left[\lambda_q(\mu,\nu)\, \phi_q\, \chi_\mu\, \chi_\nu^\dagger + \text{H.c.} \right] \tag{36}$$

so that

$$S_{int}^T[Q,X;\phi_q] = S_{int}^A[Q,\phi_q] + S_{int}^B[X,\phi_q] \tag{37}$$

Here we have introduced a set of eigenstates $|\chi_\mu\rangle$ for system B, such that

$$[\mathcal{H}_0^B - \varepsilon_\mu^0]\, \chi_\mu = 0 \tag{38}$$

and a pair of interaction matrix elements $g_q(n,m)$ (between states $|n\rangle$ and $|m\rangle$ of system A, mediated by ϕ_q) and $\lambda_q(\mu\nu)$ (between states $|\mu\rangle \equiv |\chi_\mu\rangle$ and $|\nu\rangle = |\chi_\nu\rangle$ of system B).

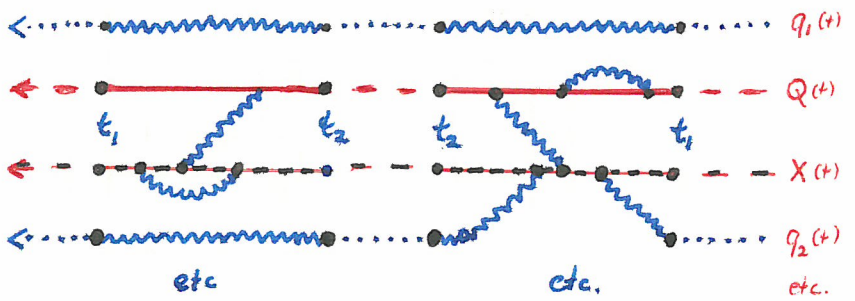
With these interactions one writes a propagator $K(22',11')$ for a density matrix ρ which now describes the simultaneous propagation of Q, X, and the set of $\{\phi_q\}$ (we will assume $q = 1, 2, \ldots N_B$), i.e.,

$$\hat{\rho} = \prod_q \hat{\rho}_q = \prod_q |n\mu q_\alpha\rangle \rho_{n\mu q_\alpha, m\nu q_\beta} \langle m\nu q_\beta| \tag{39}$$

where the different states of each mode ϕ_q of the external field are labelled by α, β. The propagator for ρ then takes the form

$$\left.\begin{aligned} K(22',11') = \int \mathcal{D}q(\tau) \int \mathcal{D}q'(\tau) \int \mathcal{D}x(\tau) \int \mathcal{D}x'(\tau) \prod_{q=1}^{N_B} \int \mathcal{D}\phi_q(\tau) \int \mathcal{D}\phi_q'(\tau) \\ \times \exp\left\{\tfrac{i}{\hbar}\left(S_\tau[q,x;\phi_q] - S_\tau[q',x';\phi_q']\right)\right\} \end{aligned}\right\} \tag{40}$$

and the expansion of the exponential then generates many diagrams - we show here one typical example (in Keldysh form):



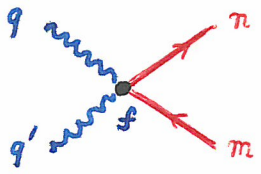
(41)

Note that in this propagator there will be N_B lines for ϕ_q that enter the graph to the right, and leave on the left. Many of the ϕ_q quanta will interact with either $Q(t)$ or $X(t)$ on the way, but the number entering and leaving will be conserved. The ϕ_q will also mediate interactions between the $Q(t)$ and $X(t)$ lines (and these interactions will now in general be <u>retarded</u>), as well as self-interactions for both systems A and B.

Two points are of special interest here. The first concerns the nature of the ϕ_q. The typical assumption in relativistic QFT is that the ϕ_q are the normal or "free field" modes of some bosonic field. However as we shall see, whenever we have to deal with real condensed matter systems, one also has to deal with "spin both" variables, which behave quite

differently from the oscillator modes of a bosonic field.

Notice also, in this context, that the assumption in (35) and (36) of linear interactions (linear in the $\{\phi_q\}$) is also not completely general. One must also have higher order interactions - an example is:



$$\delta S^A_{int}[\Phi,\phi_q] = -\int dt \sum_{qq'} \sum_{nm} \varepsilon [f_{qq',(n,m)}\, \phi_q \phi_{q'} \psi_n \psi^*_m + H.c.] \qquad (42)$$

Such higher-order interactions are non-linear in the "environmental" external field variables. They can be important in various circumstances; for example:

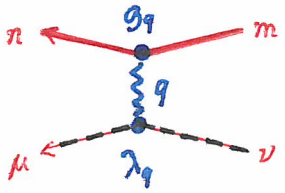
- when the couplings $g_q(n,m)$ and/or $\lambda_q(\mu,\nu)$ are small or zero (they can vanish by symmetry - or, if the coordinates Φ or X describe solitons, they have to be zero).
- The field ϕ_q is highly excited, with a large population of (quasi)particles (eg., a high-T thermal state).
- The field ϕ_q describes a spin bath, where the higher-order couplings may just as important as the 1st-order coupling.

The 2nd point here concerns the relationship between theories with a direct interaction, of form (30), and the interacting field theories by (34) - (37) and (42). Quite generally in physics, a theory with an instantaneous model interaction $V_{AB}(\Phi,X)$ like that in (30) is the result of integrating out the field modes ϕ_q, and the excited states of the systems A and B, above some UV cutoff Λ_0. This process of truncation of the high-energy field Hamiltonian to the low-energy model Hamiltonian (30), with the resulting V_{AB}, is nothing but the standard renormalization procedure of QFT. It is equivalent to a coarse-graining at time, so that all time intervals $t < t_0$, where

$$t_0 = \hbar/\Lambda_0 \qquad (43)$$

are treated as instantaneous. Thus if the timescale of interactions between A and B is $< t_0$, we can make this truncation. To see how this works, we consider how this truncation works for the interactions g_q in . Formally this is accomplished by expanding the exponential in (40), then Fourier transforming the path integrals to convert them to sums over frequency/momentum components, & then carrying out the sums for all frequencies

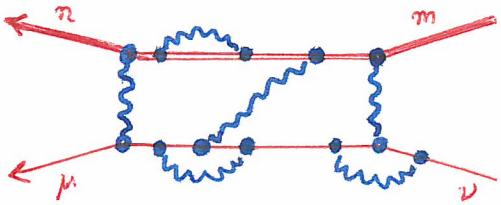
ω_ℓ such that $\omega_\ell > \Lambda_0/\hbar$. The lowest order term in g_ℓ, λ_ℓ that is generated by this is:



$$V_{int}^{nm,\mu\nu}(\Lambda_0) = \sum_q \left[g_q(n,m)\lambda_q(\mu\nu)\, D_q(\omega_q)\, \theta(\omega_q - \Lambda_0) + H.c. \right] \qquad (44)$$

where $D_q(\omega)$ is the propagator of the environmental field. The characteristic frequency scale of this interaction vertex is Λ_0, so that on time scales $\gg t_0$, it can be treated as a constant.

Note, however, that there will be higher order contributions to V_{int}; an example is shown at left. It can happen that such diagrams introduce a new, lower energy scale $\ll \Lambda_0$. This will happen in particular if the system is near an instability (near a 2nd-order phase transition and/or a quantum phase transition, this new frequency scale $\delta\omega_0$ will actually go to zero).



In any case, the final effective interaction $V_{AB}(\Phi, X)$ in (30) is defined by the sum of all terms generated by the exponential in (41). The Hamiltonian (30) is only valid for energy scales $< \delta\omega_0$, where $\delta\omega_0$ is the frequency scale defined by the sum of terms generated by (41). Only under these circumstances can one use (30).

We also note that the theory still contains all the field excitations with energies $< \Lambda_0$; to be consistent these should also be added to (30).

A proper discussion of all of this requires much more than we are saying here.

1(b) PROPAGATOR for REDUCED DENSITY MATRIX $\bar{\rho}$

As we have just seen, any effective theory (and ALL Hamiltonians are effective Hamiltonians) must have already integrated out / averaged over a set of high-energy degrees of freedom, above some UV cut-off.

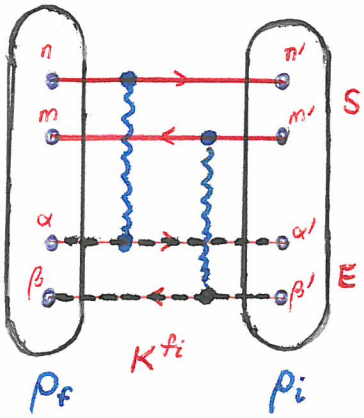
From this point of view we must inevitably deal with reduced density matrices.

Let us begin with an extended quantum system, described by variables Φ, X, where we assume that Φ is the collective coordinate of interest, and X is the "rest of the universe", which we call the "environment". Typically $X = \{x_q\}$, with $q = 1, 2, \ldots N_E$.

We write elements of the total density matrix between states $|n\rangle, |m\rangle$, etc, of the system S, and states $|\alpha\rangle, |\beta\rangle$, etc., of the environment E.

Then the equation of motion of the density matrix is written as

$$\rho^f_{\eta m;\alpha\beta}(22') = \sum_{n'm'}\sum_{\alpha'\beta'} K^{fi}_{nmn'm';\alpha\beta\alpha'\beta'}(22'11')\,\rho_{n'm';\alpha'\beta'}(11') \qquad (45)$$



or, more succinctly

$$\rho^f_{nm\alpha\beta} = K^{fi}_{nm\alpha\beta\, n'm'\alpha'\beta'}\,\rho_{n'm'\alpha'\beta'} \qquad (46)$$

Now we wish to trace over the environmental variables in this equation. This certainly means we must trace over all final states in the environment, with some weighting factor. However, there is no particular reason we have to trace over the initial states - everything depends on how the pair of systems were initially prepared. Consider the following possibilities:

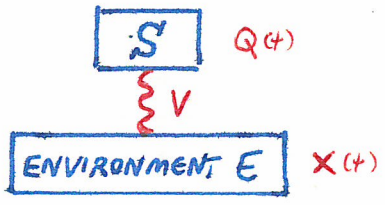
(i) S and E are completely uncorrelated at t_1, and both in pure states.

(ii) S and E are initially uncorrelated at t_1, but E is in a thermal density matrix state.

(iii) S and E are initially correlated in a "Cat" state (which is not an eigenstate of $S+E$).

and so on. In case (ii) we might have to assume some sort of trace over E, depending on how the initial environmental state was set up.

In what follows we will assume, for the most part, that the two systems S and E are initially uncorrelated, and that the final trace over the environmental states is accomplished in a straightforward way, as described below. This assumption is made for expository simplicity only. Then we define the reduced density matrix $\bar\rho$ by taking the trace over the final states of the environmental variables; ie.:



$$\bar\rho_{nm}(t) = Tr_\mu\,\rho_{nm;\mu\mu}(t) \qquad (47)$$

so that, from (46)

$$\bar\rho^f_{nm}(t_2) = Tr_\mu\,\rho^f_{nm;\mu\mu}(t_2)$$

$$= \sum_\mu K_{nm\mu\mu;\,n'm'\alpha\beta}\,\rho^i_{n'm'\alpha\beta}(t_1) \qquad (48)$$

We can therefore define a propagator $\bar{K}$ for the reduced density matrix, of form

$$\bar{K}_{nn:n'm'\alpha\beta}(t_2,t_1) = Tr_\mu K_{nn\mu\mu:n'm'\alpha\beta}(t_2,t_1) \tag{49}$$

There are a number of other useful ways of defining the propagator for the reduced density matrix. One of the most transparent is in the form of a path integral. Consider first the reduced density matrix defined between position eigenstates. By taking the trace over (33), we have

$$\left.\begin{aligned}\bar{K}(22,11') &= \int dx_f \int_{x_1}^{x_f}\mathcal{D}x(\tau)\int_{x_1'}^{x_f}\mathcal{D}x'(\tau)\int_{q_1}^{q_2}\mathcal{D}q(\tau)\int_{q_1'}^{q_2'}\mathcal{D}q'(\tau)\, e^{i/\hbar(S_T[q,x]-S_T[q'x'])} \\ &\equiv \int_{q_1}^{q_2}\mathcal{D}q(\tau)\int_{q_1'}^{q_2'}\mathcal{D}q'(\tau)\,\mathcal{F}_{x_1x_1'}[q,q']\, e^{i/\hbar(S_0[q]-S[q'])}\end{aligned}\right\} \tag{50}$$

where in the first expression we assume a final state $X_f(t_2)$ for the environmental state, and $\int dx_f$ is over all possible values of x_f. The functional $\mathcal{F}$ in (50) is thus given by (cf. (32)):

$$\mathcal{F}_{x_1x_1'}[q,q'] = \int dx_f \int_{x_1}^{x_f}\mathcal{D}x(\tau)\int_{x_1'}^{x_f}\mathcal{D}x'(\tau)\, e^{i/\hbar(S_0^E[x]+S_{int}[x,q]-S_0^E[x']-S_{int}[x',q'])} \tag{51}$$

and in the next sub-section we will study its properties.

(i) PROPERTIES OF THE INFLUENCE FUNCTIONAL

: Let's first put the influence functional in a more general form, not restricted to position eigenstates. We write

$$\mathcal{F}_{\alpha\beta}[qq'] = \sum_\mu \int_\alpha^\mu \mathcal{D}x \int_\beta^\mu \mathcal{D}x'\; e^{i/\hbar(S_0^E[x]+S_{int}[q,x]-S_0^E[x']-S_{int}[q'x'])} \tag{52}$$

so that

$$\bar{K}_{nn:n'm'\alpha\beta} = \int_{n'}^{n}\mathcal{D}q \int_{m'}^{m}\mathcal{D}q'\;\mathcal{F}_{\alpha\beta}[q,q']\, e^{i/\hbar(S_0[q]-S_0[q'])} \tag{53}$$

where the notations $\int_\alpha^\mu \mathcal{D}x(\tau)$ and $\int_{n'}^{n}\mathcal{D}q(\tau)$ are both shorthands (PTO):

$$\left.\begin{aligned} \int_{\alpha}^{\mu} \mathcal{D}x(\tau) &\equiv \langle \mu | x_f \rangle \int_{x_i}^{x_f} \mathcal{D}x(\tau)\, \langle x_i | \alpha \rangle \\ \int_{n'}^{n} \mathcal{D}q(\tau) &\equiv \langle n | Q_2 \rangle \int_{Q_1}^{Q_2} \mathcal{D}q(\tau)\, \langle Q_1 | n' \rangle \end{aligned}\right\} \text{ summation convention} \qquad (54)$$

where, as indicated, we must integrate over x_f, x_i, Q_2, and Q_1 in these expressions.

Another very illuminating way of writing the influence functional can be deduced from these results. Suppose we define the unitary operator $U^E_{x_i}[q]$ acting on the environmental variables X, assuming that the initial state of the environment is X_i, and that the system we are interested in follows a path $q(\tau)$. Under these circumstances the final state of the environment is determined - we have

$$|X_f(t_2)\rangle = \hat{U}^E_{x_i}([q(\tau)]; t_2, t_1)\, |X_i(t_i)\rangle \qquad (55)$$

But then we can write the influence functional very simply as

$$\left.\begin{aligned} \mathcal{F}_{x_i x_i'}[q,q'] &= \langle \hat{U}^E_{x_i}[q]\, \hat{U}^{E\,\dagger}_{x_i'}[q'] \rangle_E \\ &\equiv Tr_E \left\{ U^E_{x_i}[q(\tau); t_2, t_1]\, U^{E\,\dagger}_{x_i'}[q(\tau); t_2 t_i] \right\} \end{aligned}\right\} \qquad (56)$$

The physical interpretation of (50) and (53), or (56), is fairly clear. The influence functional $\mathcal{F}[q,q']$ is a WEIGHTING FACTOR, defined over the pair of paths $q(\tau)$, $q'(\tau)$. It is of course complex; in general it takes the form

$$\mathcal{F}[q,q'] = e^{-i/\hbar\,(\Phi[q,q'] - i\Gamma[q,q'])} \qquad (57)$$

so that $\mathcal{F}[q,q']$ renormalizes the phase of the density matrix, given by $\Phi_0 = -(S_0[q] - S[q'])$, and also adds a "damping" term $\Gamma[q,q']$, which embodies both dissipation and decoherence in the system dynamics. Both of these are functionals of the 2 paths $q(\tau)$ and $q'(\tau)$. We see that $\Gamma[q,q']$ suppresses transitions between $q(\tau)$ and $q'(\tau)$ in the density matrix propagator.

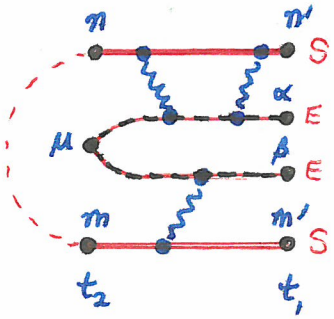
From these considerations it is obvious that

$$\mathcal{F}[q,q'] \to 1 \quad (\text{free system } S) \qquad (58)$$

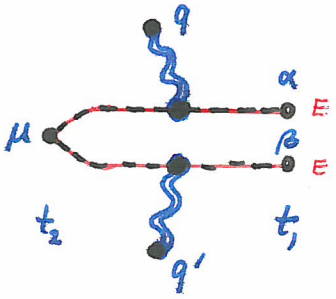
whereas in the case of strong decoherence in the position basis,

we expect $\Gamma[q,q']$ to increase rapidly as one separates the paths q and q'.

It is useful to have a diagrammatic picture of $\bar{K}$ and $\mathcal{F}$, if for no other reason than as a mnemonic device. In the diagrams below we slightly change the topology of the graphs, putting the environmental lines on the inside:



$\bar{K}_{nn;n'm'\alpha\beta}(t_2 t_1)$



$\mathcal{F}_{\alpha\beta}[q,q']$ (59)

The influence functional satisfies a number of general properties, independent of the environment E and the way in which S couples to it. Some of the most important ones are

(i) $\mathcal{F}[q,q']$ is Hermitian: $\mathcal{F}[q,q'] = \mathcal{F}^*[q',q]$ (60)

(ii) Additive property over probabilities; suppose that the environmental states are unknown, but the probability P_α of the environment being in state $|\alpha\rangle$ then we have

$$\mathcal{F}_{\alpha\beta}[q,q'] = P_\alpha \mathcal{F}_\alpha[q,q'] \delta_{\alpha\beta} \quad (61)$$

where $\mathcal{F}_\alpha[q,q']$ refer only to environmental states $|\alpha\rangle$.

(iii) Classical Forces: if the influence functional arises from either a known or an unknown classical force, it must take a certain form.

For a known classical force $F = -\partial V/\partial q$, we have

$$\mathcal{F}_V[q,q'] = e^{i\int dt\, V(t)\,(q(t)-q'(t))} \quad (62)$$

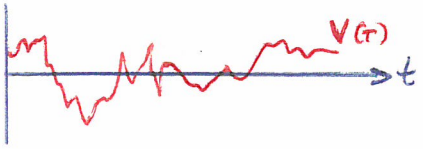
and for an unknown "noise" force, where we must functionally average over different realizations of $V(t)$, we have

$$\bar{\mathcal{F}}_V[q,q'] = P_V[q(t)-q(t')] \quad (63)$$

where $\mathcal{P}_V[q(\tau)]$ is the characteristic functional of $V(\tau)$, ie.,

$$\mathcal{P}_V[q(\tau)] = \frac{\int \mathcal{D}V(\tau)\, P[V(\tau)]\, e^{i\int d\tau\, q(\tau)V(\tau)}}{\int \mathcal{D}V(\tau)\, P[V(\tau)]} \tag{64}$$

where $P[V(\tau)]$ is the probability of a given realization of $V(\tau)$, ie., of the "path" $V(\tau)$; a typical path is shown below.



The most common kind of unknown noise force we have to deal with is one with Gaussian correlations, ie., one for which we have the probability distribution

$$\mathcal{P}_G[V(\tau)] = \exp\left\{-\tfrac{1}{2}\int d\tau \int d\tau'\, V(\tau)\,\Phi(\tau-\tau')\,V(\tau')\right\} \tag{65}$$

The further study of these processes is pursued elsewhere. Notice that the influence functional for this random force is REAL.

(ii) INFLUENCE FUNCTIONALS for MODEL ENVIRONMENTS

Elsewhere we have seen that one can classify the environmental variables into either "oscillator" or "spin" bath variables. It is then useful to see what general forms result for $\mathcal{F}[q,q']$ in these 2 cases.

(a) Oscillator Baths : Here the environment is a set of independent oscillators, with coordinates $\{x_j\}$ and momenta $\{p_j\}$; the oscillator Hamiltonian is

$$\mathcal{H}^E_{osc}(X) = \tfrac{1}{2}\sum_j^{N_0} \frac{p_j^2}{m_j} + m_j\omega_j^2 x_j^2 \tag{66}$$

and the interaction is

$$V^{osc}_{int}(Q,X) = \sum_j^{N_0} F_j(P,Q)\,x_j + G_j(Q,P)\,p_j \tag{67}$$

where the couplings are weak: $$F_j, G_j \sim O(N_0^{-1/2}) \tag{68}$$

because they describe extended modes (either bosonic or fermionic).

The original development of the influence functional formalism by Feynman et al. was accomplished for oscillator bath modes. The general form for

$\mathcal{F}[q,q']$ for an oscillator bath can be written down using fairly general arguments. Here we simply give the result for the case where $G_j(P,Q) = 0$ (we can always canonically transform the Hamiltonian to accomplish this). Then one easily finds that

$$\mathcal{F}_{osc}[q,q'] = \prod_{j=1}^{N_o} \int \mathcal{D}x_j(\tau) \int \mathcal{D}x_j'(\tau) \times \exp\left\{\frac{i}{\hbar}\int d\tau \left(\frac{M_j}{2}\left[\dot{x}_j^2(\tau) - \dot{x}_j'^2(\tau) - \omega_j^2\left(x_j^2(\tau) - x_j'^2(\tau)\right)\right] - \left[F_j(q(\tau))x_j(\tau) - F(q'(\tau))x_j'(\tau)\right]\right)\right\} \tag{69}$$

This form may seem rather forbidding but in fact the integration over the $x_j(\tau)$, $x_j'(\tau)$ may be accomplished in standard fashion, since the integrals are all Gaussian. We will give a detailed discussion below.

(b) Spin Baths : Now the environment describes a set of localized states, which we will assume to be 2-levels systems. We can therefore map the system onto a set $\{\underline{\sigma}_k\}$ of spin-½ terms, with an environmental Hamiltonian

$$\mathcal{H}_{SB}^{E}(X) = \sum_{k}^{N_s} \underline{h}_k \cdot \underline{\sigma}_k + \sum_{kk'} V_{kk'}^{\alpha\beta} \sigma_k^{\alpha} \sigma_{k'}^{\beta} \tag{70}$$

and an interaction term

$$\mathcal{H}_{int}^{SB}(Q,\sigma_k) = \sum_{k}^{N_s} \underline{F}_k(P,Q) \cdot \underline{\sigma}_k \tag{71}$$

Typically we assume that the interactions $V_{kk'}^{\alpha\beta}$ between the bath spins are weak, ie., that

$$|V_{kk'}| \ll |\underline{h}_k|, |\underline{F}_k| \tag{72}$$

but nothing is assumed about the ratios $|\underline{h}_k / \underline{F}_k|$.

One then immediately finds an influence functional

$$\mathcal{F}_{SB}[q,q'] = \prod_{k=1}^{N_s} \int \mathcal{D}\underline{\sigma}_k(\tau) \int \mathcal{D}\underline{\sigma}_k'(\tau) \times \exp\left\{\frac{i}{\hbar}\int d\tau \left(\underline{A}_k \cdot \left[\dot{\underline{\sigma}}_k(\tau) - \dot{\underline{\sigma}}_k'(\tau)\right] - \underline{h}_k \cdot \left[\underline{\sigma}_k(\tau) - \underline{\sigma}_k'(\tau)\right] - \left[\underline{F}_k(P,Q)\cdot\underline{\sigma}_k - F_k(P'Q')\cdot\underline{\sigma}_k'\right] - \sum_{k'} V_{kk'}^{\alpha\beta}\left[\sigma_k^{\alpha}\sigma_{k'}^{\beta} - \sigma_k'^{\alpha}\sigma_{k'}'^{\beta}\right]\right)\right\} \tag{73}$$

where $\underline{A}_k$ is the vector potential of a unit monopole at the centre of the Bloch sphere $\mathcal{S}_k$ upon which the $\underline{\sigma}_k$ moves.