Correlations in Quantum Mechanics: Path Integral Approach

We seek here to set up a path integral formulation of the problem of calculating operator expectation values. We will see that the results look a little unweildy - it is not obvious why one would want to do this. The reason is of course that there is a very straightforward generalization to field theory.

A. Operator Expectations: Path Integral Formulation

In standard quantum mechanics we deal with operators $\hat{A}(\hat{p},\hat{q})$ acting in real space, or operators $\hat{\alpha}(\underline{\sigma})$ acting in spin space; and more generally we deal with products of such operators, in the form of a sequence like $\hat{S} = \hat{T}\{\hat{A}_j\} = \hat{T}(\hat{A}_1(t_1)\hat{A}_2(t_2)\cdots A_n(t_n))$, where $\hat{T}$ is the time-ordering operator. A special case of such sequences is a correlator between 2 or more operators, of the form $[\hat{A}(t)\hat{B}(t')] = \hat{A}(t)\hat{B}(t') - \hat{B}(t')\hat{A}(t)$.

To calculate such correlators we need to make assumptions about which states we are taking the operators to act on. Thus it is quite common to take a vacuum expectation value of a series of operators - a simple example is

$$\left.\begin{aligned} \langle \hat{A}(t)B(t')\rangle_0 &= \langle 0|A(t)B(t')|0\rangle \\ &= \sum_n A_{0n}B_{n0}\, e^{+i/\hbar(\epsilon_n-\epsilon_0)(t-t')} \end{aligned}\right\} \qquad (A.1)$$

where we use $\hat{A}(t) = e^{+i/\hbar Ht}\hat{A}e^{-i/\hbar Ht}$, and the eigenstates $|n\rangle$ of the system have eigenenergies ϵ_n; and we write $\langle 0|\hat{A}|n\rangle = A_{0n}$, etc. We can also Fourier transform this, to get

$$\left.\begin{aligned} \chi^{00}_{AB}(\omega) &= \int_{-\infty}^{\infty} dt\, \langle 0|A(t)B(0)|0\rangle\, e^{i\omega t} \\ &= 2\pi\sum_n A_{0n}B_{n0}\,\delta(\omega + (\epsilon_n-\epsilon_0)) \end{aligned}\right\} \qquad (A.2)$$

We can of course calculate the operators sandwiched between any states; another obvious choice is the correlator $\langle A(t)B(t')\rangle_{\psi}$ sandwiched between a pair of states $|\psi\rangle$. It is also useful to calculate thermal averages, of the form

$$\left.\begin{aligned} \langle A(t)B(t')\rangle_\beta &= \frac{1}{Z}\sum_m e^{-\beta\epsilon_m}\langle m|A(t)B(t')|m\rangle \\ &= \frac{1}{Z}\sum_m\sum_n e^{-\beta\epsilon_m} A_{mn}B_{nm}\, e^{i/\hbar(\epsilon_n-\epsilon_m)(t-t')} \end{aligned}\right\} \qquad (A.3)$$

where $Z = \sum_m e^{-\beta\epsilon_m}$ is the partition function. If we develop all of this formalism, we end up with the apparatus of time-dependent thermal Green functions, a very useful set of techniques.

Consider now how we might set up a path integral framework to find correlation functions. We recall that the basic object in path integral theory is the 1-particle propagator, given by

$$\left.\begin{aligned} G(x,x') \equiv G(\underline{r},t;\underline{r}'t') &= \int_{x'}^{x} \mathcal{D}q(\tau)\, e^{i/\hbar \int_{t'}^{t} d\tau\, L(q,\dot{q};\tau)} \\ &\equiv \langle \underline{r},t| e^{-i/\hbar H(t-t')} |\underline{r}'t'\rangle \\ &\equiv \langle x|x'\rangle \end{aligned}\right\} \qquad (A.4)$$

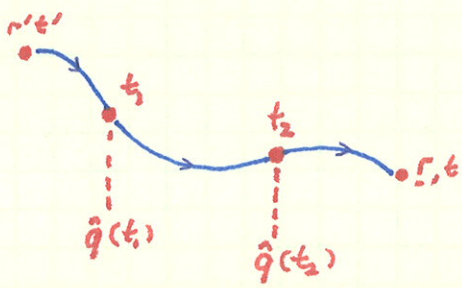
where $\int_{x'}^{x} \mathcal{D}q(\tau) \equiv \int_{q(t')=\underline{r}'}^{q(t)=\underline{r}} \mathcal{D}q(\tau)$ is a shorthand, as is $\langle x|x'\rangle$.

Now since path integral theory is naturally formulated in real space (ie., the space of the corresponding classical theory) it makes sense to consider a general correlation function of the form

$$\left.\begin{aligned} \chi_n^{xx'}(A_1(t_1)\cdots A_n(t_n)) &\equiv \langle x| T\{A_j(t_j)\}|x'\rangle \\ &\equiv \langle \underline{r},t|\, A_1(t_1)\, A_2(t_2)\cdots A_n(t_n)\,|r't'\rangle \\ &\equiv \langle r,t| e^{-i/\hbar H(t-t_1)}\hat{A}_1 e^{-i/\hbar H(t_1-t_2)}\hat{A}_2\cdots\hat{A}_n e^{-i/\hbar H(t_n-t')}|\underline{r}'t'\rangle \end{aligned}\right\} (A.5)$$

Rather than develop the general theory for such a large object, let's just consider a simple example, viz., the very important correlator between the positions of a particle at 2 different times, ie.,

$$\chi_2^{xx'}(q_1,q_2) \equiv \langle \underline{r},t|\, T\{\hat{q}(t_1)\,\hat{q}(t_2)\}\,|\underline{r}'t'\rangle \qquad (A.6)$$



which is shown in diagrammatic form at left. Thus we can interpret this correlation function as a measurement of the operator q at 2 different times t_1 and t_2, subject to the condition that at an earlier time $t'<t$, the particle is at $\underline{r}'$, and that at a later time $t>t_2$, the particle will be at $\underline{r}$.

Now, without any formal proof (which is in any case not difficult), we can simply state the expression for (A.6) in path integral form:

$$\chi_2^{xx'}(q_1,q_2) = \int_{x'}^{x} \mathcal{D}q(\tau)\, e^{i/\hbar \int_{t'}^{t} d\tau\, L(q,\dot{q},\tau)}\; q(t_1)\, q(t_2) \qquad (A.7)$$

ie., we simply weight each path by the product $q(t_1)q(t_2)$ (as well as the usual weighting factor $e^{i/\hbar S}$). Note that the time-ordering does not appear in this expression.

Let us also state the result for some general correlator, where we also no longer assume that the Hamilton / Lagrangian are quadratic functions of velocity. Thus, for the correlator in (A.5), we have

$$\left.\begin{aligned} \chi_n^{xx'}\Big(\prod_{j=1}^{n} \hat{A}_j(t_j)\Big) &= \langle x | T\{\hat{A}_1(t_1)\cdots\hat{A}_n(t_n)\} | x'\rangle \\ &= \int \mathcal{D}p(\tau) \int_{x'}^{x} \mathcal{D}q(\tau)\, e^{i/\hbar \int d\tau [p\dot{q} - H(q,p)]} \prod_{j=1}^{n} A_j(p(t_j), q(t_2)) \end{aligned}\right\} \qquad (A.8)$$

where now
$$A_j(t_j) = A_j(p(t_j), q(t_j)) \qquad (A.9)$$

is some function of the variables p and q, taken at time t_j (as opposed to a function of the operators $\hat{p}$ and $\hat{q}$). In the case where $H(p,q)$ depends quadratically on p, this reduces to

$$\chi_n^{xx'}\Big(\prod_{j=1}^{n} A_j(t_j)\Big) \longrightarrow \int_{x'}^{x} \mathcal{D}q(\tau)\, e^{i/\hbar \int_{t'}^{t} d\tau\, L(q\dot{q},\tau)} \prod_{j=1}^{n} A_j(q(t_j), \dot{q}(t_j)) \qquad (A.10)$$

with $A_j(q(t_j), \dot{q}(t_j))$ now the relevant function of the variables q and $\dot{q}$.

Formal demonstrations of formulas (A.7), (A.8), and (A.10), as well as a systematic discussion of the theory that one can develop from (A.5), is given in a Supplementary Appendix.

Finally, let us note that we can write these results in another way, which is more directly connected with the functional formulation of QFT, in the form invented by Schwinger. Consider the "source" Green function

$$\left.\begin{aligned} G(x,x'; J(t)) &= \int_{x'}^{x} \mathcal{D}q \int \mathcal{D}p\, e^{i/\hbar \int d\tau ([p\dot{q} - H(pq)] + J(t)q(t))} \\ &\xrightarrow[\text{quadratic } H]{} \int_{x'}^{x} \mathcal{D}q\, e^{i/\hbar \int d\tau (L(q,\dot{q};t) + J(t)q(t))} \end{aligned}\right\} \qquad (A.11)$$

which is the propagator for a particle between x' and x, supposing that there is an external "source" field acting on the particle through the coupling $J(t)q(t)$ (so that $J(t)$ is some arbitrary force, varying with time).

We now see that we can write the 2-time position correlator $\chi_2^{xx'}(q_1q_2)$ of (A.6) and (A.7) as

$$\left.\begin{aligned} \chi_2^{xx'}(q_1q_2) &= \langle r,t | T\{\hat{q}(t_1)\hat{q}(t_2)\} | r't'\rangle \\ &= (-i\hbar)^2 \frac{\delta^2}{\delta J(t_1)\,\delta J(t_2)} G(xx'|J)\Big|_{J=0} \end{aligned}\right\} \qquad (A.12)$$

This result, when generalized to cover an infinite set of field variables, is central to a functional / path integral formulation of QFT. Obviously we can generalize it to cover some arbitrary correlation function, by just adding the coupling $\sum q(t) A_j(q(t_j), p(t))$ to the original Hamiltonian; but we will not pursue this here.

It is useful to discuss an example of this — it will be done below.

B. VACUUM STATE CORRELATORS

In relativistic field theory, and to a lesser extent in non-relativistic field theory, a central role is played by the expectation value of operators taken between the vacuum state. What we are going to do here is set up the theory for a single particle in the form where it is directly generalized to QFT. Thus the reasons for considering particular limits of correlation functions will not be immediately obvious, at least until we make the jump to QFT.

Let's start from the vacuum correlator $\chi_2^{00}(q_1, q_2; t, t')$ given by

$$\chi_2^{00}(\hat{q}(t_1)\hat{q}(t_2); t, t') = \langle 0, t | T\{q(t_1) q(t_2)\} | 0, t' \rangle \qquad (B.1)$$

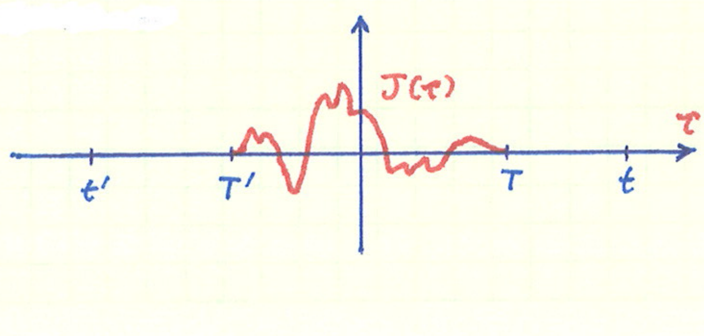
by which we denote that the initial state is the vacuum at time t', and the final state is the vacuum at time t. Clearly we can also write this as

$$\left.\begin{aligned} \chi_2^{00}(q_1 q_2; t t') &= \int d\underline{r} \int d\underline{r}' \langle 0 | \underline{r}, t\rangle \langle \underline{r}, t | T\{q(t_1) q(t_2)\} | \underline{r}' t' \rangle \langle r' t' | 0 \rangle \\ &\equiv \int dr \int dr' \langle 0 | x \rangle \langle x | T\{q(t_1) q(t_2)\} | x' \rangle \langle x' | 0 \rangle \\ &\equiv \int d\underline{r} \int d\underline{r}' \, \psi_0^*(\underline{r}, t) \, \chi_2^{xx'}(q_1 q_2) \, \psi_0(r' t') \end{aligned}\right\} \qquad (B.2)$$

where, eg., $\langle 0 | x \rangle = \psi_0^*(r, t)$ is the complex conjugate of the vacuum wave-function at time t; which for an ordinary QM particle we just call the ground state wave-function.

We now consider a special case of this vacuum correlator. First, we add a source term, so that we have

$$\left.\begin{aligned} H(p,q) \rightarrow H(p,q; J) &= H(p,q) - q(t) J(t) \\ L(q,\dot{q}) \rightarrow L(q\dot{q}; J) &= L(q,\dot{q}) + q(t) J(t) \end{aligned}\right\} \qquad (B.3)$$



Then we assume that the "driving" function $J(t)$ is zero except between times T' and T; and that $t' < T$, and $t > T$, as shown at left.

The point of this manoeuvre is we want to start the system off in its ground state, and then, after the perturbation $J(t)\,q(t)$ has acted, we want to see where it has ended up; and in particular, we want to see the overlap afterwards with the ground state. While the perturbation is acting, we have

$$\left.\begin{aligned} \psi_J(\tau) &= U_J(\tau,\tau')\,\psi_J(\tau') \\ \text{with}\quad i\hbar\,\partial_\tau U_J(\tau,\tau') &= [\hat{H} - J(\tau)\,q(\tau)]\,U_J(\tau,\tau') \end{aligned}\right\} \qquad (B.4)$$

where $U_J(\tau,\tau')$ is the time evolution operator for the Schrodinger eqtn. Notice that we can write the propagator from initial to final states as

$$\left.\begin{aligned} G(xx';J) &= \int dR \int dR'\, G_0(r,t;RT)\, G(R,T;R'T'|J)\, G_0(RT;r't') \\ &\equiv \int dR \int dR'\, \langle rt|R'T'\rangle_0\, \langle RT|R'T'\rangle_J\, \langle R'T'|r't'\rangle_0 \end{aligned}\right\} \qquad (B.5)$$

where $G_0(xx')$ signifies the propagator in the absence of a driving force. The result (B.5) of course just expresses the linearity of QM – it is the standard composition rule for amplitudes.

Now if we wanted to pick out the ground state in the way described above, the simplest thing to do would be to sandwich $G(xx'|J)$ between 2 vacuum states, to give

$$\left.\begin{aligned} G_{00}(t,t'|J) &= \int d\underline{r} \int d\underline{r}'\, \langle 0t|\underline{r}t\rangle\, G(xx'|J)\, \langle r't'|0t'\rangle \\ &\equiv \int d\underline{r} \int d\underline{r}'\, \psi_0^*(\underline{r},t)\, G(rr';tt'|J)\, \psi_0(\underline{r}'t') \end{aligned}\right\} \qquad (B.6)$$

However one would like to separate out explicitly the regions where $J(t) = 0$ from those where it is not. This we do using the following trick. Consider the matrix element

$$\left.\begin{aligned} \langle \underline{r},t|RT\rangle_0 &= \langle \underline{r}|e^{-i/\hbar H(t-T)}|\underline{R}\rangle \\ &= \sum_m \psi_m(\underline{r})\,\psi_m^*(\underline{R})\, e^{-i/\hbar\,\epsilon_m(t-T)} \end{aligned}\right\} \qquad (B.7)$$

Now let $t \to -i\infty$; we then get

$$\lim_{t\to -i\infty} \langle \underline{r},t|\underline{R},T\rangle_0 = \lim_{|t|\to\infty} \sum_m \psi_m(\underline{r})\,\psi_m^*(R)\, e^{i/\hbar\,\epsilon_m T}\, e^{-\epsilon_m|t|} \to 0 \qquad (B.8)$$

However, if we premultiply by $e^{i/\hbar\,\epsilon_0 t}$, we then get

$$\left.\begin{aligned} \lim_{t\to -i\infty} e^{i/\hbar\,\epsilon_0 t}\langle r,t|R,t\rangle_0 &= \lim_{t\to -i\infty} \sum_m \psi_m(r)\,\psi_m^*(R)\, e^{i/\hbar\,\epsilon_m T}\, e^{-i/\hbar(\epsilon_m-\epsilon_0)t} \\ &= \psi_0(\underline{r})\,\psi_0^*(\underline{R})\, e^{i/\hbar\,\epsilon_0 T} \equiv \psi_0(\underline{r})\,\psi_0^*(R,T) \end{aligned}\right\} \qquad (B.9)$$

and we have managed to pick out only the ground state from the sum! In the same way we see that we can deal with $\langle R'T'|r't'\rangle_0$ in (B.5), this time by taking the limit $t' \to i\infty$, and thus we find that

$$\lim_{t' \to i\infty} e^{-\frac{i}{\hbar}\epsilon_0 t'} \langle R'T' | r't' \rangle = \psi_0(R',T')\,\psi_0^*(\underline{r}') \qquad (B.10)$$

and so, substituting (B.9) and (B.10) into (B.5), we get

$$\lim_{\substack{t \to -i\infty \\ t' \to i\infty}} e^{\frac{i}{\hbar}\epsilon_0(t-t')}\, G(xx'|J) = \psi_0(\underline{r})\,\psi_0^*(\underline{r}')\, G_{00}(T\,T'|J) \qquad (B.11)$$

where $G_{00}(T,T'|J)$ is the "vacuum-to-vacuum" transition amplitude in the time period between T' and T, in the presence of $J(t)$, ie.,

$$\left.\begin{aligned} G_{00}(T,T'|J) &= \int d\underline{R}\int d\underline{R}' \,\langle 0T|R\rangle\langle R|\hat{G}(T,T'|J)|R'\rangle\langle R'|0T'\rangle \\ &\equiv \int dR\int dR'\, \phi_0^*(R,T)\,\langle RT|R'T'\rangle_J\, \phi_0(R',T') \\ &\equiv \langle 0|\hat{G}(T,T'|J)|0\rangle \end{aligned}\right\} \qquad (B.12)$$

Thus, inverting (B.11), we have the following result for this vacuum/vacuum amplitude:

$$G_{00}(T,T'|J) = \lim_{\substack{t \to -i\infty \\ t' \to i\infty}} e^{-\frac{i}{\hbar}\epsilon_0(t-t')}\,\frac{G(x,x'|J)}{\psi_0(r)\,\psi_0^*(r')} \qquad (B.13)$$

where $\underline{r}, \underline{r}'$ are arbitrary.

Now what do we learn from this? First, that $G_{00}(T,T'|J)$ is proportional to $G(xx'|J)$. We can actually show that the constant of proportionality is trivial. Suppose we consider (B.13) in the case where $J=0$ (ie, no external field at any time. Then we have

$$\left.\begin{aligned} G_{00}(T,T'|J=0) &= \lim_{\substack{t \to -i\infty \\ t' \to i\infty}} e^{\frac{i}{\hbar}\epsilon_0(t-t')}\,\frac{G(xx'|J=0)}{\psi_0(r)\,\psi_0^*(r')} \\ &= \langle 0|e^{\frac{i}{\hbar}\hat{H}T}\, U_{J=0}(T,T')\, e^{-\frac{i}{\hbar}\hat{H}T'}|0\rangle \\ &= 1 \end{aligned}\right\} \qquad (B.14)$$

where we have used (B.5), and the last result simply follows because when $J(t)=0$, a particle starting in the ground state must remain in the ground state provided ~~it~~ it is only acted on by $\hat{H}$. Thus, dividing both sides of (B.13) by $G_{00}(T,T'|J=0)$, we can simply identify $G_0(T,T'|J)$ with $G(xx'|J)$ in the limit $t' \to i\infty$, $t' \to -i\infty$.

Before proceeding to the punch line here, note that there are a few minor variations one can introduce in this derivation. The time contour involved in the limits of (B.11) – (B.14) are rather clumsy. But we notice that we can simplify them somewhat by just writing, for the time variable of integration, that $\tau \to \tau(1-i\delta)$, where δ is some arbitrarily small (but finite) constant. Then we achieve exactly the same goal as before, when we let the times go to $\pm\infty$. Another variation is to let $J(t)$ go to $\hbar J(t)$, which has the advantage of removing the factors of $\hbar$ in eqtns like (A.12).

In any case, the key result we have can now be obtained by looking at (B.13) and (B.14), and comparing with (A.11); we see we can write the vacuum state correlator as a path integral. We introduce a new notation here – we write

$$Z[J] = G_{00}(T, T' | J) \qquad (B.15)$$

where as before, $J(t) = 0$ for $t > T$, and $t < T'$. Then we have

$$\left.\begin{aligned} Z[J] &= \lim_{\substack{t \to -i\infty \\ t' \to i\infty}} \frac{1}{Z(0)} \int \mathcal{D}p \int_{r'}^{r} \mathcal{D}q \, e^{\frac{i}{\hbar}\int_{t'}^{t} d\tau \left([p\dot{q} - H(p,q)] + q(\tau)J(\tau)\right)} \\ &\xrightarrow[H(p,q)]{\text{quad.}} \lim_{\substack{t \to -i\infty \\ t' \to i\infty}} \frac{1}{Z(0)} \int \mathcal{D}q(\tau) \, e^{\frac{i}{\hbar}\int_{t'}^{t} d\tau \left(L(q\dot{q}) + q(\tau)J(\tau)\right)} \end{aligned}\right\} \qquad (B.16)$$

where we divide by $Z[0] = Z[J=0]$ for convenience of comparison with QFT results (here $Z[0] = 1$, as we just saw); and both $Z[J]$ & $Z[0]$ are taken between (arbitrary) points $r' = q(t')$ and $r = q(t)$.

In the same way we can write correlators – thus, comparing with (A.12) we see we can write

$$\left.\begin{aligned} \chi_2^{00}(q_1 q_2) &\equiv \langle 0 | T\{\hat{q}(t_1)\hat{q}(t_2)\} | 0 \rangle \\ &= \frac{(-i\hbar)^2}{Z[0]} \left.\frac{\delta^2 Z[J]}{\delta J(t_1)\,\delta J(t_2)}\right|_{J=0} \end{aligned}\right\} \qquad (B.17)$$

Let's recap what we've found. We see that we can write the amplitudes for Green functions and for correlators between vacuum states – the "vacuum amplitudes", in terms of a function $Z[J]$, which can be written as the path integral for propagation between the vacuum states in the presence of a "source" or "noise" field $J(\tau)$; correlators are found by taking functional derivatives of $Z[J]$, and then taking the limit $J(\tau) \to 0$.

The reason for denoting the vacuum amplitude by $Z[J]$ will become obvious when we change time variables to "Euclidean time"; we will then see that $Z[J]$ becomes the partition function.

Finally, let's note that we can easily write down the results for more general correlators, using the same formalism. Thus

$$\chi_n^{00}(\{q_j\}) = \langle 0 | T\{q(t_1) \cdots q(t_n)\} | 0 \rangle = \frac{(-i\hbar)^n}{Z[0]} \frac{\delta^n Z[J]}{\delta J(t_1) \cdots \delta J(t_n)} \qquad (B.18)$$

and indeed we can in the same way set up a more general coupling to external sources, of form

$$\hat{\mathcal{H}}(q,p) \rightarrow \hat{\mathcal{H}}(q,p) - \sum_{\mu=1}^{p} \hat{J}(\tau)\, A_\mu(\hat{p}(\tau), \hat{q}(\tau)) \tag{B.19}$$

and then we have

$$\langle 0 | T\{ \hat{A}_1(t_1), \ldots A_n(t_n) \} | 0 \rangle = \frac{(-i\hbar)^n}{Z[0]} \frac{\delta^2 Z[J]}{\delta J(t_1) \cdots \delta J(t_n)} \tag{B.20}$$

where now

$$Z[J] = \int \mathcal{D}p(\tau) \int \mathcal{D}q(\tau)\, e^{i/\hbar \int d\tau \left([p\dot{q} - H(p,q)] + \sum_{\mu=1}^{p} J(\tau) A_\mu(p(\tau), q(\tau)) \right)} \tag{B.21}$$

where the $\hat{A}_\mu$ are functions of the operators $\hat{p}, \hat{q}$, and we suppose that the n different operators $A_j(t_j)$, with $j = 1, 2, \ldots n$, are drawn from the collection A_μ of p different functions.

C. EUCLIDEAN TIME FORMULATION

We have already seen how clumsy it is to formulate the path integral expressions for vacuum correlators in real time. A simple remedy is to go to a "Euclidean time" formulation. For ordinary QM this merely solves an inconvenience, but for QFT it is more important, because of the connection with Minkowski $\leftrightarrow$ Euclidean rotations, and because it makes the mathematics well-behaved.

In ordinary QM, the "Euclidean rotation" is very simple. We let

$$t \rightarrow -i\tau \qquad (\tau \text{ real}) \tag{C.1}$$

so that

$$\left.\begin{aligned} G(xx') = G(\underline{r},\underline{r}'; t,t') &= \langle \underline{r} | e^{-\frac{i}{\hbar} H(t-t')} | r' \rangle \\ &\rightarrow \langle \underline{r} | e^{-H(\tau-\tau')/\hbar} | r' \rangle \\ &\equiv G(r,r'; -i(\tau-\tau')) \end{aligned}\right\} \tag{C.2}$$

which we write as

$$G_E(\underline{r}\underline{r}', \tau\tau') \equiv G(r,r'; -i\tau, -i\tau') \tag{C.3}$$

The path integral expression for this propagator is then

$$G_E(\underline{r},\underline{r}'; \tau,\tau') = \int_{r'(\tau')}^{r(\tau)} \mathcal{D}q(s)\, \exp\left\{ -\frac{1}{\hbar} \int_{\tau'}^{\tau} ds\, L_E(q,\dot{q}) \right\} \tag{C.4}$$

where the "Euclidean Lagrangian" $L_E(q,\dot{q})$ is produced formally by the substitutions

$$\left.\begin{aligned} dt &\to -i\,d\tau \\ \left(\frac{dq}{dt}\right)^2 &\to \left(i\frac{dq}{d\tau}\right)^2 = -\left(\frac{dq}{d\tau}\right)^2 \end{aligned}\right\} \qquad (C.5)$$

So that for a Lagrangian with a source term, we have

$$\left.\begin{aligned} L(q,\dot{q}\,|J) &= \tfrac{1}{2}m\dot{q}^2 - V(q) + q(t)J(t) \\ \longrightarrow \quad L_E(q\dot{q}J) &= \tfrac{1}{2}m\dot{q}^2 + V(q) - q(\tau)J(\tau) \end{aligned}\right\} \qquad (C.6)$$

where $\dot{q} \equiv dq/d\tau$ in $L_E(q,\dot{q})$.

We see that L_E looks the exponent of a partition function, and indeed

$$G_E(r,r';\tau,\tau') \equiv \rho(r,r';(\tau-\tau')/\hbar) \qquad (C.7)$$

where $\rho(xx')$ is just the density matrix. Conversely, we see that we can write

$$\left.\begin{aligned} Z_0(\beta) = \mathrm{Tr}\,e^{-\beta H} &= \int dr \langle r|e^{-\beta H}|r\rangle \\ &\equiv \int dr\, \rho(r,r;\hbar\beta,0) \\ &\equiv \int\limits_{r(0)=r(\beta\hbar)} \mathcal{D}q(\tau)\, \exp\left\{-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau\left[\tfrac{1}{2}m\dot{q}^2 + V(q)\right]\right\} \end{aligned}\right\} \qquad (C.8)$$

Thus, if we wish, we can use the path integral formalism in imaginary time to study the dynamics of the density matrix; and the field theoretical generalization of this will allow us to study statistical mechanics in a non-perturbative field theory, in which one sums over different configurations with a statistical weighting factor $e^{-\beta H}$, where the configurations are represented by paths in imaginary time.

However from the present point of view, the most important thing about the Euclidean form is that the path integral is much better behaved than the standard form. This is because the integrand function $e^{i/\hbar S}$ oscillates wildly as one changes the paths, making it hard to give a precise mathematical meaning to the functional. On the other hand $e^{-S_E/\hbar}$ is much better behaved, and unimportant contributions with large S_E are exponentially small. As a consequence, many treatments of path integration, particularly in QFT, make all their formal manoeuvres in Euclidean spacetime, only analytically continuing to real spacetime at the end.

From this point of view, it is not the time integral between 0 and $\hbar\beta$ that interests us, but the integral over τ from $\pm\infty$. Thus we can rewrite the "partition function", or vacuum amplitude, of eqtns (B.15) and (B.16) as

$$Z_E[J] = \lim_{\substack{\tau \to \infty \\ \tau' \to -\infty}} \frac{1}{Z_E[0]} \int \mathcal{D}p \int_{\tau'}^{\tau} \mathcal{D}q \;\; \exp\left\{ -\frac{1}{\hbar} \int d\tau \left[i p \dot{q} - H[p,q] + q(\tau) J(\tau) \right] \right\}$$

$$\xrightarrow[\mathcal{H}(p,q)]{\text{quadratic}} \lim_{\substack{\tau \to \infty \\ \tau' \to -\infty}} \frac{1}{Z_E[0]} \int_{\tau'}^{\tau} \mathcal{D}q(\tau) \;\; \exp\left\{ \frac{-1}{\hbar} \int_{-\infty}^{\infty} d\tau' \, L_E(q, \dot{q}\,; J(\tau)) \right\} \qquad (C.9)$$

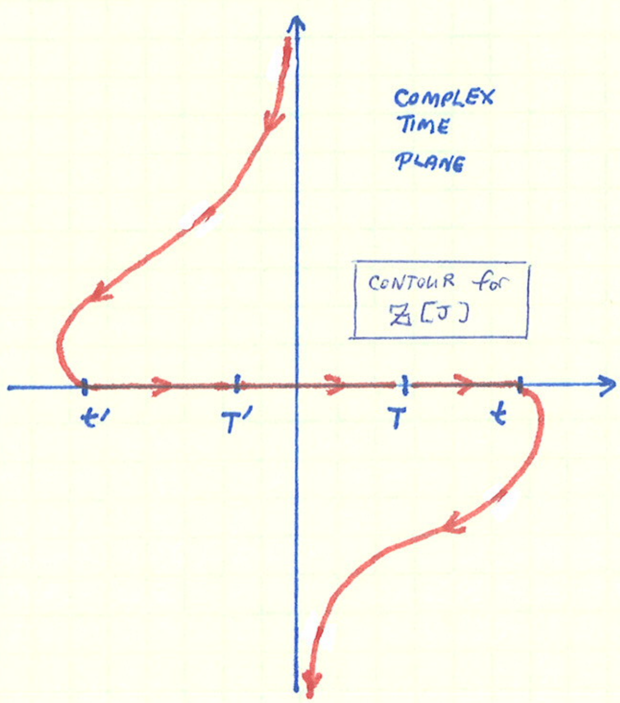
where we now assume a "source" or driving term $J(\tau)$ in imaginary time, which has been produced from $J(t)$ by analytic continuation. In the same way we have, for the correlation functions, expressions like

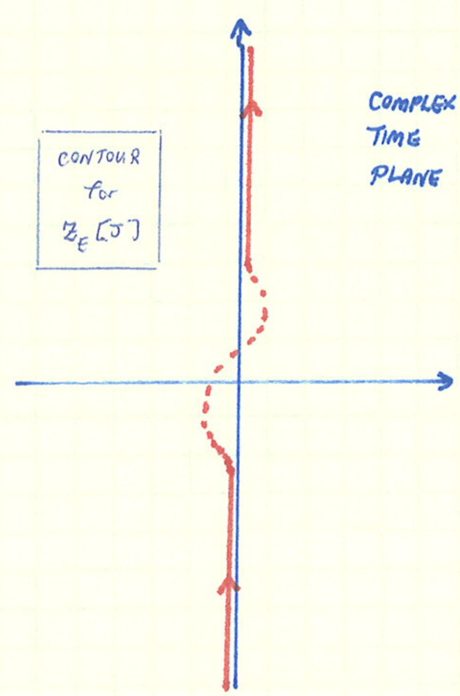
$$\chi_n^{00}(\{q_j\}) \equiv \langle 0 | T\{q(\tau_1) \ldots q(\tau_n)\} | 0 \rangle$$

$$= \frac{(-\hbar)^{-n}}{Z_E[0]} \; \frac{\delta^2 Z_E[J]}{\delta J(\tau_1) \ldots\ldots \delta J(\tau_n)} \Bigg|_{J=0} \qquad (C.10)$$

where the time-ordering is now done along the imaginary axis.

To see exactly what is going on, it is useful to look at the integral





contours in the complex plane. The original contour discussed for $Z[J]$, which appears, eg., in (B.13)-(B.16), is shown at left; and we recall that we take the limits $t \to$ $t' \to \pm i\infty$; what this means is that we fix t and t' as shown previously, so that $t' < T'$, and $t > T$, and then continue the integration path from these points to rejoin the imaginary axis, and extend off to $\pm i\infty$. On the other hand to τ-integrals which define the Euclidean function $Z_E[J]$ are already on the imaginary axis. The only proviso we note is that if the functions in the integrand have any poles or branch cuts on or around this axis, we need to prescribe a contour which circumvents them – we will see this in examples.

Finally, we note that in the discussion of a relativistic theory, the rotation to Euclidean time possesses a further advantage – it changes the metric from a Lorentzian to a Euclidean one. This has a number of formal advantages. Since this is properly part of field theory, we delay discussion of it for the moment.

D. HARMONIC OSCILLATOR REDUX

The standard problem of the simple harmonic oscillator is treated in introductions to path integral methods. Let us recall the results. We have a Hamiltonian

$$\left.\begin{aligned} \mathcal{H}_0(p,q) &= \tfrac{1}{2}\left[\frac{p^2}{m} + m\omega_0^2 q^2\right] \\ \text{so that}\qquad L_0(q,\dot{q}) &= \frac{m}{2}\left[\dot{q}^2 - \omega_0^2 q^2\right] \end{aligned}\right\} \qquad (D.1)$$

for which we recall that the spacetime propagator is given by

$$\left.\begin{aligned} G_0(x,x') \equiv G_0(\mathbf{r},\mathbf{r}';t,t') &= \int_{\mathbf{r}'}^{\mathbf{r}} \mathcal{D}q(t)\, e^{i/\hbar \int_{t'}^{t} dt\, L_0(q,\dot{q})} \\ &= A_0(t-t')\, e^{i/\hbar\, S_0(x,x'|0)} \end{aligned}\right\} \qquad (D.2)$$

where the action $S_0(x,x'|0)$ is labelled so as to indicate that there is no driving force $J(t)$, ie, $J=0$, and where

$$\left.\begin{aligned} A_0(t-t') &= \frac{m\omega_0}{2\pi i\hbar \sin \omega_0(t-t')} \\ S_0(x,x'|0) &= \frac{m\omega_0}{2\sin\omega_0(t-t')}\left[(r^2+r'^2)\cos\omega_0(t-t') - 2rr'\right] \end{aligned}\right\} \qquad (D.3)$$

In the presence of some arbitrary driving force $-J(t)$, we have

$$\left.\begin{aligned} \mathcal{H}_0^J(p,q;J) &= \tfrac{1}{2}\left[\frac{p^2}{m} + m\omega_0^2 q^2\right] - J(t)q(t) \\ L_0(q\dot{q};J) &= \frac{m}{2}\left[\dot{q}^2 - \omega_0^2 q^2\right] + J(t)\,q(t) \end{aligned}\right\} \qquad (D.4)$$

and the propagator $G_0(x,x'|J)$ then takes on the rather complicated form (PTO):

$$G_0(xx'|J) = A_0(t-t')\, e^{i/\hbar\, S_0(xx'|J)} \qquad (D.5)$$

$$\left.\begin{aligned} \text{with}\quad S_0(xx'|J) &= S_0(xx'|0) + \Delta S_J(xx'|J) \\ \Delta S_J(xx'|J) &= \frac{1}{\sin\omega_0(t-t')}\Big\{ \int_{t'}^{t} ds\, J(s)\left[r \sin\omega_0(s-t') + r'\sin\omega_0(t-s)\right] \\ &\qquad - \frac{1}{m\omega_0}\int_{t'}^{t} ds \int_{t'}^{t} ds'\, J(s)\,\gamma(s,s')\, J(s') \Big\} \end{aligned}\right\} \qquad (D.6)$$

in which the "correlator" between the external forces $J(s)$ and $J(s')$ is given by

$$\gamma(s,s') = \theta(s-s')\sin\omega_0(t-s)\sin\omega_0(s'-t') \qquad (D.7)$$

These results are standard for the SHO system. Let us now, in order to make contact with the earlier discussion (and to get some very useful and interesting results), look at the matrix elements of the operator $\hat{G}_0$, but now between the bare SHO eigenstates $\{|n\rangle\}$, instead of the position eigenstates $|r\rangle$, $|r'\rangle$, etc. Thus we consider

$$\left.\begin{aligned} G^0_{nm}(t,t'|J) &= \langle n|\hat{T}\{ e^{-i/\hbar \int ds\,[\hat{H}_0 - J(s)q(s)]}\}|m\rangle \\ &\equiv \int dr \int dr'\, \langle n|rt\rangle_0\, G_0(rr',tt'|J)\,\langle r't'|m\rangle_0 \\ &\equiv \int dr\int dr'\, \phi^*_n(r,t)\,\langle r|\hat{G}_0(t,t'|J)|r'\rangle\,\phi_m(r't') \\ &\equiv \langle n|\hat{G}_0(t,t'|J)|m\rangle \end{aligned}\right\} \qquad (D.8)$$

and in particular we consider the vacuum-vacuum amplitude

$$\left.\begin{aligned} G^0_{00}(t,t'|J) &= \langle 0|\hat{G}_0(t,t'|J)|0\rangle \\ &\equiv \int dr\int dr'\, \phi^*_0(r,t)\, G_0(xx'|J)\,\phi_0(r't') \end{aligned}\right\} \qquad (D.9)$$

where the $\phi_n(r,t)$ are just the bare SHO eigenstates, and we write all these different equivalent forms just for reference. Now we notice that the vacuum amplitude (D.9) is just exactly the same quantity we dealt with previously (compare eqtn (B.12)), and that $G^0_{nm}(t,t'|J)$ is just the generalization of this to arbitrary transition matrix elements - all specialized here to the SHO, of course.

The calculation of $G^0_{00}(tt'|J)$ and of $G^0_{nm}(t,t'|J)$ are of course standard problems in QM (they are, for example, discussed in the book of Feynman & Hibbs). Let's just recall the results.

(i) <u>Vacuum Amplitude $G^0_{00}(t,t'|J)$</u>: The simplest way to compute this directly is by using eqtn (D.9), and just substituting in (D.5) and (D.6) for $G_0(xx'|J)$, along with the standard forms for the SHO ground state wave-functions, viz.

$$\phi_0(r,t) = \left(\frac{m\omega_0}{\pi\hbar}\right)^{1/4} e^{-\frac{1}{2}\frac{m\omega_0}{\hbar}r^2}\, e^{-\frac{1}{2}i\omega_0 t} \qquad (D.10)$$

where we have not forgotten the time-dependence in (D.10).

The calculation of the vacuum amplitude from (D.5)-(D.7), (D.9), and (D.10) is a little tedious but elementary, since we are dealing with Gaussian integrals. The result is

$$G^0_{00}(t,t'|J) = e^{-\frac{1}{2m\omega_0\hbar}\int_{t'}^{t}ds\int_{t'}^{s}ds'\, J(s)J(s')\,e^{-i\omega_0(s-s')}} \qquad (D.11)$$

which we can write in symmetrized form as

$$\left.\begin{aligned} G^0_{00}(t,t'|J) &= \exp\left\{-\frac{1}{2\hbar}\int_{t'}^{t}ds\int_{t'}^{t}ds'\, J(s)\,D_0(s-s')\,J(s')\right\} \\ D_0(s-s') &= \frac{1}{2m\omega_0}\left[\theta(s-s')\,e^{-i\omega_0(s-s')} + \theta(s'-s)\,e^{i\omega_0(s-s')}\right] \end{aligned}\right\} \qquad (D.12)$$

and, finally, the "partition function", of generating functional $Z_0[J]$, is seen to be the limit where the integration time variable $s \to \pm\infty(1-i\delta)$ (cf. discussion after (B.14)), ie.,

$$Z_0[J] = e^{-\frac{1}{2\hbar}\int_{-\infty}^{\infty}ds\int_{-\infty}^{\infty}ds'\, J(s)\,D_0(s-s')\,J(s')} \qquad (D.13)$$

where the integration limits are understood as above.

Now let us rederive this result in a completely different way, starting directly from the path integral result for $Z_0[J]$ in eqtn (B.16), now adapted to the SHO; thus we start from

$$Z_0[J] = \int \mathcal{D}q(s)\, e^{\frac{i}{\hbar}\int_{-i\infty}^{i\infty}ds\left[\frac{m}{2}(\dot{q}^2-\omega_0^2q^2) + J(s)q(s)\right]} \qquad (D.14)$$

Now this is a Gaussian functional integral, and so we should be able to first integrate by parts (recall how one derives the classical action for a SHO), to get:

$$Z_0[J] = \int \mathcal{D}q(s)\, e^{\frac{i}{\hbar}\int_{-i\infty}^{i\infty}ds\left[\left[-\frac{1}{2}q(s)\left[m\left(\frac{d^2}{ds^2}+\omega_0^2\right)\right]q(s) + J(s)q(s)\right]\right]} \qquad (D.15)$$

and then just do this Gaussian integral, to get (defining $\hat{K}_0 = im\left(\frac{d^2}{ds^2}+\omega_0^2\right)$):

$$Z_0[J] = \exp\left\{\frac{-1}{2\hbar}\int_{-\infty}^{\infty}ds\int_{-\infty}^{\infty}ds'\, J(s)\,K_0^{-1}(s-s')\,J(s')\right\} \qquad (D.16)$$

and by comparing (D.13) and (D.16), we see that our task is to show that

$D_0(s-s')$ and $K_0^{-1}(s-s')$ are the same, where the precise definition of $K_0^{-1}(s-s')$ is:

$$im\left(\frac{d^2}{dt^2}+W_0^2\right)K_0^{-1}(t-t') = \delta(t-t') \qquad (D.17)$$

ie, we want to show that $\hat{D}_0(t,t')$ is acting as the "inverse operator" to the operator $m(d^2/dt^2+W_0^2) = K_0(t-t')$

We will show this by the obvious manoeuvre of Fourier transforming (D.17), to get

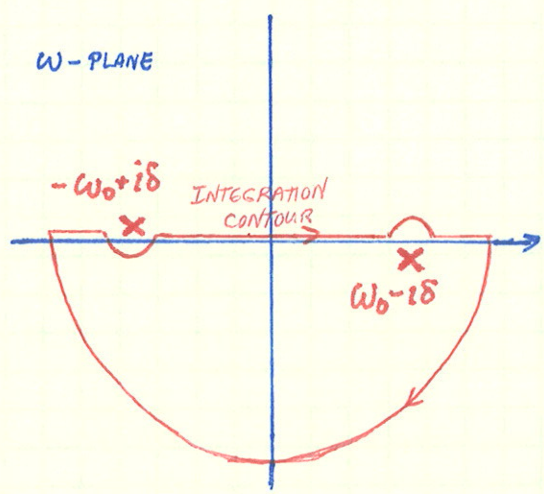
$$(\omega_0^2-\omega^2)K_0^{-1}(\omega) = i/m \qquad (D.18)$$

However this implies a singular solution in ω-space for $K_0(\omega)$, since it has, according to (D.18), poles at $\omega = \pm W_0$. The prescription for avoiding these is to write

$$\left.\begin{aligned} K_0^{-1}(\omega) \rightarrow D_0(\omega) &= \frac{i}{m}\frac{1}{2W_0}\left[\frac{1}{\omega-(W_0-i\delta)} - \frac{1}{\omega+(W_0-i\delta)}\right] \\ &\equiv \frac{i}{m}\frac{1}{\omega^2-\omega_0^2+i\delta} \end{aligned}\right\} \qquad (D.19)$$

from which we immediately verify that:

$$\left.\begin{aligned} D_0(t) &= \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}e^{-i\omega t}D_0(\omega) \\ D_0(\omega) &= \int_{-\infty}^{\infty}dt\, e^{i\omega t}D_0(t) \end{aligned}\right\} \qquad (D.20)$$



with $D_0(t)$ defined in (D.12).

The integration contour in the integral over ω, in (D.20), is shown in the Figure at left.

The propagator in (D.20), with the explicit expressions given in (D.12) and (D.20), is usually known as the Feynman propagator — as one sees when this formal development is generalized to an infinite set of independent oscillators, we are dealing here with the propagator for a scalar field (and, once polarisation degrees of freedom and gauge invariance is added, with a photon propagator). As such it is the essential ingredient in the propagator for any bosonic field.

Note that we can incorporate this pole structure directly into the generating functional with the substitution $W_0^2 \rightarrow W_0^2 - i\delta$, to write

$$Z_0[J] = \int \mathcal{D}q(s)\, \exp\left\{\frac{i}{\hbar}\int_{-\infty}^{\infty}ds\left[\frac{m}{2}\left(\dot{q}^2-(W_0-i\delta)^2q^2\right)+J(s)q(s)\right]\right\} \qquad (D.21)$$

Finally, we notice that the correlator $D_0(t)$ is itself nothing but the propagator of the oscillator itself, between vacuum states at 2 different times; we see that

$$\left.\begin{aligned} \chi_2^{00}(q_1,q_2) &\equiv \langle 0|\,T\{q(t_1)\,q(t_2)\}\,|0\rangle \\ &= \frac{(-i\hbar)^2}{Z_0[0]}\;\frac{\delta^2 Z_0[J]}{\delta J(t_1)\,\delta J(t_2)}\bigg|_{J=0} \\ &= D_0(t_1-t_2) \end{aligned}\right\} \qquad (D.22)$$

by simple differentiation of (D.13)

Note also that we can rederive all these results in a Euclidean framework (indeed, it is somewhat simpler). We have a Euclidean generating functional

$$\left.\begin{aligned} Z_0^E[J] &= \int \mathcal{D}q(\tau)\,\exp\Big\{-\frac{1}{\hbar}\int_{-\infty}^{\infty} d\tau\;\tfrac{1}{2}m\,[\dot{q}^2+w_0^2q^2] - J(\tau)\,q(\tau)\Big\} \\ &= \exp\Big\{\frac{1}{2\hbar}\int d\tau \int d\tau'\; J(\tau)\,D_0^E(\tau-\tau')\,J(\tau')\Big\} \end{aligned}\right\} \qquad (D.23)$$

where the Euclidean propagator $D_0^E(\tau)$ is the solution of

$$m\left(\frac{d^2}{d\tau^2}-w_0^2\right)D_0^E(\tau-\tau') = \delta(\tau-\tau') \qquad (D.24)$$

and is given by

$$D_0^E(\tau) = \frac{1}{2mw_0}\,e^{-w_0|\tau|} \qquad (D.25)$$

from which we see that $D_0^E(\tau)$ is the "Euclidean continuation" of the real-time propagator $D_0(t)$; in fact

$$D_0(-it) = D_0^E(t) \qquad (D.26)$$

(ii) Higher Matrix Elements $G^0_{nm}(t,t'|J)$: For ordinary relativistic field

theory, all we need is the vacuum generating functional. However in application to statistical mechanics and condensed matter systems, we need to know, at finite T, about transition amplitudes between excited states. For the SHO this means we need to compute the transition matrix element $G^0_{nm}(t,t'|J)$ given in (D.8)

A direct evaluation of $G^0_{nm}(t,t'|J)$ from (D.8) is of course extremely tedious and lengthy. One short cut is given by Feynman & Hibbs; one gets

$$G^0_{nm}(t,t'|J) = \frac{G^0_{00}(t,t'|J)}{(n!\,m!)^{1/2}}\sum_{\ell=0}^{\mathrm{Max}[n,m]} \ell!\;C^n_\ell\,C^m_\ell\,\big(iJ_{w_0}(t,t')\big)^{n-\ell}\big(iJ^*_{w_0}(t,t')\big)^{m-\ell} \qquad (D.27)$$

where $$C^n_\ell = \frac{n!}{\ell!(n-\ell)!} \qquad \text{(D.28)}$$

is just the usual binomial coefficient, and

$$J_{\omega_0}(t,t') = \frac{1}{(2\omega_0 m^2)^{1/2}} \int_{t'}^{t} ds\, e^{-i\omega_0 s} J(s) \qquad \text{(D.29)}$$

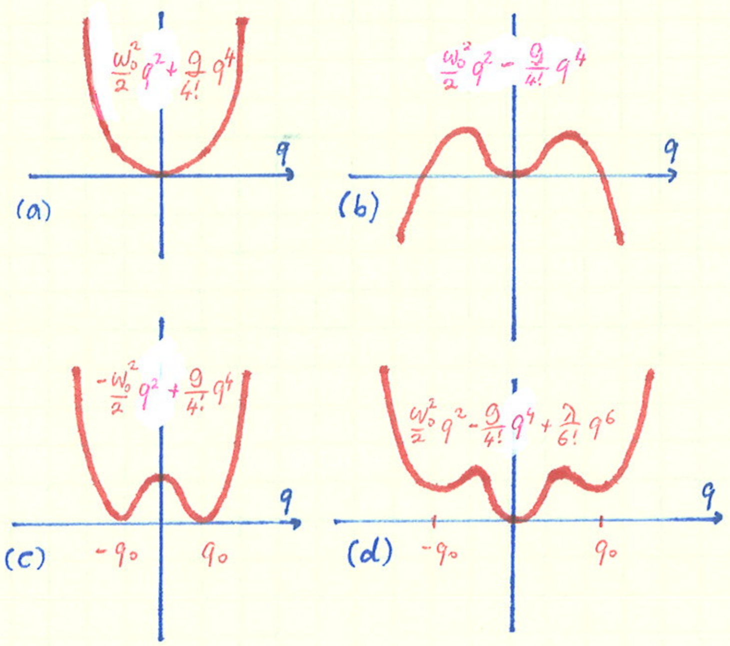
is, roughly speaking, the Fourier component of $J(t)$ at frequency ω_0 (ie., which resonates with the oscillator). We can think of (D.27) as describing a sequence of transitions through a set of intermediate states, each one driven by the factor $J_{\omega_0}(t,t')$; the combinatorial factors label the many different ways this can be done.

Results like this are important when one comes to deal with, eg., response functions for condensed matter systems at finite T.

E. NON-HARMONIC POTENTIALS : PERTURBATION THEORY

We have just seen that the SHO problem is of key importance, because a set of N oscillators, with $N \to \infty$, models a scalar quantum field. However it is a FREE field – it has no interactions in it.

It is then clear that a prototype for the study of interacting fields is provided by the simple problem of a non-parabolic potential $V(q)$. There are a few examples we can think of, all of which are simple in the sense that we are simply adding polynomial terms, in q, to the original quadratic potential.



Each of the examples shown at left presents its own features. The model in (a) is the "ϕ^4" model, with a positive 4th order coupling, and a stable low-energy state at $q = 0$.

The model in (b) has a metastable ground state at $q = 0$, and the model in (c) has 2 metastable "vacua" at $q = \pm q_0$ (they are metastable because the system can tunnel between the two, and the correct vacuum is a symmetric superposition of the two). Finally (d) has a stable vacuum at $q = 0$, and 2 metastable excited states at $\pm q_0$. We see that models (b), (c), and (d) all involve tunneling, which is a non-perturbative process (it lies outside a perturbative expansion in powers of g or λ; in fact WKB tells us that tunneling processes are $O(e^{-1/\tilde{g}})$ or $O(e^{-1/\tilde{\lambda}})$, where $\tilde{g}$ and $\tilde{\lambda}$ are dimensionless parameters obtained from the energies λ and g.

The development given below is fairly easily adapted to include such tunneling processes, (the field-theoretical analogue of these being instanton processes). However we shall stick here with a perturbative development. Thus we shall be developing the path integral approach to a potential like model (a) above.

We begin by writing the Hamiltonian and Lagrangian of the system as

$$\left.\begin{aligned} \mathcal{H}(p,q;J) &= H_0(p,q) + V(q) - J(t)q(t) \\ L(q\dot{q};J) &= L_0(q\dot{q}) - V(q) + J(t)q(t) \end{aligned}\right\} \qquad (E.1)$$

where the SHO forms were given in eqtn. (D.1). We now write the Green function and the propagator for the system in the form (compare eqtn. (D.15)):

$$\mathcal{G}(xx'|J) = \int_{x'}^{x}\mathcal{D}q\, e^{-i/\hbar\int_{t'}^{t}ds\left[\frac{1}{2}q(s)K_0(s-s')q(s') + V(q(s)) - q(s)J(s)\right]} \qquad (E.2)$$

where again we define: $\qquad K_0(t-t') = m\left(\frac{d^2}{dt^2} + \omega_0^2\right)\delta(t-t') \qquad (E.3)$

as the SHO "kinetic" or free field operator; and in the same way we have for the generating functional ("partition function") the functional form:

$$Z[J] = \int\mathcal{D}q(s)\, e^{-i/\hbar\int_{-\infty}^{\infty}ds\left[\frac{1}{2}q(s)K_0(s-s')q(s') + V(q(s)) - q(s)J(s)\right]} \qquad (E.4)$$

What we would now like to do is rewrite such expressions in such a way as to pull out the factor $G_0(xx'|J)$ and $Z_0[J]$, referring solely to the SHO — this is because we have exact expressions for these. The resulting functional forms can be used to generate perturbative expansions for the effect of the anharmonic part $V(q)$ of the potential, in a path integral language.

Result 1: Differentiate $\delta/\delta J$.: To get our first result we note that we can think of forms like (E.2) and (E.4) as straightforward generalizations of ordinary 1-d integrals to infinite-dimensional integrals. Thus consider the following integral

$$I_P(J) = \int dq\, P(q)\, e^{-\Phi_J(q)} \qquad (E.5)$$

where $\qquad \Phi_J(q) = \frac{1}{2}qK_0q + Jq + c \qquad (E.6)$

is a quadratic form in the variable q, $P(q)$ is some polynomial in q, and K_0, J, and c are constants. This integral is a standard form — we are dealing with Gaussian integrals, and we know that if $P(q) = 1$, then we just have the usual result

$$I(J) = \int dq\, e^{-Q_J(q)} = \frac{1}{K_0^{1/2}}\, e^{\frac{1}{2} J K_0^{-1} J - C} \tag{E.7}$$

and if we write the polynomial $P(q) = \sum_n c_n q^n$, then it is easy to see that

$$\left.\begin{aligned} I_P(J) &= \int dq \sum_n c_n q^n e^{-Q_J(q)} \\ &= \int dq \sum_n c_n (-d/dJ)\, e^{-Q_J(q)} = P(-d/dJ) \int dq\, e^{-Q_J(q)} \\ &= P(-d/dJ)\, I(J) \end{aligned}\right\} \tag{E.8}$$

Now this result is straightforwardly adapted to functional integrals, in the form

$$\int \mathcal{D}q\, P[q]\, e^{-Q_J[q]} = P(-\delta/\delta J) \int \mathcal{D}q\, e^{-Q_J[q]} \tag{E.9}$$

and moreover we see that in our case, the polynomial in question is just the exponential $\exp[-i/\hbar \int ds\, V(q(s))]$, which can always be expanded in a power series in the integral over $q(s)$. If we now put in the factors of i and $\hbar$, etc., we get the important result that

$$\mathcal{G}(xx'|J) = e^{-i/\hbar \int_{t'}^{t} ds\, V(-i\hbar\, \delta/\delta J(s))}\, G_0(x,x'|J) \tag{E.9}$$

so that in particular the vacuum amplitude is given by

$$\left.\begin{aligned} \mathcal{G}_{00}(t,t'|J) &= e^{-i/\hbar \int_{t'}^{t} ds\, V(-i\hbar\, \delta/\delta J(s))}\, G^0_{00}(t,t'|J) \\ &= e^{-i/\hbar \int_{t'}^{t} ds\, V(-i\hbar\, \delta/\delta J(s))}\, e^{-\frac{1}{2\hbar} \int_{t'}^{t} ds \int_{t'}^{t} ds'\, J(s) D_0(s-s') J(s')} \end{aligned}\right\} \tag{E.10}$$

where we use the explicit form in (D.12) for G^0_{00}. Now (E.10) is a very convenient form – it is simply a polynomial operator in $\delta/\delta J$ acting on the simple quadratic form $e^{-\frac{1}{2} J D_0 J}$. Moreover, if we take the limit $J \to 0$ in (E.10) after doing the differentiation, we get a result for $\mathcal{G}_{00}(t,t')$ in the absence of an external driving field. The result (E.9) can also be written out in a similar explicit form, using our result in (D.5)-(D.7) for $G_0(xx'|J)$, but the result is more unweildy. If we write $\mathcal{G}(xx'|J)$ in the form

$$\left.\begin{aligned} \mathcal{G}(xx'|J) &= G_0(xx'|J)\, e^{-i/\hbar \int ds\, [L_1(s) J(s) + \frac{1}{2} \int ds'\, J(s') L_2(s,s') J(s')]} \\ &\equiv G_0(xx'|J)\, e^{-i/\hbar\, [(L_1, J) + \frac{1}{2}(J, L_2, J)]} \end{aligned}\right\} \tag{E.11}$$

then the result for $\mathcal{G}(xx'|J)$ can be written as

$$\left.\begin{aligned}\mathcal{G}(xx'|J) &= e^{-i/\hbar \int_{t'}^{t} ds\, V(-i\hbar\, \delta/\delta J(s))}\; G_0(xx'|J) \\ &= G_0(xx'|J=0)\, e^{-i/\hbar \int ds\, V(-i\hbar\, \delta/\delta J(s))}\; e^{-i/\hbar [(L_1, J) + 1/2 (J, L_2, J)]}\end{aligned}\right\} \quad (E.12)$$

where the function $G_0(xx') = G_0(xx'|J=0)$ is just the free oscillator in the absence of any driving field (see eqtns. (D.2) & (D.3)).

Finally, by noticing the the correct time limits of (E.10) just give us the generating functional, we get

$$\left.\begin{aligned}Z[J] &= e^{-i/\hbar \int_{-\infty}^{\infty} ds\, V(-i\hbar\, \delta/\delta J(s))}\; Z_0(J) \\ &\equiv e^{-i/\hbar \int_{-\infty}^{\infty} ds\, V(-i\hbar\, \delta/\delta J(s))}\; e^{-1/2\hbar \int_{-\infty}^{\infty} ds \int_{-\infty}^{\infty} ds'\, J(s) D_0(s-s') J(s')}\end{aligned}\right\} \quad (E.13)$$

To see how this works in practise, we will consider an example below. The real use of an expression like (E.13), however, is in QFT, where it can be used to generate all the Feynman diagrams for $Z[J]$ (and, by functional differentiation of $Z[J]$ w.r.t. J, all the diagrams for any correlator).

Result 2 : Differentiate $\delta/\delta q$: Since the external field $J(t)$ couples to $q(t)$, and in this sense is conjugate to it, we see that we can also, in principle, generate an expansion for the propagator and for Z in terms of $\delta/\delta q(t)$, instead of $\delta/\delta J(t)$. The following result can also be used to generate a diagrammatic expansion, in a somewhat more obvious way.

Let us go back again to ordinary integrals, and notice that for 2 functions f and g, we have

$$f(-i\partial_{\underline{j}})\, g(\underline{j}) = g(-i\partial_{\underline{q}})\, f(\underline{q})\, e^{i\underline{q}\cdot\underline{j}}\Big|_{q=0} \qquad (E.14)$$

for two vectors $\underline{q}$ and $\underline{j}$.

Applying this to our result (E.13) for $Z[J]$, and converting to functional integrals & differentials, we see we can write

$$e^{-i/\hbar \int_{-\infty}^{\infty} ds\, V(-i\hbar\, \delta/\delta J(s))}\; Z_0[J] = Z_0[-i\, \delta/\delta q(s)]\, e^{-i/\hbar \int ds [V(q(s)) - q(s) J(s)]}\Big|_{q=0} \qquad (E.15)$$

which, using (D.13), gives explicitly

$$Z[J] = e^{1/2 \int ds \int ds'\, D_0(s-s')\, \delta/\delta q(s)\, \delta/\delta q(s')}\; e^{-i/\hbar \int ds [V(q(s)) - q(s) J(s)]}\Big|_{q=0} \qquad (E.16)$$

where we are now computing functional derivatives w.r.t. the path variable $q(t)$, as opposed to the external force variable $J(t)$.

Such an expression is not obviously useful in QM (and nor is its generalization to describe $\mathcal{G}(xx'|J)$ in terms of $\delta/\delta q(t)$); but in QFT it corresponds to taking field derivatives of the interaction part of the generating functional, and then putting the field to zero (ie, to its vacuum state); in this case it is very useful.

Result 3 : Equation of Motion for $Z[J]$, etc.

: Just as the ordinary Green function w/o external driving field $J(t)$ satisfies an eqtn of motion, so does the driven Green function $\mathcal{G}(xx'|J)$. However in a path integral framework, where we deal with classical paths, we may be more interested in just looking at the eqtns of motion of the paths $q(t)$ themselves, or at the generating functional of $J(t)$.

To do this, let's consider a rather simple question first, viz., what is the "functional Fourier transform" of $\mathcal{G}(xx'|J)$ to its "conjugate variable" $q(t)$, ie., to a functional $\mathcal{G}(xx'|q)$, which depends on the particular path $q(t)$ followed by the system. Actually the answer is really obvious and illuminating - if we simply write out the path integral expression for $\mathcal{G}(xx'|J)$, we see it has an obvious Fourier transform pair:

$$
\left.\begin{aligned}
\mathcal{G}(xx'|J(t)) &= \int_{x'}^{x} \mathcal{D}q\, e^{i/\hbar S[q(t)]}\, e^{i/\hbar \int_{t'}^{t} dt\, q(t) J(t)} \\
&= \int_{x'}^{x} \mathcal{D}q(t)\, \mathcal{G}(xx'|q(t))\, e^{i/\hbar \int_{t'}^{t} dt\, q(t) J(t)} \\
\text{so that} \quad \mathcal{G}(xx'|q(t)) &= \int \mathcal{D}J(t)\, \mathcal{G}(xx'|J(t))\, e^{-i/\hbar \int dt\, q(t) J(t)} \\
&= e^{i/\hbar S[q(t)]} \equiv e^{i/\hbar \int_{t'}^{t} dt\, L(q(t))}
\end{aligned}\right\} \qquad (E.17)
$$

ie., the propagator $\mathcal{G}(xx'|q(t))$ is simply the probability amplitude to follow ONE SPECIFIC PATH $q(t)$ between $x' = (\underline{r}, t')$ and $x = (\underline{r}, t)$.

Now, where we want to write down eqtns of motion, we typically functionally differentiate the action to get Lagrange's eqtns. Here we will simply differentiate not the action, but the propagator itself; and we will use the fact that the integral of this total derivative is zero, to derive a variational result.

Start first with the "sourceless" propagator (ie., for which $J = 0$); then we have

$$\int \mathcal{D}q(\tau) \frac{\delta}{\delta q(\tau)} \mathcal{G}(xx'|q(\tau)) = 0 \qquad (E.18)$$

However this eqtn. simply reads

$$\int \mathcal{D}q(\tau) \left[\hat{K}(t) q(\tau) - \frac{\partial V}{\partial q}(q) \right] e^{\frac{i}{\hbar} S[q]} = 0 \qquad (E.19)$$

where we have assumed the Lagrangian takes the form

$$L(q) = \tfrac{1}{2} q \hat{K}_0 q - V(q) \qquad (E.20)$$

given in (E.1) and (E.3). Since (E.19) is true for different paths, we see that

$$\hat{K}_0(t) q(t) - V'(q) = 0 \qquad (E.21)$$

which is just Newton's 2nd law.

Now let's consider the full Green function $\mathcal{G}(x,x'|J)$, and apply the same treatment. We then have

$$\int \mathcal{D}q(\tau) \left[\frac{\delta S[q]}{\delta q(\tau)} - J(\tau) \right] e^{\frac{i}{\hbar}(S[q] - \int d\tau\, J(\tau) q(\tau))} = 0 \qquad (E.22)$$

Now lets use the functional identity

$$-i\hbar \frac{\delta}{\delta J(t)} e^{\frac{i}{\hbar}\int dt\, J(t) q(t)} = q(t) e^{\frac{i}{\hbar}\int dt\, J(t) q(t)} \qquad (E.23)$$

which can be applied any number of times to deal with some polynomial $q^n(t) \exp\{\frac{i}{\hbar}\int dt\, J(t) q(t)\}$, by operating n times with $-i\hbar\, \delta/\delta J$; since $\delta S/\delta q$ is just such a polynomial, we can transform (E.22) to give (once the variation has been removed) the equation

$$\left[\left.\frac{\delta S[q]}{\delta q(\tau)}\right|_{q = -i\hbar \delta/\delta J} - J(\tau) \right] \mathcal{G}(x,x'|J(\tau)) = 0 \qquad (E.24)$$

where we use the notation $\left.\frac{\delta S}{\delta q}\right|_{q=-i\hbar\frac{\delta}{\delta J}}$ to mean that $-i\hbar\frac{\delta}{\delta J}$ is substituted for q, in whatever polynomial in q represents $\delta S/\delta q$. For the specific Lagrangian of (E.20), this just gives

$$\left[i\hbar K_0(t) \frac{\delta}{\delta J(t)} + \left.\frac{\partial V(q)}{\partial q}\right|_{q = -i\hbar \delta/\delta J} + J(t) \right] \mathcal{G}(xx';J) = 0 \qquad (E.25)$$

an eqtn. of motion for $\mathcal{G}(xx'|J)$ which is usually known as the "Schwinger-Dyson" eqtn. Again, for ordinary QM this doesn't give us anything more than Newton's 2nd law. However, we will see its power once we get to

QFT, and it's use to generate a hierarchy of coupled eqtns of motion.

Just as before, we can specialize these results to discuss the generating functional. The derivations are the same, and the result is just like (E.24); we have

$$\left[\frac{\delta S[q]}{\delta q(t)} \Bigg|_{q = -i\hbar\, \delta/\delta J(t)} - J(t) \right] Z[J] = 0 \tag{E.26}$$

which gives, for the Lagrangian in (E.20), the result

$$\left[i\hbar K_0(t) \frac{\delta}{\delta J(t)} + \frac{\partial V}{\partial q}\Bigg|_{q = -i\hbar\, \delta/\delta J} + J(t) \right] Z[J] = 0 \tag{E.27}$$

Now, this is an eqtn. of motion for $Z[J]$, and it is of considerable methodological interest to show that its solution is just the result we already found in eqtn (E.13), essentially by direct calculation.

Let's first verify that the free generating functional $Z_0[J]$ satisfies (E.27) (with $V = 0$). We want to show that

$$\left. \begin{aligned} \left[i\hbar \hat{K}_0 \frac{\delta}{\delta J(t)} + J(t) \right] Z_0[J] &= \left[i\hbar \hat{K}_0\, \delta/\delta J + J \right] e^{-\frac{1}{2\hbar} \int ds \int ds'\, J(s)\, D_0(s-s')\, J(s')} \\ &= 0 \end{aligned} \right\} \quad (E.27)$$

However, it is easily verified that $(i\hbar \hat{K}_0\, \delta/\delta J)\, Z_0 = -J Z_0$; and so we get (E.27). Now consider the interacting case. To do this we need a few handy identities, as follows:

(i) We have the commutator $\left[J(t), -i\hbar\, \delta/\delta J(t') \right] = i\hbar\, \delta(t-t')$ (E.28)

as can be shown by acting upon a wave-function like $\psi_J(t) = e^{-\frac{i}{\hbar} \int dt\, J(t) q(t)}$. This of course is reminiscent of the usual $[x, -i\hbar \partial_x] = i\hbar$.

(ii) In the same way, we have $\left[J(t), \left(-i\hbar\, \delta/\delta J(t')\right)^n \right] = i\hbar n\, \delta(t-t') \left(-i\hbar\, \delta/\delta J(t')\right)^{n-1}$ (E.29)

so that the commutator reduces to power of the derivative by one. This can then be used to show that for some function $f(-i\hbar\, \delta/\delta J)$, which can be expanded in a power series, will be writeable in the same way — if we then integrate over this function to get rid of the δ-fn, we get

(iii) the commutator

$$\left. \begin{aligned} \left[J(t), \int dt'\, f\left(-i\hbar\, \delta/\delta J(t')\right) \right] &= i\hbar F'\left(-i\hbar\, \delta/\delta J(t)\right) \\ &\equiv i\hbar \frac{\partial F}{\partial x}\Bigg|_{x = -i\hbar\, \delta/\delta J(t)} \end{aligned} \right\} \quad (E.30)$$

With these generalizations of the simpler commutation relations one meets in elementary QM, we can now provide a generalization of the unitary (Heisenberg) transformation that one uses to shift operators & and to generate canonical transformations. Defining the operators

$$\left.\begin{aligned} \hat{A} &= J(t) \\ \hat{B} &= i/\hbar\, V\left[\int dt\, (-i\hbar\, \delta/\delta J(t))\right] \end{aligned}\right\} \tag{E.31}$$

then, using the usual Baker-Hausdorff formula $e^{B} A e^{-B} = A + [B,A] + \cdots$, we get the result

$$\left.\begin{aligned} e^{i/\hbar \int dt' V(-i\hbar\, \delta/\delta J(t'))}\, J(t)\, e^{-i/\hbar \int dt' V(-i\hbar\, \delta/\delta J(t'))} &= J(t) + V'(-i\hbar\, \delta/\delta J(t)) \\ &\equiv J(t) + \left.\frac{\partial V}{\partial x}\right|_{x = -i\hbar\, \delta/\delta J(t)} \end{aligned}\right\} \tag{E.32}$$

From this it now becomes obvious how to prove that $Z[J]$ in (E.13) is going to satisfy the eqtn of motion (E.27). Symbolically we write (E.13) as $Z = e^{iV_J} Z_0$, so that $JZ = Je^{iV_J} Z_0 = e^{iV_J}(e^{-iV_J} J e^{iV_J}) Z_0$, which by (E.32) is equal to $e^{iV_J}(J + V_J') Z_0$, ie., we have

$$J(t) Z[J] = e^{i/\hbar \int dt' V(-i\hbar\, \delta/\delta J(t'))} \left[J(t) + V'(-i\hbar\, \delta/\delta J(t))\right] Z_0[J] \tag{E.33}$$

Using (E.27) for $J(t) Z_0[J]$, and then reversing the order of e^{iV_J} and V_J' in the 2nd part of (E.33) (since they commute), this then becomes

$$J(t) Z[J] = \left[-i\hbar \hat{K}_0(t) \frac{\delta}{\delta J(t)} - V'(-i\hbar\, \delta/\delta J(t))\right] Z[J] \tag{E.44}$$

which is just the original eqtn of motion (E.27). We have thus verified that $Z[J]$ written in the form (E.13), ie., $Z = e^{iV_J} Z_0$, is the solution to the eqtn of motion.

This is all I want to do on this topic, in the context of ordinary QM. Some of what is done above will seem pretty esoteric, and indeed is so for ordinary QM – it's use is only obvious in QFT, where it is very powerful. Nevertheless it is useful to try out examples - Try $V(q) = gq^4/4$!