Selected topics in solid state physics 2

Part 4

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I. FEYNMAN-VERNON INFLUENCE FUNCTIONAL

A. Crash course on path integrals

Consider a particle described by a canonical pair $\hat{x}, \hat{p}$, such that $[\hat{x}, \hat{p}] = i\hbar$. The particle's dynamics is described by the hamiltonian $H(x,p)$. We want to calculate the propagator

$$K(x_f, t_f; x_i, t_i) \equiv \langle x_f | \, e^{-(i/\hbar)(t_f - t_i)H} \, | x_i \rangle \tag{1}$$

We present the exponent as a product of many

$$K(x_f, t_f; x_i, t_i) = \langle x_f | \prod_{n=1}^{N} e^{-(i/\hbar)(t_n - t_{n-1})H} \, | x_i \rangle \ , \tag{2}$$

where $t_0 = t_i$ and $t_N = t_f$. We assume that $t_{n+1} - t_n = \Delta t$, i.e., the time interval $t_f - t_i$ is divided into N equal intervals. We insert $N-1$ unity operators $\hat{1} = \int dx_n \, |x_n\rangle \langle x_n|$ $(n = 1, \ldots, N-1)$.

$$K(x_f, t_f; x_i, t_i) = \int dx_1 \ldots \int dx_{N-1} \prod_{n=1}^{N} \langle x_n | \, e^{-(i/\hbar)\Delta t H} \, | x_{n-1} \rangle \ , \tag{3}$$

where $x_0 = x_i$ and $x_N = x_f$. We now insert N unity operators $\hat{1} = \int dp_m \, |p_m\rangle \langle p_m|$ $(m = 1, \ldots, N)$, where $|p\rangle = (2\pi\hbar)^{-1/2} e^{(i/\hbar)px}$.

$$K(x_f, t_f; x_i, t_i) = \int dx_1 \ldots dx_{N-1} dp_1 \ldots dp_N \prod_{n=1}^{N} \langle x_n | \, e^{-(i/\hbar)\Delta t H} \, | p_n \rangle \langle p_n | x_{n-1} \rangle \ , \tag{4}$$

Assume $H = K(p) + V(x)$. Then

$$\begin{aligned} \langle x_n | \, e^{-(i/\hbar)\Delta t H} \, | p_n \rangle &\approx \langle x_n | \, 1 - (i/\hbar)\Delta t H + O(\Delta t^2) \, | p_n \rangle \\ &= \langle x_n | p_n \rangle \left(1 - \frac{i\Delta t}{\hbar} \left[K(p_n) + V(x_n) \right] + O(\Delta t^2) \right) \\ &\approx \langle x_n | p_n \rangle \, e^{-(i/\hbar)\Delta t H(p_n, x_n)} \ . \end{aligned} \tag{5}$$

Thus we obtain

$$\begin{aligned} K(x_f, t_f; x_i, t_i) &= \int dx_1 \ldots dx_{N-1} dp_1 \ldots dp_N \prod_{n=1}^{N} \langle x_n | p_n \rangle \, e^{-(i/\hbar)\Delta t H(p_n, x_n)} \langle p_n | x_{n-1} \rangle \\ &= \int \prod_{n=1}^{N-1} dx_n \prod_{n=1}^{N} \frac{dp_n}{2\pi\hbar} \, e^{(i/\hbar) \sum_{n=1}^{n=N} [p_n (x_n - x_{n-1}) - \Delta t \, H(x_n, p_n)]} \ . \end{aligned} \tag{6}$$

The symbolic way to write this in the limit $N \to \infty$ reads

$$K(x_f, t_f; x_i, t_i) = \int DxDp \, \exp\left[(i/\hbar) S_H \right] \ , \tag{7}$$

where

$$S_H = \int_{t_i}^{t_f} dt(p\dot{x} - H(p,x)) \ . \tag{8}$$

If the kinetic energy is quadratic, $K(p) = p^2/(2m)$, it is possible to perform the integration over the momenta. Using

$$\int \frac{dp_n}{2\pi\hbar} e^{(i/\hbar)\left[p_n(x_n - x_{n-1}) - \Delta t \frac{p_n^2}{2m}\right]} = C e^{(i/\hbar)\frac{m(x_n - x_{n-1})^2}{2\Delta t}} \ , \tag{9}$$

where $C = \sqrt{\frac{m}{2\pi i\hbar\Delta t}}$. This gives

$$K(x_f, t_f; x_i, t_i) = C^N \int \prod_{n=1}^{N-1} dx_n e^{(i/\hbar)\sum_{n=1}^{n=N} \Delta t \left[\frac{m(x_n - x_{n-1})^2}{2(\Delta t)^2} - V(x_n)\right]} \ , \tag{10}$$

which is symbolically written

$$K(x_f, t_f; x_i, t_i) = \int Dx \exp\left[(i/\hbar) S_L\right] \ , \tag{11}$$

where

$$S_L = \int_{t_i}^{t_f} dt\, L(x, \dot{x}) = \int_{t_i}^{t_f} dt \left[\frac{m\dot{x}^2}{2} - V(x)\right] \ . \tag{12}$$

1. *Amplitudes*

The amplitude to go from state i to state f is given by

$$\begin{aligned} A_{nm} = \langle \phi_f | \, e^{-(i/\hbar)H(t_f - t_i)} \, |\phi_i\rangle \ &= \int dx_f dx_i \langle \phi_f \, |x_f\rangle \, \langle x_f | \, e^{-(i/\hbar)H(t_f - t_i)} \, |x_i\rangle \, \langle x_i | \, \phi_i\rangle \\ &= \int dx_f dx_i \langle \phi_f \, |x_f\rangle \, K(x_f, t_f; x_i, t_i) \, \langle x_i | \, \phi_i\rangle \\ &= \int dx_f dx_i \phi_f^*(x_f) K(x_f, t_f; x_i, t_i) \phi_i(x_i) \ . \end{aligned} \tag{13}$$

B. Feynman-Vernon (density matrix evolution)

Consider now a degree of freedom denoted by Q and the degrees of freedom of the bath denoted by X. For simplicity we consider the Lagrangian such that the coupling is via coordinates Q, X, whereas the velocities appear only in the Lagrangians of the system and the bath:

$$L(Q, \dot{Q}, X, \dot{X}) = L_S(Q, \dot{Q}) + L_B(X, \dot{X}) + L_I(X, Q) \tag{14}$$

Assume initially at time t_i the whole system was in a factorised state described by the density matrix $\rho_i(Q_i, X_i, Q_i', X_i') = \rho_{Si}(Q_i, Q_i')\rho_{Bi}(X_i, X_i')$. Then, at later time t_f the density matrix of the whole system reads

$$\rho_f(Q_f, X_f, Q_f', X_f') = \int dQ_i dQ_i' dX_i dX_i' \\ K(Q_f, X_f, t_f; Q_i, X_i, t_i) K^*(Q_f', X_f', t_f; Q_i', X_i', t_i) \rho_i(Q_i, X_i, Q_i', X_i') \ . \tag{15}$$

Here

$$K(Q_f, X_f, t_f; Q_i, X_i, t_i) = \int DQDX \exp\left((i/\hbar)\left[S_S[Q] + S_B[X] + S_I[Q, X]\right]\right) \ , \tag{16}$$

Since the initial state was factorised we obtain for the reduced density matrix of the system (taking trace over the bath)

$$\rho_{Sf}(Q_f, Q_f') \\ = \int dQ_i dQ_i' \int DQ \int DQ' \exp\left((i/\hbar)\left[S_S[Q] - S_S[Q']\right]\right) \times F[Q, Q'] \rho_{Si}(Q_i, Q_i') \ . \tag{17}$$

where $F[Q, Q']$ is the so called influence functional given by

$$F[Q, Q'] = \int dX_i dX_f \int dX_i' dX_f' \delta(X_f - X_f') \rho_{Bi}(X_i, X_i') \\ \int DXDX' \exp\left((i/\hbar)\left[S_B[X] - S_B[X'] + S_I[Q, X] - S_I[Q', X']\right]\right) \ . \tag{18}$$

In the influence functional the two paths $Q(t)$ and $Q'(t)$ serve as external parameters.

C. Linear coupling to one harmonic oscillator

Assume $S_I = \int dt Q X$, where $X = \lambda x$ and x is the coordinate of a linear oscillator with mass m and eigenfrequency ω_0. We will also need the equilibrium density matrix of an oscillator

$$\rho_T(x, x') = \sqrt{\frac{m\omega_0}{2\pi\hbar \sinh(\hbar\omega_0/k_B T)}} e^{-\frac{m\omega_0}{2\hbar \sinh(\hbar\omega_0/k_B T)}\left[\left(x^2 + x'^2\right)\cosh(\hbar\omega_0/k_B T) - 2xx'\right]} \tag{19}$$

We observe that in this case the influence functional is given by the Gaussian integral.

To understand this deeper we transform again to the discrete time representation. The Keldysh contour is shown in Fig. 1 Using the numeration of Fig. 1 we introduce $x_n = x(t_n)$.

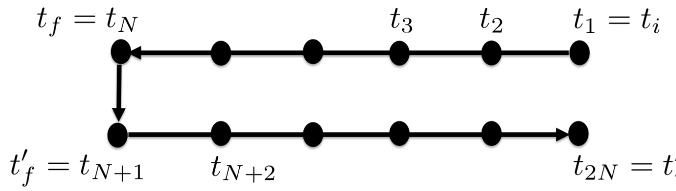

FIG. 1: Keldysh contour with discrete times.

Then $x_i = x_0$, $x'_i = x_{2N}$, $x_f = x_N$, and $x'_f = x_{N+1}$. The influence functional reads

$$F[Q,Q'] \;=\; \mathcal{N}\int \prod_{n=1}^{n=2N} dx_n \delta(x_N - x_{N+1})\rho_T(x_1,x_{2N}) \exp\left((i/\hbar)\left[S_B[x] - S_B[x']\right]\right) \exp\left((i\lambda\Delta t/\hbar)\left[\sum_{n=1}^{n=N} x_n Q_n - \sum_{n=N+1}^{n=2N} x_n Q_n\right]\right) . \tag{20}$$

Here

$$S_B[x] = \sum_{n=2}^{n=N} \Delta t \left[\frac{m(x_n - x_{n-1})^2}{2(\Delta t)^2} - \frac{m\omega_0^2 x_n^2}{2}\right] \tag{21}$$

and

$$S_B[x'] = \sum_{n=N+2}^{n=2N} \Delta t \left[\frac{m(x_n - x_{n-1})^2}{2(\Delta t)^2} - \frac{m\omega_0^2 x_n^2}{2}\right] . \tag{22}$$

We can present this as

$$F[Q,Q'] \;=\; \mathcal{N}\int \prod_{n=1}^{n=2N} dx_n \exp\left[\frac{i}{2}\sum_{n,m=1}^{2N} x_n \left(G^{-1}\right)_{nm} x_m\right] \times\; \exp\left((i\lambda\Delta t/\hbar)\left[\sum_{n=1}^{n=N} x_n Q_n - \sum_{n=N+1}^{n=2N} x_n Q_n\right]\right) . \tag{23}$$

The matrix G^{-1} has a close to diagonal form given by Eqs. (21,22). However is has a far off-diagonal matrix element $(G^{-1})_{1,2N}$ given by the initial density matrix of the oscillator and also for $(G^{-1})_{N,N+1}$ there is a special entry due to the delta function $\delta(x_N - x_{N+1})$ in Eq. (20).

1. *Continuous representation*

To eliminate the minus sign we introduce $\Delta t_n = \Delta t$ for $n = 1,\ldots,N$ and $\Delta t_n = -\Delta t$ for $n = N+1,\ldots,2N$. Then, there is a substantial temptation to rewrite Eq. (23) as

$$F[Q,Q'] \;=\; \int Dx \exp\left[\frac{i}{2}\int_K dt_1 dt_2\, x(t_1) G^{-1}_{(t_1,t_2)} x(t_2)\right] \times\; \exp\left(i(\lambda/\hbar)\int_K dt\, Q(t)x(t)\right) . \tag{24}$$

However one should remember that the inverse matrix (Green's function) G^{-1} is NOT just given by its expressions on the upper and lower contours, i.e.,

$$\hbar G^{-1}_{(t_1,t_2)} = \pm \left[m \left(\frac{\partial}{\partial t_1}\right)^T \delta(t_1 - t_2) \frac{\partial}{\partial t_2} - m\omega_0^2\, \delta(t_1 - t_2) \right] \ , \tag{25}$$

(plus when $t_1 = t_2$ on upper contour, minus when $t_1 = t_2$ on lower contour) but one should take into account the off-diagonals (terms connecting the upper and the lower contours). These terms are very difficult to present in the continuous form.

Performing the usual Gaussian integration we obtain

$$F[Q, Q'] = \frac{\mathcal{N}_1}{\sqrt{Det(-iG^{-1})}} \exp\left[-\frac{i\lambda^2}{2\hbar^2} \int_K dt_1 dt_2\, Q(t_1) G_{(t_1,t_2)} Q(t_2) \right] \ . \tag{26}$$

The pre-factor is however identically equal to unity. Indeed

$$\frac{\mathcal{N}_1}{\sqrt{Det(-iG^{-1})}} = \int Dx \exp\left[\frac{i}{2} \int_K dt_1 dt_2\, x(t_1) G^{-1}_{(t_1,t_2)} x(t_2) \right] = \mathrm{Tr}(\rho_B(t_f)) = 1 \ . \tag{27}$$

Thus, finally

$$F[Q, Q'] = \exp\left[-\frac{i\lambda^2}{2\hbar^2} \int_K dt_1 dt_2\, Q(t_1) G_{(t_1,t_2)} Q(t_2) \right] \ . \tag{28}$$

D. Relation of matrix G to the correlators

This relation is easiest to understand using the already mentioned relation

$$1 = \mathrm{Tr}(\rho_B(t_f)) = \int Dx \exp\left[\frac{i}{2} \int_K dt_1 dt_2\, x(t_1) G^{-1}_{(t_1,t_2)} x(t_2) \right] \ . \tag{29}$$

Consider now the time ordered correlation function

$$ig(\tau_1, \tau_2) = \langle T_K \hat{x}(\tau_1) \hat{x}(\tau_2) \rangle \ . \tag{30}$$

One can calculate this correlation function exactly the same way as the influence functional using the path integral. Let us for example consider the case when both τ_1 and τ_2 are on the upper Keldysh contour and $\tau_1 > \tau_2$. Then

$$\begin{aligned} ig(\tau_1, \tau_2) &= \langle T_K \hat{x}(\tau_1) \hat{x}(\tau_2) \rangle \\ &= \mathrm{Tr}\left[\hat{x}(\tau_1) \hat{x}(\tau_2) \rho_B(t_i) \right] = \mathrm{Tr}\left[e^{iH_B\tau_1} \hat{x} e^{-iH_B\tau_1} e^{iH_B\tau_2} \hat{x} e^{-iH_B\tau_2} \rho_B(t_i) \right] \ . \end{aligned} \tag{31}$$

Using the fact that the initial density matrix $\rho_B(t_i)$ and the Hamiltonian H_B commute we can write

$$
\begin{aligned}
ig(\tau_1,\tau_2) &= \mathrm{Tr}\left[e^{-iH_Bt_f}e^{iH_B\tau_1}\hat{x}e^{-iH_B\tau_1}e^{iH_B\tau_2}\hat{x}e^{-iH_B\tau_2}e^{iH_Bt_i}\rho_B(t_i)e^{-iH_Bt_i}e^{iH_Bt_f}\right] \\
&= \mathrm{Tr}\left[e^{-iH_B(t_f-\tau_1}\hat{x}e^{-iH_B(\tau_1-\tau_2)}\hat{x}e^{-iH_B(\tau_2-t_i)}\rho_B(t_i)e^{iH_B(t_f-t_i)}\right] \ . \qquad (32)
\end{aligned}
$$

We rewrite this formula in terms of propagators and, ultimately, as a path integral:

$$
\begin{aligned}
&ig(\tau_1,\tau_2) = \int dx_f dx'_f \delta(x_f - x'_f) \int dx_i dx'_i \int dx_1 dx_2 \\
&K(x_f,t_f;x_1,\tau_1)x_1K(x_1,\tau_1;x_2,\tau_2)x_2K(x_2,\tau_2;x_i,t_i)\rho_{Bi}(x_i,x'_i)K^*(x'_f,t_f;x'_i,t_i) \ . \qquad (33)
\end{aligned}
$$

Thus we get

$$
ig(\tau_1,\tau_2) \ = \ \int Dx\, x(\tau_1)\, x(\tau_2)\, \exp\left[\frac{i}{2}\int_K dt_1 dt_2\, x(t_1)G^{-1}_{(t_1,t_2)}x(t_2)\right] \ . \qquad (34)
$$

Finally, using the identity (99) we get

$$
ig(\tau_1,\tau_2) = iG(\tau_1,\tau_2) \ . \qquad (35)
$$

Analogously for all other arrangements of times τ_1 and τ_2.

E. Keldysh correlators

We use

$$
x = \sqrt{\frac{\hbar}{2m\omega_0}}(a + a^\dagger) \ . \qquad (36)
$$

$$
\begin{aligned}
iG^> = iG_{-+} = \langle T_K x_-(t_1)x_+(t_2)\rangle &= \frac{\hbar}{2m\omega_0}\langle(ae^{-i\omega_0 t_1} + a^\dagger e^{i\omega_0 t_1})(ae^{-i\omega_0 t_2} + a^\dagger e^{i\omega_0 t_2})\rangle \\
&= \frac{\hbar}{2m\omega_0}\left(n_B e^{i\omega_0(t_1-t_2)} + (n_B+1)e^{-i\omega_0(t_1-t_2)}\right) \ , \qquad (37)
\end{aligned}
$$

$$
\begin{aligned}
iG^< = iG_{+-} = \langle T_K x_+(t_1)x_-(t_2)\rangle &= \frac{\hbar}{2m\omega_0}\langle(ae^{-i\omega_0 t_2} + a^\dagger e^{i\omega_0 t_2})(ae^{-i\omega_0 t_1} + a^\dagger e^{i\omega_0 t_1})\rangle \\
&= \frac{\hbar}{2m\omega_0}\left(n_B e^{-i\omega_0(t_1-t_2)} + (n_B+1)e^{i\omega_0(t_1-t_2)}\right) \ , \qquad (38)
\end{aligned}
$$

$$iG^c = iG_{++} = \langle T_K x_+(t_1) x_+(t_2) \rangle \;=\; \theta(t_1-t_2) iG^>(t_1-t_2) + \theta(t_2-t_1) iG^<(t_1-t_2) \;, \tag{39}$$

$$iG^{ac} = iG_{--} = \langle T_K x_-(t_1) x_-(t_2) \rangle \;=\; \theta(t_1-t_2) iG^<(t_1-t_2) + \theta(t_2-t_1) iG^>(t_1-t_2) \;. \tag{40}$$

Here $n_B(\omega_0) = (e^{\beta\hbar\omega_0} - 1)^{-1}$. It is easy to see that these four components are not linearly independent. Namely,

$$G^> + G^< = G^c + G^{ac} \;. \tag{41}$$

For the Fourier transforms we obtain

$$G^>(\omega) = G_{-+}(\omega) = -i\frac{2\pi\hbar}{2m\omega_0}\left[(n_B+1)\delta(\omega-\omega_0) + n_B\delta(\omega+\omega_0)\right] \;, \tag{42}$$

$$G^<(\omega) = G_{+-}(\omega) = -i\frac{2\pi\hbar}{2m\omega_0}\left[n_B\delta(\omega-\omega_0) + (n_B+1)\delta(\omega+\omega_0)\right] \;, \tag{43}$$

$$\begin{aligned} G^c(\omega) = G_{++}(\omega) \;&=\; \frac{\hbar}{2m\omega_0}\left[\frac{n_B}{\omega+\omega_0+i\delta} + \frac{n_B+1}{\omega-\omega_0+i\delta} - \frac{n_B}{\omega-\omega_0-i\delta} - \frac{n_B+1}{\omega+\omega_0-i\delta}\right] \\ &=\; -i\frac{\pi\hbar}{2m\omega_0}(2n_B+1)\left[\delta(\omega-\omega_0)+\delta(\omega+\omega_0)\right] \\ &+\; \frac{\hbar}{2m\omega_0}\left[P\frac{1}{\omega-\omega_0} - P\frac{1}{\omega+\omega_0}\right] \;, \end{aligned} \tag{44}$$

$$\begin{aligned} G^{ac}(\omega) = G_{--}(\omega) \;&=\; \frac{\hbar}{2m\omega_0}\left[\frac{n_B+1}{\omega+\omega_0+i\delta} + \frac{n_B}{\omega-\omega_0+i\delta} - \frac{n_B+1}{\omega-\omega_0-i\delta} - \frac{n_B}{\omega+\omega_0-i\delta}\right] \\ &=\; -i\frac{\pi\hbar}{2m\omega_0}(2n_B+1)\left[\delta(\omega-\omega_0)+\delta(\omega+\omega_0)\right] \\ &+\; \frac{\hbar}{2m\omega_0}\left[P\frac{1}{\omega+\omega_0} - P\frac{1}{\omega-\omega_0}\right] \;, \end{aligned} \tag{45}$$

In the matrix form we have thus $-i\langle T_K x_\alpha(t_1) x_\beta(t_2) = G_{\alpha,\beta}(t_1,t_2)$, where $\alpha = \pm$ and $\beta = \pm$.

It is much more convenient to use the quantum and the classical components of x defined by

$$\begin{pmatrix} x_c \\ x_q \end{pmatrix} = L \begin{pmatrix} x_+ \\ x_- \end{pmatrix} \ , \tag{46}$$

where

$$L = L^{-1} = L^{\dagger} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \ . \tag{47}$$

This transformation gives

$$\hat{G} = LGL = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} G_{++} & G_{+-} \\ G_{-+} & G_{--} \end{pmatrix} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \begin{pmatrix} G^K & G^R \\ G^A & 0 \end{pmatrix} \ , \tag{48}$$

where

$$G^K = -i\langle T_K x_c(t_1) x_c(t_2)\rangle = \frac{1}{2}\left(G_{++} + G_{--} + G_{+-} + G_{-+}\right) = G_{+-} + G_{-+} = G_{++} + G_{--} \ , \tag{49}$$

$$G^R = -i\langle T_K x_c(t_1) x_q(t_2)\rangle = \frac{1}{2}\left(G_{++} - G_{--} + G_{-+} - G_{+-}\right) = G_{++} - G_{+-} = G_{-+} - G_{--} \ , \tag{50}$$

$$G^A = -i\langle T_K x_q(t_1) x_c(t_2)\rangle = \frac{1}{2}\left(G_{++} - G_{--} - G_{-+} + G_{+-}\right) = G_{++} - G_{-+} = G_{+-} - G_{--} \ . \tag{51}$$

We obtain

$$G^K = \frac{\hbar}{2m\omega_0}(-2\pi i)(2n_B + 1)\left[\delta(\omega - \omega_0) + \delta(\omega + \omega_0)\right] \ , \tag{52}$$

$$G^R = \frac{\hbar}{2m\omega_0}\left(\frac{1}{\omega - \omega_0 + i\delta} - \frac{1}{\omega + \omega_0 + i\delta}\right) \ , \tag{53}$$

$$G^A = \frac{\hbar}{2m\omega_0}\left(\frac{1}{\omega - \omega_0 - i\delta} - \frac{1}{\omega + \omega_0 - i\delta}\right) \ , \tag{54}$$

For the inverse matrix we obtain formally

$$\hat{G}^{-1} = \begin{pmatrix} 0 & \left[G^A\right]^{-1} \\ \left[G^R\right]^{-1} & -\left[G^R\right]^{-1} G^K \left[G^A\right]^{-1} \end{pmatrix} \tag{55}$$

We obtain (cf. Eq. 25)

$$\left[G^{R/A}\right]^{-1} = \frac{m}{\hbar}\left[(\omega \pm i\delta)^2 - \omega_0^2\right] \ . \tag{56}$$

For the (q,q) element of $\hat{G}^{-1}$ we get

$$\begin{aligned}
\Sigma^K &\equiv \left[G^R\right]^{-1} G^K \left[G^A\right]^{-1} \\
&= \frac{m}{\hbar}\left[(\omega+i\delta)^2-\omega_0^2\right]\frac{(-2\pi i\hbar)}{2m\omega_0}(2n_B+1)\left[\delta(\omega-\omega_0)+\delta(\omega+\omega_0)\right]\frac{m}{\hbar}\left[(\omega-i\delta)^2-\omega_0^2\right] \\
&= -\frac{i\pi m}{\hbar\omega_0}(2n_B+1)\left[(\omega+i\delta)^2-\omega_0^2\right]\left[(\omega-i\delta)^2-\omega_0^2\right]\left(\frac{1}{\pi}\frac{\delta}{\delta^2+(\omega-\omega_0)^2}+\frac{1}{\pi}\frac{\delta}{\delta^2+(\omega+\omega_0)^2}\right) .
\end{aligned} \tag{57}$$

We were forced to use the Lorentzian representation of the delta-functions in order to be able to go to $\omega = \pm\omega_0$. We, thus, obtain an infinitesimal quantity

$$\Sigma^K = -\frac{4im\omega_0}{\hbar}(2n_B+1)\,\delta \tag{58}$$

We can rewrite then

$$\hat{G}^{-1} = \begin{pmatrix} 0 & G_0^{-1}-\Sigma^A \\ G_0^{-1}-\Sigma^R & -\Sigma^K \end{pmatrix} , \tag{59}$$

where $G_0^{-1} \equiv (m/\hbar)(\omega^2-\omega_0^2)$ and $\Sigma^R = (\Sigma^A)^* = -2i(m\omega_0/\hbar)\,\mathrm{sign}(\omega)\,\delta$. We also rewrite

$$\hat{G} = \begin{pmatrix} G^R\Sigma^K G^A & G^R \\ G^A & 0 \end{pmatrix} , \tag{60}$$

which emphasises the importance of the infinitesimal Σ_K.

F. Many oscillators (bath of oscillators)

We now consider a bath of harmonic oscillators, such that $X = \sum_n \lambda_n x_n$. Each oscillator is characterised by mass m_n and frequency ω_n. In analogy to (28) the influence functional will be now given by

$$F[Q,Q'] = \exp\left[-\frac{i}{2\hbar^2}\int_K dt_1 dt_2\, Q(t_1)G_{(t_1,t_2)}Q(t_2)\right] , \tag{61}$$

where

$$G_{(t_1,t_2)} = -i\langle T_K X(t_1)X(t_2)\rangle . \tag{62}$$

For the components of the Green's function we obtain

$$G^K = \sum_n \frac{\hbar\lambda_n^2}{2m_n\omega_n}(-2\pi i)(2n_B(\omega_n)+1)\left[\delta(\omega-\omega_n)+\delta(\omega+\omega_n)\right] , \tag{63}$$

$$G^R = \sum_n \frac{\hbar\lambda_n^2}{2m_n\omega_n}\left(\frac{1}{\omega-\omega_n+i\delta} - \frac{1}{\omega+\omega_n+i\delta}\right) \ , \tag{64}$$

$$G^A = \sum_n \frac{\hbar\lambda_n^2}{2m_n\omega_n}\left(\frac{1}{\omega-\omega_n-i\delta} - \frac{1}{\omega+\omega_n-i\delta}\right) \ . \tag{65}$$

it is easy to show that

$$G^K(\omega) = (G^R(\omega) - G^A(\omega)) \coth\frac{\hbar\omega}{2k_BT} \ . \tag{66}$$

We define the spectral function as

$$J(\omega) \equiv -\frac{1}{\pi}\,\mathrm{Im}G^R(\omega) = \sum_n \frac{\hbar\lambda_n^2}{2m_n\omega_n}\left[\delta(\omega-\omega_n) - \delta(\omega+\omega_n)\right] \ . \tag{67}$$

It is an antisymmetric function of frequency ω. Then $G^K(\omega) = -2\pi i J(\omega) \coth\frac{\hbar\omega}{2k_BT}$.

G. Influence functional in classical-quantum components

The influence functional reads

$$\begin{aligned} F[Q,Q'] &= \exp\left[-\frac{i}{2\hbar^2}\int_K dt_1dt_2\, Q(t_1)G(t_1,t_2)Q(t_2)\right] \\ &= \exp\left[-\frac{i}{2\hbar^2}\int dt_1dt_2\, Q_\alpha(t_1)(\tau_z)_{\alpha,\alpha}G_{\alpha,\beta}(t_1,t_2)(\tau_z)_{\beta,\beta}Q_\beta(t_2)\right] \ , \end{aligned} \tag{68}$$

where $\alpha = \pm$. Here we have replaced the (double) integration over contour by the integration over the physical time. The matrices τ_z stand there for the fact that the integration along the lower contour was backward in time.

Analogously to the bath variable it is convenient to introduce quantum and classical components of the variable Q:

$$\begin{pmatrix} Q_c \\ Q_q \end{pmatrix} = L \begin{pmatrix} Q_+ \\ Q_- \end{pmatrix} \ , \tag{69}$$

Now we can perform the rotation to classical and quantum components. We obtain

$$F[Q,Q'] = \exp\left[-\frac{i}{2\hbar^2}\int dt_1dt_2\hat{Q}^T(t_1)\tau_x\hat{G}(t_1,t_2)\tau_x\hat{Q}(t_2)\right] \ . \tag{70}$$

Here $\hat{Q}^T = (Q_c, Q_q)$. We thus obtain $F[Q,Q'] = e^{(i/\hbar)\mathcal{S}_F}$ [2], where

$$i\mathcal{S}_F = -\frac{i}{2\hbar}\int\limits_{-\infty}^{\infty} dt_1 \int\limits_{-\infty}^{\infty} dt_2 \begin{pmatrix} Q_c(t_1) & Q_q(t_1) \end{pmatrix} \begin{pmatrix} 0 & G^A \\ G^R & G^K \end{pmatrix}_{(t_1-t_2)} \begin{pmatrix} Q_c(t_2) \\ Q_q(t_2) \end{pmatrix} \ , \tag{71}$$

Another popular definition of the classical and quantum components is $\tilde{Q}_c = Q_c/\sqrt{2} = (Q_+ + Q_-)/2$, $\tilde{Q}_q = \sqrt{2}Q_c = Q_+ - Q_-$. It is physically motivated but is less convenient in calculations. In terms of these variables we have

$$i\mathcal{S}_F = -\frac{i}{\hbar}\int\limits_{-\infty}^{\infty} dt_1 \int\limits_{-\infty}^{\infty} dt_2 \begin{pmatrix} \tilde{Q}_c(t_1) & \frac{\tilde{Q}_q(t_1)}{2} \end{pmatrix} \begin{pmatrix} 0 & G^A \\ G^R & G^K \end{pmatrix}_{(t_1-t_2)} \begin{pmatrix} \tilde{Q}_c(t_2) \\ \frac{\tilde{Q}_q(t_2)}{2} \end{pmatrix} . \tag{72}$$

II. QUANTUM DISSIPATIVE DYNAMICS

We return back to Eq. (17), which we now rewrite as

$$\begin{aligned} &\rho_{Sf}(Q_f, Q'_f) \\ &= \int dQ_i dQ'_i \int DQ \int DQ' \exp\left((i/\hbar)\left[S_S[Q] - S_S[Q'] + \mathcal{S}_F[Q,Q']\right]\right)\rho_{Si}(Q_i, Q'_i) . \end{aligned} \tag{73}$$

From now on we will only write down the effective action, keeping in mind the path integral above. The action reads

$$\mathcal{S} = S_S[Q] - S_S[Q'] + \mathcal{S}_F[Q,Q'] . \tag{74}$$

Consider, first, the case of a free particle, $S_S[Q] = \int dt M\dot{Q}^2/2$. We obtain

$$S_S[Q] - S_S[Q'] = \int dt \left[\frac{M\dot{Q}_+^2}{2} - \frac{M\dot{Q}_-^2}{2}\right] = \int dt M\dot{Q}_c\dot{Q}_q \tag{75}$$

Thus,

$$\mathcal{S} = \int dt M\dot{Q}_c(t)\dot{Q}_q(t) - \frac{1}{2\hbar}\int\limits_{-\infty}^{\infty} dt_1 \int\limits_{-\infty}^{\infty} dt_2 \begin{pmatrix} Q_c(t_1) & Q_q(t_1) \end{pmatrix} \begin{pmatrix} 0 & G^A \\ G^R & G^K \end{pmatrix}_{(t_1-t_2)} \begin{pmatrix} Q_c(t_2) \\ Q_q(t_2) \end{pmatrix} . \tag{76}$$

Taking into account $G^A(t_1,t_2) = G^R(t_2,t_1)$ (this is so since X is hermitian) we obtain

$$\begin{aligned} \mathcal{S} = \int dt M\dot{Q}_c(t)\dot{Q}_q(t) \; &- \; \frac{1}{\hbar}\int dt_1 dt_2\, Q_q(t_1) G^R(t_1,t_2) Q_c(t_2) \\ &- \; \frac{1}{2\hbar}\int dt_1 dt_2\, Q_q(t_1) G^K(t_1,t_2) Q_q(t_2) \end{aligned} \tag{77}$$

A. Quasi-classical trajectories

The trajectories, for which the action (77) is extremal should satisfy two conditions: $\delta S/\delta Q_c = 0$ and $\delta S/\delta Q_q = 0$. Since the action (77) is at least of first order in Q_q (this will always be the case, since for $Q_q = 0$ the action must vanish), one can always achieve

$\delta S/\delta Q_c = 0$ trivially by choosing $Q_q = 0$. Such trajectories are called *classical*. These are, in general, not the only extremal trajectories to be considered.

To find a classical trajectory, we consider variation with respect to Q_q around such a trajectory, that is we vary and then put $Q_q = 0$. Then the third term of (77) drops out. We, thus, obtain

$$-M\ddot{Q}_c(t) - \frac{1}{\hbar}\int dt_2\, G^R(t,t_2)Q_c(t_2) = 0\ . \tag{78}$$

Taking into account

$$G^R(\omega) = \sum_n \frac{\hbar\lambda_n^2}{2m_n\omega_n}\left(\frac{1}{\omega-\omega_n+i\delta} - \frac{1}{\omega+\omega_n+i\delta}\right)\ , \tag{79}$$

we observe that $[G^R(\omega)]^* = G^R(-\omega)$ and $G^R(t_1-t_2)$ is real. For the imaginary part of $G^R(\omega)$ we obtain

$$\mathrm{Im}G^R(\omega) = -\pi J(\omega)\ . \tag{80}$$

Consider an Ohmic bath, such that $J(\omega) = (\hbar\gamma/\pi)\omega$ (up to some high-frequency cut-off ω_c). Then

$$\int\frac{d\omega}{2\pi}\, i\,\mathrm{Im}G^R(\omega)e^{-i\omega t} = \hbar\gamma\int\frac{d\omega}{2\pi}\,(-i\omega)\,e^{-i\omega t} = \hbar\gamma\frac{d}{dt}\,\delta(t)\ . \tag{81}$$

For the real part we have

$$\mathrm{Re}G^R(\omega) = \frac{1}{\pi}P\int d\nu\,\frac{\mathrm{ImG^R}(\nu)}{\nu-\omega} = P\int d\nu\,\frac{J(\nu)}{\omega-\nu}\ . \tag{82}$$

For $\omega = 0$ this is a linearly divergent integral $\mathrm{Re}G(\omega=0) = -(2\hbar\gamma/\pi)\omega_c$. The Fourier transform of this part can be approximated as

$$\int\frac{d\omega}{2\pi}\,\mathrm{Re}G^R(\omega)e^{-i\omega t} = -\hbar C\delta(t)\ , \tag{83}$$

where $C = 2\gamma\omega_c/\pi$. The equation of motion, thus, reads

$$-M\ddot{Q}_c - \gamma\dot{Q}_c + CQ_c = 0\ . \tag{84}$$

The second term gives friction (good!). The third term corresponds to a potential of the inverted parabolic form with a diverging ($\propto\ \omega_c$) curvature. Thus the problem appears extremely unstable (bad!?). In physical models this infinite renormalisation is subtracted from the very beginning (a parabolic potential with positive diverging curvature appears in the Hamiltonian along with the linear coupling) and, thus the problem remains stable and the proper equation of motion reads

$$-M\ddot{Q}_c - \gamma\dot{Q}_c = 0\ . \tag{85}$$

B. Langevin equation

We explore now fluctuations around the classical trajectory, i.e., the trajectories for which $Q_q \neq 0$. One elegant way to do so was proposed in Ref. [1]. The main idea is that the third (quantum-quantum) term in the action (77) suppresses the deviation of Q_q from zero, but allows some small ones. To take this into account we use the Hubbard-Stratonovich transformation

$$e^{-\frac{i}{2\hbar^2}\int dt_1 dt_2\, Q_q(t_1)G^K(t_1,t_2)Q_q(t_2)} = \int D\xi\, e^{i/\hbar\int dt\xi(t)Q_q(t)}\, e^{\frac{i}{2}\int dt_1 dt_2\,\xi(t_1)(G^K)^{-1}(t_1,t_2)\xi(t_2)} \,. \tag{86}$$

Here $D\xi$ means functional integration over the realisations of $\xi(t)$. The path integral in, e.g., Eq. (73) now reads

$$\int D\xi\, e^{\frac{i}{2}\int dt_1 dt_2\,\xi(t_1)(G^K)^{-1}(t_1,t_2)\xi(t_2)} \int DQ_c DQ_q e^{(i/\hbar)S_\xi} \,, \tag{87}$$

where

$$S_\xi = \int dt Q_q(t)\xi(t) + \int dt M\dot{Q}_c(t)\dot{Q}_q(t) - \frac{1}{\hbar}\int dt_1 dt_2\, Q_q(t_1)G^R(t_1,t_2)Q_c(t_2) \,. \tag{88}$$

Variation of S_ξ with respect to Q_q produces the Langevin equation of motion:

$$M\ddot{Q}_c(t) + \gamma\dot{Q}_c(t) = \xi(t) \,, \tag{89}$$

where the (diverging) renormalisation of the potential has been removed as discussed above. The realisations of the random variable $\xi(t)$ are chosen according to the weight (distribution) function

$$e^{\frac{i}{2}\int dt_1 dt_2\,\xi(t_1)(G^K)^{-1}(t_1,t_2)\xi(t_2)} \,. \tag{90}$$

Thus the field $\xi(t)$ has a Gaussian distribution with the correlation function

$$\langle\xi(t_1)\xi(t_2)\rangle = iG^K(t_1 - t_2) \,. \tag{91}$$

For the Fourier transform we obtain

$$\langle\xi(t_1)\xi(t_2)\rangle_\omega = 2\pi J(\omega)\coth\frac{\hbar\omega}{2k_BT} \,. \tag{92}$$

Thus, this Langevin equation contains also quantum noise at $\omega \gg k_BT/\hbar$.

III. APPENDIX: GAUSSIAN INTEGRALS

$$\int dx\, e^{-ax^2/2} = \sqrt{\frac{2\pi}{a}} \ . \tag{93}$$

$$\int d^N\vec{x}\, \exp\left[-\frac{\vec{x}\cdot A\cdot\vec{x}}{2}\right] = \frac{(2\pi)^{N/2}}{\sqrt{\mathrm{Det}(A)}} \tag{94}$$

Since $\vec{x}$ is real, the matrix A is by construction symmetric.

$$\int d^N\vec{x}\, \exp\left[-\frac{\vec{x}\cdot A\cdot\vec{x}}{2} + \vec{b}\cdot\vec{x}\right] = \frac{(2\pi)^{N/2}}{\sqrt{\mathrm{Det}(A)}}\, \exp\left[\frac{\vec{b}\cdot A^{-1}\cdot\vec{b}}{2}\right] \tag{95}$$

We will also need the following property

$$\langle x_n x_m\rangle \equiv \left[\frac{(2\pi)^{N/2}}{\sqrt{\mathrm{Det}(A)}}\right]^{-1} \int d^N\vec{x}\ x_n x_m\ \exp\left[-\frac{\vec{x}\cdot A\cdot\vec{x}}{2}\right] = (A^{-1})_{nm}\ . \tag{96}$$

This can be proven by introducing, first, the vector of sources $\vec{\eta}$ and calculating the generating function

$$\chi(\vec{\eta}) \equiv \left[\frac{(2\pi)^{N/2}}{\sqrt{\mathrm{Det}(A)}}\right]^{-1} \int d^N\vec{x}\, \exp\left[-\frac{\vec{x}\cdot A\cdot\vec{x}}{2} + \vec{\eta}\cdot\vec{x}\right]\ . \tag{97}$$

Using (95) we obtain

$$\chi(\vec{\eta}) = \exp\left[\frac{\vec{\eta}\cdot A^{-1}\cdot\vec{\eta}}{2}\right]\ . \tag{98}$$

Finally,

$$\langle x_n x_m\rangle = \frac{\partial}{\partial\eta_n}\frac{\partial}{\partial\eta_m}\,\chi(\vec{\eta})\Big|_{\vec{\eta}\to 0} = (A^{-1})_{nm}\ . \tag{99}$$

[1] A. Schmid, J. of Low Temp. Phys. **49**, 609 (1982).

[2] Different notations could be used here. For example, $i\mathcal{S}_{FV}$ for Feynman-Vernon or $i\mathcal{S}_{CL}$ for Caldeira-Leggett.