

DERIVATION OF COLLECTIVE MASS PARAMETERS IN THE PATH INTEGRAL
APPROACH TO NUCLEAR DYNAMICS

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1. Introduction.

The path integral approach has been used in former works ^{1,2)} in the description of large amplitude motion to derive friction and diffusion coefficients arising from the coupling between the collective and intrinsic subspaces characterized by the variables $\{q\}$ and $\{\xi\}$. We now show that the same formalism can also be used to generate mass parameters corresponding to the presence of conservative forces. They are derived in the framework of a fixed and an adiabatic basis of intrinsic states.

2. Equation of motion in the collective subspace.

In the path integral formalism, the average probability amplitude to go from an initial intrinsic state $|a\rangle$ at t_0 to an ensemble of final states $|b\rangle$ at t can be written as a double path integral ¹⁾ :

$$\sum_b |K_{ba}|^2 = \iint \mathcal{D}_q \mathcal{D}_{\tilde{q}} e^{\frac{i}{\hbar} [S(q) - S(\tilde{q})]} \sum_b \rho_{ba}(q, \tilde{q}) \quad (2.1)$$

where the two paths $q(t')$ and $\tilde{q}(t')$ both start at $q_0 = q(t_0)$ and end at $q = q(t)$ and $S(q)$ is the collective action integral.

If the influence function ρ_{ba} is

$$\rho(q, \tilde{q}) \equiv \sum_b \rho_{ba}(q, \tilde{q})$$

is cast in the form

$$\rho(q, \bar{q}) = e^{\frac{i}{\hbar} \int dt_1 \eta(t_1) F(t_1) - \frac{1}{2\hbar^2} \int dt_1 \eta(t_1) \int dt_2 \eta(t_2) G(t_1, t_2) + \theta(\eta^3)} \quad (2.2)$$

with $\eta = q - \bar{q}$

the application of the stationary phase approximation to the integrand of (2.1) leads to the classical equation of motion

$$\frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{q}} - \frac{\partial \mathcal{L}}{\partial q} - F(t) = 0 \quad (2.3)$$

where F is a force generated by the coupling between q and ξ and G can be interpreted as a diffusion coefficient³).

3. Mass parameters.

In the limit of slow collective motion (\dot{q} small) and high temperature, the expression of F can be worked out explicitly by introducing statistical assumptions on the relevant matrix elements⁴). These are supposed to be Gaussian distributed quantities with zero mean.

The generalized influence functional

$$P(T, \tau) = \sum_b e^{i\epsilon_b \tau} \bar{\rho}_{ba}(T + \frac{\tau}{2}, T - \frac{\tau}{2}) \quad (3.1)$$

where ϵ_b are the intrinsic energies and $\bar{\rho}$ the average of ρ over the random distribution of matrix elements obeys an integro-differential equation¹).

Seeking a solution of P in the form

$$P(T, \tau) = P_{eq}(T, \tau) e^{\int^T dT' L(T', \tau)}$$

where P_{eq} obeys $\partial P_{eq} / \partial T = 0$ when T goes to ∞ , we can show that

$$L(T, 0) = i\eta \dot{q} - i\eta M \dot{q} - \frac{\eta^2}{2} D + \theta(\ddot{q}, \eta^3) \quad (3.2)$$

This formula is obtained by Taylor expanding q around T . The first and third term in (3.2) were worked in refs. ^{1,2}).

The derivation of M can be performed for weak and strong coupling. The calculations are done in a fixed basis of intrinsic states as well as in the adiabatic basis.

In the adiabatic basis and the strong coupling limit one gets :

$$M = \frac{2\hbar}{\sigma_1^2} \int_0^\infty d\tau' e^{-\left[\frac{\Gamma^{\downarrow 2}}{2\hbar^2} + \frac{2\pi q^{\downarrow 2}}{\sigma_1^2}\right] \tau'^2} \sin\delta\tau' - \frac{6\hbar q^{\downarrow 2}}{\sigma_1^4} \int_0^\infty d\tau \tau'^2 e^{-\left[\frac{\Gamma^{\downarrow 2}}{2\hbar^2} + \frac{2\pi q^{\downarrow 2}}{\sigma_1^2}\right] \tau'^2} \sin\delta\tau'$$

with

$$\delta = \frac{\beta\Gamma^{\downarrow 2}}{2\hbar} + \frac{2\pi\beta\Gamma^{\downarrow 2} q^{\downarrow 2}}{\hbar\sigma_1^2} \left[\left(\frac{q}{\sigma_1}\right)^2 + \frac{\Gamma^{\downarrow 2}}{2\hbar^2} \right]^{-1}$$

where σ_1 is the correlation length in q , Γ^{\downarrow} the spreading width of the intrinsic states over a Slater determinant basis, β the inverse temperature.

Hence the influence functional approach allows for the derivation of collective inertia parameters whatever the strength of the coupling between intrinsic and collective degrees of freedom. The mass parameters can be worked out analytically and used in conjunction with the friction and diffusion coefficient in order to construct a Fokker-Planck equation for the classical distribution function of the variable q .

References.

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