TDHFB-Langevin approach to the nuclear collective dynamics\footnote{in Proc. Int. Symposium \textit{Large-Scale Collective Motion of Atomic Nuclei}, October 15-19, 1996, Brolo (Messina), Italy, Edited by G. Giardina, G. Fazio, M. Lattuada, World Scientific, Singapore, 1997, p. 222.}

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Stochastic mean-field equations are derived applying the time-dependent variational principle to a quantum many-body system in interaction with a classical heat bath. This approach is tested on the case of a charged particle in thermal radiation field, and is used to include frictional and random forces in the TDHFB equations. Dynamical estimates of the diffusion coefficient for the quadrupole deformation are obtained.

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1 Introduction

The simulation of the non-equilibrium fluctuation phenomena observed in hot nuclei represents a fundamental problem of the many-body theory, demanding stochastic extensions of the kinetic or mean-field equations.

At the level of the semiclassical description provided by the phase-space density, the fluctuations can be accounted by the Boltzmann-Langevin approach [1]. Within this approximation the nuclear Boltzmann equation is modified, so that a random component (Brownian force [2]) is included in the collision term.

The time-dependent variational calculations on coherent states trial manifolds, as time-dependent Hartree-Fock (TDHF), or antisymmetrized molecular-dynamics (AMD), lead to deterministic mean-field equations, but recipes to introduce a random behavior have been proposed [3, 4, 5, 6, 7]. The basic assumption is that some decoherence mechanism exists, interrupting the deterministic evolution of the quantum wave packet by spontaneous collapse to the neighbouring states of the same trial manifold. The collapse rate is obtained using the Fermi’s golden rule, for a suitable residual interaction.

The mechanism of the random spontaneous collapse induced by environmental (residual) fluctuations remains obscure, beyond the framework of the quantum many-body theory. This ambiguous mechanism can be avoided if the residual interactions and the unretained degrees of freedom are accounted from the very beginning in the time-dependent variational principle. Particularly suited for this purpose is the model of bilinear coupling between a particle and a heat bath of harmonic oscillators, applied with success to derive the classical Langevin equation [8]. This model can be used also to include stochastic forces in the mean-field equations, and was applied to study the effects of pairing, dissipation and temperature on the giant quadrupole resonance (GQR) [9].

The dynamical approach to the coupling between a quantum many-body system and the heat bath is presented in Sec. 2, together with a test on the important case provided by a charged particle in blackbody radiation field. The stochastic mean-field equations are used in Sec. 3 to calculate the diffusion coefficient of the quadrupole deformation coordinate. Conclusions are drawn in Sec. 4.
2 Brownian quantum dynamics

The phenomenology of the Brownian diffusion in classical mechanics can be described by two external force terms in the Hamilton equations of motion for the particle: a random force with zero mean, $\xi(t)$, (the noise), and a dissipative friction force, $f$. The type of friction is determined by the memory function $\Gamma(t)$, or the spectral density of the environment, $J(\omega)$, so that for a linear dissipation mechanism

$$f(t) = -\int_0^t \Gamma(t-t')\dot{Q}(t')dt' , \quad \Gamma(t) = \frac{2}{\pi} \int_0^\infty d\omega \frac{J(\omega)\cos(\omega t)}{\omega} ,$$

with $\dot{Q}$ the particle velocity. The memory function gives also the noise correlation function, and $\xi(t)$ should obey the fluctuation-dissipation theorem,

$$<< \xi(t)\xi(t') >> = k_B T \Gamma(t-t') ,$$

where $<< .. >>$ denotes the average over an ensemble of trajectories.

Noise and friction forces having these properties may be derived following a Hamiltonian treatment of the whole system consisting of the particle in interaction with a heat bath of $N_c$ harmonic oscillators via the bilinear coupling term [8]

$$H_{coup} = Q \sum_{j=1}^{N_c} C_j q_j ,$$

where $C_j$ are coupling constants and $q_j$ the time-dependent bath coordinates.

The advantage of the bilinear coupling model over the phenomenological Langevin approach becomes striking when the particle is a quantum object. For example, below a certain crossover temperature, the mechanism of chemical reactions changes from thermal activation to tunneling, becoming sensitive to destruction of the phase coherence and dissipation produced by environment. The temperature effect on the tunneling rate can be accounted by the thermal average of the quantum penetrability factors [10]. However, dissipation requires a more elaborate treatment, based essentially on Euclidean path integral calculations for the bilinear coupling Hamiltonian [11].

The problem of dynamical coupling between a quantum system and its environment is even more complex, having not yet a satisfactory solution. Thus, no standard method exists to treat a mixed system composed of a
quantum particle interacting with a classical heat bath. In quantum gravity
the similar problem of a quantum system coupled to the classical space-
time foam could be treated by Hamilton-Heisenberg equations derived from
a variational principle [12]. In the quantum many-body theory, the collective
mean-field obtained from time-dependent variational calculations has already
a hybrid character, including both quantum and classical aspects. Thus, it is
natural to define its dynamical coupling to a classical heat bath of oscillators
using the variational equation
\[
\delta \int dt \left[ \sum_{i=1}^{N_c} m_i (\dot{q}_i)^2 + \langle \Psi | i\hbar \partial_t - (H_0 + H_b) | \Psi \rangle \right] = 0
\] (4)
where \( H_0 \) is the Hamiltonian operator for the isolated quantum system, and
\( H_b \) contains the bath energy plus the coupling interaction.

Let us consider variations of the quantum wave function \( \Psi \) in Eq. (4)
restricted to a finite dimensional trial manifold \( S = \{|\Psi\rangle(X)\} \), parameterized
by \( 2N \) coordinates \( X \equiv \{x^i\}, i = 1, 2N \), so that the matrix \( \omega^S = [\omega^S_{ij}(\Psi)] \),
defined by
\[
\omega^S_{ij}(\Psi) = 2\hbar Im \langle \partial_i \Psi | \partial_j \Psi \rangle
\] (5)
is non-singular [13]. Supposing a coupling interaction \( H_{coup} = K \sum_{j=1}^{N_c} C_j q_j \),
linear in the coordinate operator \( K \), the equations of motion determined by
variations in Eq. (4) with respect to \( X(t) \) and the bath trajectories \( q_i(t) \) are
\[
\sum_{j=1}^{2N} \dot{x}^j \omega^S_{jk}(\Psi) = \frac{\partial \langle \Psi | H_0 | \Psi \rangle}{\partial x^k} + \frac{\partial \langle \Psi | K | \Psi \rangle}{\partial x^k} \sum_{i=1}^{N_c} C_i q_i
\] (6)
for the quantum system and
\[
\dot{q}_i = \frac{p_i}{m_i}, \quad \dot{p}_i = -m_i \omega_i^2 q_i - C_i \langle \Psi | K | \Psi \rangle
\] (7)
for the classical oscillators. The classical equations can be solved in terms
of the unknown function of time \( Q_\psi = \langle \Psi | K | \Psi \rangle \), and when their retarded
solution is inserted in Eq. (6), a Langevin-like equation is obtained,
\[
\sum_{j=1}^{2N} \dot{x}^j \omega^S_{jk}(\Psi) = \frac{\partial \langle \Psi | H_0 + W_{ren} | \Psi \rangle}{\partial x^k} - \frac{\partial \langle \Psi | K | \Psi \rangle}{\partial x^k} [\xi(t) + f_\psi]
\] . (8)

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Here \( f_\psi \) is given by Eq. (1) with \( Q_\psi \) instead of \( Q \). The term \( W_{\text{ren}} = K[Q_\psi(0)\Gamma(t) - Q_\psi(t)\Gamma(0)] \) will be neglected, supposing that it can be accounted by renormalizing \( H_0 \).

If \( S \) is the whole Hilbert space of the quantum system, then Eq. (8) becomes a non-linear time-dependent Schrödinger equation

\[
\frac{i\hbar}{\partial t} \Psi = [H_0 - K(\xi(t) + f_\psi)]\Psi .
\]

The non-linearity appears in the friction term \( f_\psi \), accounting for the back-reaction of the environment on the quantum system. When friction is neglected, the rate of the noise-induced excitation between two eigenstates \( |E_i\rangle \) and \( |E_f\rangle \) of \( H_0 \) can be easily calculated in the first-order approximation for the time-dependent perturbation represented by \( H_{\text{noise}} = -K\xi(t) \). The result is

\[
\Gamma_{fi} = \frac{|K_{fi}|^2}{\hbar^2} \lim_{t \to \infty} \frac{1}{t} \int_0^t \xi(s) e^{i\omega_{fi} s} ds^2
\]

and can be further averaged over the statistical ensemble before the time-integral making use of Eq. (2), so that

\[
\Gamma_{fi}^{\text{noise}} \equiv << \Gamma_{fi} >> = \frac{2}{\hbar^2} |K_{fi}|^2 k_B T \frac{J(\omega_{fi})}{\omega_{fi}} .
\]

Here \( K_{fi} = \langle E_f | K | E_i \rangle \) is the matrix element of the coupling operator \( K \), and \( \omega_{fi} = |E_f - E_i|/\hbar \).

The rate provided by Eq. (11) may be used to test the formalism presented above on the case of a single charged particle in thermal radiation field, considered as a classical heat bath of oscillators continuously distributed in frequency. In the dipolar approximation, the coupling of the electromagnetic field to the charge \( e \) has the form \( H_{\text{noise}}^{\text{rad}} = -\vec{d} \cdot \vec{E} = -d_x E_x - d_y E_y - d_z E_z \) where \( \vec{d} = er \) is the electric dipole operator, and \( \vec{E} \) the radiation electric field. For isotropic radiation \( H_{\text{noise}}^{\text{rad}} \) is a sum of three terms of the form \(-K\xi\) assumed above, each with the spectral density \( J^{\text{rad}}(\omega) = 2\hbar e^2 \omega^4 \langle n \rangle_\omega / (3c^3k_B T) \).

The total transition rate \( \Gamma_{fi}^{\text{rad}} \), is the sum of three terms provided by Eq. (11), and the result

\[
\Gamma_{fi}^{\text{rad}} = \frac{4e^2}{3\hbar c^3} |\vec{r}_{fi}|^2 \omega_{fi}^3 \langle n \rangle_{\omega_{fi}} , \quad \langle n \rangle_{\omega} = 1/(e^{\hbar\omega/k_B T} - 1) ,
\]
coincides with the known transition rate in thermal radiation field \[14\]. At high temperatures the memory function corresponding to \( J^{\text{rad}}(\omega) \) can be expressed in terms of the second derivative of the delta function, \( \Gamma(t) = -4e^2 \delta(t)/(3c^3) \), and the related friction force

\[
\vec{f}_{\psi}^{\text{rad}} = \frac{2e^2}{3c^3} \frac{d^3(\vec{r})}{dt^3}
\]  

is the classical radiation reaction in vacuum \[15\].

In the case of Ohmic dissipation \( \Gamma(t) = 2\gamma_K \delta(t) \), with \( \gamma_K \) the static friction coefficient, and Eq. (8) becomes

\[
\sum_{j=1}^{2N} \dot{x}^j \omega_j S(\Psi) = \frac{\partial \langle \Psi | H_0 | \Psi \rangle}{\partial x^k} - \frac{\partial \langle \Psi | K | \Psi \rangle}{\partial x^k} [\xi(t) - \gamma_K \frac{d \langle \Psi | K | \Psi \rangle}{dt}].
\]  

3 \hspace{1em} TDHFB-Langevin dynamics and the shape diffusion coefficient

An important application of the stochastic mean-field techniques concerns the calculation of the shape diffusion coefficient. The thermal equilibrium state of a highly excited nucleus can be represented \[7\] by an ensemble of incoherent self-consistent Hartree-Fock configurations \( |\Psi_k\rangle \), with energies \( E_k = \langle H_0 | \Psi_k \rangle \) and quadrupole deformations

\[
\beta_k = \frac{4\pi}{5} \frac{Q_0^p + Q_0^n}{A<r^2>} \quad Q_0^\nu = \sqrt{\frac{5}{16\pi}} (2z^2 - x^2 - y^2)^\nu_i .
\]  

Within this ensemble the transitions induced by the residual interactions occur with a rate

\[
\Gamma_{fi} = \frac{2\pi}{\hbar} |\langle \Psi_f | H_{\text{res}} | \Psi_i \rangle|^2 \delta(E_f - E_i)
\]  

and a diffusion coefficient of the quadrupole deformation can be defined by \[7\]

\[
D_\beta = \sum_f (\beta_f - \beta_i)^2 \Gamma_{fi} ,
\]  

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where the sum involves states $|\Psi_f\rangle$ different by $|\Psi_i\rangle$ in the occupation number of two orbital levels. However, the value predicted by this calculation is only a fraction ($\approx 10\%$) of the estimate provided by the Einstein formula$^2$

$$D^E_\beta = \frac{k_B T}{\gamma_\beta}$$

with the friction coefficient $\gamma_\beta$ extracted from experiment.

A dynamical calculation of $D_\beta$ can be performed using an ensemble of Brownian trajectories $\beta(t)$ generated by Eq. (14) for a nucleon system in contact with a heat bath. The study of the axially symmetric quadrupole shape vibrations in the sd shell nucleus $^{28}\text{Si}$ including pairing, friction and temperature shows that the occupation numbers $p_r, r = 1, 6$ of the orbital levels depend on time and may switch between different configurations, but each configuration is quasi-stable for relatively long periods, despite the shape fluctuations. For $^{28}\text{Si}$ this switching means a change of $\{p_r\}$ from the oblate configuration of the metastable ground state (mgs), $\{p^0_r\}$, to an unstable prolate configuration, $\{p^*_r\}$. The rate of these oblate→prolate configuration transitions can be defined in terms of the mean-first-passage-time $[8], \tau^*$, which is the average time elapsed until the system switches the configuration for the first time. Therefore, a diffusion coefficient of the (quasi-stable) quadrupole deformation can be defined by the average

$$D^*_\beta = \frac{1}{N_b} \sum_b \frac{(\beta^b_i - \beta^b_f)^2}{\tau^*_b}, \quad \beta^b_i \equiv \beta^b(0), \quad \beta^b_f \equiv \beta^b(\tau^*_b)$$

where the sum is taken over $N_b$ trajectories generated with random initial conditions at a fixed energy $E_i$. For such calculations, the trial manifold $S$ in Eq. (4), which is the best suited to account for the occupation number degrees of freedom, consists of a set $S^{HFB}$ of normalized Hartree-Fock-Bogolyubov functions. In this case, without environment coupling, Eq. (14) corresponds to the deterministic time-dependent Hartree-Fock-Bogolyubov (TDHFB) equations. The sd shell contains $N_s = 12$ states, and $S^{HFB}$ is parameterized by $N_s(N_s - 1) = 132$ variables $\{x^i\}$. This number is large, and therefore it is convenient to restrict $S^{HFB}$ to a submanifold with lower dimensionality, accounting only for the quadrupole and occupation numbers

$^2$When $x_t$ is a classical Brownian trajectory, $\lim_{t \rightarrow \infty} \langle \langle (x_t - x_0)^2 \rangle \rangle /t = 2k_B T/\gamma_x$.  

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degrees of freedom. For the 6 protons and 6 neutrons of $^{28}$Si outside the $^{16}$O core, the 132-dimensional manifold $S^{HFB}$ can be reduced by the cranking technique [17] to a 14-dimensional submanifold corresponding to 7 degrees of freedom: $\beta$ and the occupation numbers $p_r, r = 1, 6$ of the sd shell orbital levels.

The model Hamiltonian $H_0$ includes the spherical harmonic oscillator one-body term $h_0$ and the quadrupole-quadrupole plus pairing two-body interactions:

$$H_0 = h_0 - \chi K^2 - \frac{G_{\text{pair}}}{4} P^\dagger P.$$  \hfill (20)

Here $K \equiv Q_0/c_0$, $c_0 = (5/4\pi)^{1/2}\hbar/m\omega_0 = 26.17\text{MeV}\cdot\text{fm}^2/\hbar\omega_0$, $\omega_0 = 41A^{-1/3}$ MeV/$\hbar$, and the interaction strengths are chosen to be $\chi = 0.186$ MeV and $G_{\text{pair}} = 1.23$ MeV. The mgs configuration ($\beta^0, p^0_6$) corresponds to an oblate shape ($\beta^0 = -0.43$), and is obtained by frictional cooling [18]. This procedure ensures the self-consistency of the quadrupole and pairing mean-fields [9].

The operator $K$ is also the coordinate appearing in the coupling to the heat bath. The corresponding friction coefficient is related to $\gamma_\beta$ by $\gamma_K = 0.0083\gamma_\beta$, and at $T = 0$ the rate $\Gamma$ of the energy dissipation is the same as the decay width of the GQR, $\Gamma_{GQR} \approx 4.5$ MeV, when $\gamma_\beta \sim 6.4\hbar$.

The average in Eq. (19) was calculated using 300 trajectories starting at the GQR energy of 19.1 MeV, with random initial conditions. When $k_B T$ is between 1.5 and 2.5 MeV, and $\gamma_\beta$ is near 6.4$\hbar$, then $D_\beta^*$ can be accurately interpolated by the formula

$$D_\beta^*(T) = \frac{k_B T}{u + v k_B T + \gamma_\beta(a + b k_B T)} \quad \hfill (21)$$

where $u = 0.27\hbar$, $v = 1.1\hbar/\text{MeV}$, $a = 0.14$ and $b = 0.1\text{MeV}^{-1}$. This result indicates that the effective friction coefficient for shape diffusion with configuration change, $\gamma_{\beta}^* = u + v k_B T + \gamma_\beta(a + b k_B T)$ is not the same as the fixed model parameter $\gamma_\beta$, but depends on temperature. For $k_B T = 2.5$ MeV, Eq. (21) predicts a diffusion coefficient $D_\beta^* = 453$ keV/$\hbar$, about a factor ten larger than the microscopic estimate [7] of 30 keV/$\hbar$ in the neighboring nucleus $^{24}\text{Mg}$. Though, assuming an $A^{-1}$ dependence of $D_\beta^*$ on the mass number, for $^{158}\text{Er}$ one obtains $D_\beta^* \sim 80$ keV/$\hbar$, which is close to the value of $\sim 70$ keV/$\hbar$ extracted from experimental data.
4 Conclusions

The variational principle applied to a quantum many-body system and its thermal environment provides stochastic mean-field equations (Eq. (8)). Depending on the trial manifold, a non-linear Schrödinger-Langevin equation (Eq. (9)), or a system of TDHFB-Langevin equations can be obtained. The example of a charged particle in blackbody radiation field shows that this formalism predicts correctly the transition rate and radiation reaction.

The stochastic mean-field equations (TDHFB-Langevin) have been applied to calculate the diffusion coefficient of the quadrupole deformation (Eq. (21)). The effective friction coefficient $\gamma^*_\beta$ for shape diffusion with change of the internal configuration is not the same as the model parameter $\gamma_\beta$ and depends on temperature. The results of the present calculations within the sd shell are consistent with the measured values of the GQR decay width and shape diffusion coefficient, proving the relevance of the TDHFB-Langevin formalism.

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