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Towards Inclusion of Dissipation in Quantum Time-Dependent Mean-field Theories

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Abstract. We discuss the extension of standard quantum mean-field theories in order to account for dissipative effects. We take examples from nuclear and electronic dynamics. We show that many questions remain largely open, especially from the formal point of view.

Dissipation is an essential mechanism to understand dynamics, especially beyond the linear domain, as soon as one is not accounting for *all* degrees of freedom (which is the general case). Dissipation reflects the fact that a certain amount of energy is transferred from the degrees of freedom chosen to describe a system in the direction of neglected ones. This is usually accounted for in an approximate manner, precisely because of the lack of a complete description of the system under consideration. This also implies that the effect of this dissipation will be usually packed into simple gross quantities such as in particular a temperature. Dissipative dynamics is thus intrinsically linked to thermalization. Dissipation has been observed in most physical systems and the topic as such thus covers a certainly too large field. We will restrict here the discussion to finite systems as described by quantum mean-field. This covers typically nuclei and clusters or molecules. Illustrative examples will then be taken from these two fields.

1 Dissipation in Nuclei, Clusters and Molecules

The probably first hint of the appearance of temperature effects inside nuclei goes back to the seminal paper of Bohr [1] where the impact of neutrons on nuclei is discussed in a qualitative, but quite pertinent, manner. The argument is illustrated in Figure 1 including both the excitation mechanism (ball picture) and the ensuing relaxation of the system, in particular via nucleon emission. The mechanism is qualitatively simple. The incoming neutron transfers (dissipates) in a global manner its kinetic energy to the nucleus which gradually thermalizes. The thus acquired finite temperature leads to neutron emission according to a statistical process [2]. The study of "hot" nuclei has been widely performed

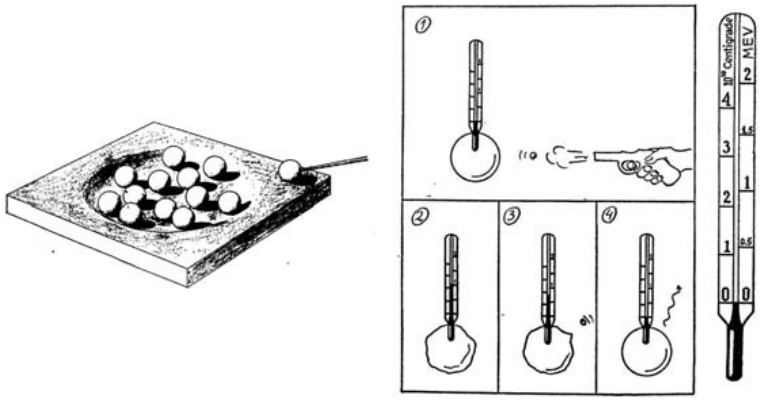

Figure 1. Sketch of neutron impact on nucleus and resulting excitation/deexcitation of the nucleus in terms of a nuclear temperature. From [1].

later on, especially in the 1980's and 1990's with help of heavy ions facilities, in particular the ones delivering beam energies in the Fermi domain [3].

Temperature effects at the side of the electron clouds in clusters and molecules is also a topic of intense investigations those days, especially with the developments of new light sources during the past two decades. As an illustration we take the example of a C_{60} fullerene irradiated by an intense laser pulse [4]. The laser ionizes the system and leads to a heating of the system. The emission temperature is plotted in Figure 2 as a function of the fluence of the laser, namely basically as a function of the total amount of deposited energy. It is interesting

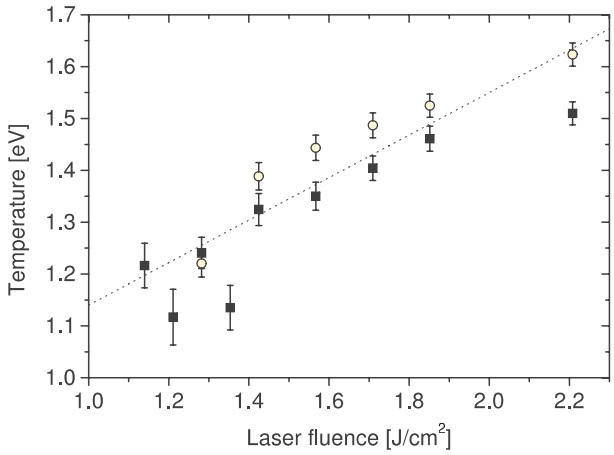

Figure 2. Extracted temperatures from electrons emitted from irradiated C_{60} (open circles) and C_{70} (close squares) as a function of laser fluence. From [4].

to note here the rather large temperatures attained, of order of 20% of the ionization potential of the irradiated system. Such a fraction is similar to the typical temperatures attained in nuclei, namely 20% of the Fermi energy.

2 Theory: Mean-Field and Beyond

The above examples have demonstrated the importance of dissipation and thermal effects in finite quantum systems. We want now to briefly introduce the typical mean-field theories used in these domains to describe the dynamics of such systems. However, as is well known, pure mean-field is generally speaking insufficient to account for observed dissipative features. The question of extending the quantum mean-field by complementing it by dissipative features is thus essential. Such extensions of the mean-field have been actively explored, especially in the nuclear domain, as early as the late 1970's [9]. However, up to the best of knowledge, they do not exist yet. In turn, and because they are reasonably justified in strongly dissipative situations, semi-classical approximations, on the basis of the Vlasov extension and its kinetic theory generalization, have been extensively used over the years. We want here to briefly present these approaches before discussing their validity.

2.1 Basic Scales and Constraints

The electronic and nuclear cases cover a wide range of systems. For the sake of simplicity, we restrict the discussion/comparisons to the simpler case of nuclei versus metal cluster for which direct scaling are more easily attainable. A few key characteristics of nuclei and metal clusters are summarized in Table 1.

Table 1. Gross characteristics of nuclei and clusters. One successively considers the radii of systems of size A (nuclei) or N (clusters), the typical distance between constituents, and the typical mean free path. Distances are expressed in terms of r_0 for nuclei and Wigner Seitz radius r_s for clusters.

	Nuclei (A)	Metal clusters (N)
Radius	$R \sim r_0 A^{1/3}$	$R \sim r_s N^{1/3}$
Interconstituents distance	$d \sim 1.5 - 2r_{0,s}$	
Mean free path	$\lambda \sim R$	

Both nuclei and metal clusters exhibit a "saturating" behavior with radii scaling as a power 1/3 of system's size. Each electron or nucleon thus occupies the same volume $(4/3)\pi {r_{0,s}}^3$, so that the average density of these systems is $\rho \sim 3/(4\pi {r_{0,s}}^3)$ independent of the system size. The parameter $r_{0,s}$ fixes characteristic scales in these systems, for example the typical interconstituent distance. The mean free path is typically of the order of magnitude of the actual size of the system, which motivates a mean-field approach (see next section).

2.2 How to Justify a Mean-Field Picture?

The free nucleon-nucleon interaction is strongly repulsive at short range [7] which at first glance makes a mean-field theory questionable. But the strong Pauli correlations in nuclei suppress low energy scattering, which renormalizes the short-range part of the nuclear interaction in medium. The finally delivered interaction is smooth enough to justify a mean-field picture [7]. A somewhat similar reasoning holds in the case of metal clusters. While the general atomic problem is originally singular, only valence electrons actually take part in the binding of molecular systems or clusters. The case of simple metals is especially forgiving in this respect, as the valence shell is well separated from core levels. Electrons can then easily delocalize to form the rather "soft" metal bonds. This provides again a good candidate for a mean-field treatment, as exemplified by the many successes of Density Functional Theory (DFT), even in its simplest Local Density Approximation (LDA) version [8].

2.3 Mean-Field and Beyond

2.3.1 Quantum Mean-Field: A Starting Point

In both cases (nuclei and metal clusters), a mean-field theory thus provides a sound starting point. The mean-field Hamiltonian are "effective" as correlations are packed in density-dependent terms of the effective interactions, or density functionals respectively.

We start with a set of one-body wave functions (nucleons or electrons) φ_i which provides the time-dependent one-body density matrix $\hat{\rho}(\mathbf{r}, \mathbf{r}', t)$ and the local time-dependent one-body density $\varrho(\mathbf{r}, t) = \hat{\rho}(\mathbf{r}, \mathbf{r}, t)$. The φ_i follow effective Schrödinger equations

$$i\hbar \frac{\partial |\varphi_i\rangle}{\partial t} = \hat{h}[\varrho(\mathbf{r}, t)]|\varphi_i\rangle \quad . \tag{1}$$

The Hamiltonian $\hat{h}$ is expressed as functionals of the density $\varrho(\mathbf{r}, t)$.In nuclei, a standard form is provided by the Skyrme expression with parameters fitted to basic nuclear properties [7]. The Skyrme Hamiltonian is complemented by a Coulomb contribution acting on protons. In metal clusters, the one-body Hamiltonian is primarily constituted of the Hartree term $V_H[\varrho]$ complemented by the DFT-LDA expression for exchange and correlation $V_{\rm xc}$

$$\hat{h}[\varrho] = \frac{\hat{p}^2}{2m} + V_H[\varrho] + V_{\rm xc}[\varrho] + V_{\rm ext}(\mathbf{r}, t) \tag{2}$$

The external one-body potential here accounts for ions (via pseudopotentials) and for coupling to an external excitation field (a by-passing projectile or a time-dependent electric field from a laser).

2.3.2 From Quantum to Semi-Classical Mean-Field

The quantum mean-field constitutes a good starting basis for deriving a semi-classical approximation on the basis of the Vlasov equation. We rewrite the mean-field equation in the equivalent matrix form Passing to the semi-classical limit then amounts to transform the density operator $\hat{\rho}$ into a one-body phase space distribution $f(\mathbf{r}, \mathbf{p}, t)$ and the commutator into Poisson brackets :

$$\begin{array}{ccc} \hat{\rho}(\mathbf{r}, \mathbf{r}', t) & \longrightarrow & f(\mathbf{r}, \mathbf{p}, t) \\ [\,.\,,\,.\,] & \longrightarrow & \{\,.\,,\,.\,\} \end{array} \tag{3}$$

which leads to the Vlasov equation The one-body Hamiltonian has the same expression in terms of the density $\varrho(\mathbf{r})$ as in the quantal form, but the density is now computed from the phase space density as The Vlasov equation has been derived discarding all higher order terms in $\hbar$, thus neglecting all quantum diffraction effects, as e.g. shell structure or tunnelling.

It should be noted here that nothing distinguishes the resulting (semi-classical) Vlasov equation from the strictly classical one, not mentioning Fermi stability of simulations. This question is by no means trivial, nor is the more formal issue of the smoothness to be delivered to $f(\mathbf{r}, \mathbf{p}, t)$ for justifying a semi-classical approximation, see for example [10]. Finally, even if the above quantum to semi-classics step may be formally founded, the question of its actual validity remains open. mean-field is justified by long mean free paths but it remains to evaluate how far quantum effects are lost in a semi-classical picture. In other words, the semi-classical approximation is certainly not justified in *any* situation. A good indicator for that is the de Broglie wavelength (see Section 2.3.4).

2.3.3 Beyond Mean-Field: the VUU Approach

The mean-field picture may become insufficient when one enters the strongly non-linear domain. A natural step beyond Vlasov is provided by kinetic equations by addition of a collision integral mimicking dynamical correlations: particle-particle scattering can then easily be included as a Markovian collision term acting on f. This has been worked out in great detail in nuclear physics applications [11]. The Vlasov equation for metal clusters can as well be complemented by a Uehling-Uhlenbeck [5] collision term. The resulting so called VUU equation reads

$$\frac{\partial f}{\partial t} = \{h, f\} + \int \frac{\mathrm{d}^3\mathbf{p}_2 \mathrm{d}\Omega}{(2\pi\hbar)^3} \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} |\mathbf{v}_{12}| \Big\{ f_1 f_2 (1 - f_3/2)(1 - f_4/2)) - f_3 f_4 (1 - f_1/2)(1 - f_2/2)) \Big\} \tag{4}$$

where $\mathbf{v}_{12}$ is the relative velocity of the colliding particles 1 and 2. The factor $\mathrm{d}\sigma/\mathrm{d}\Omega$ is the differential cross section evaluated in the center of mass frame of the two colliding particles. Indices 3 and 4 label the moments of the two

particles after an elementary collision and we use the standard abbreviation $f_i = f(\mathbf{r}, \mathbf{p}_i, t)$. The collision is purely local in space $\mathbf{r} = \mathbf{r}_1 = \mathbf{r}_2 = \mathbf{r}_3 = \mathbf{r}_4$. Outgoing momenta $\mathbf{p}_3$ and $\mathbf{p}_4$ are deduced from $\mathbf{p}_1$ and $\mathbf{p}_2$ by conservation of energy, of total momentum, and by scattering angle Ω. Pauli blocking factors $(1 - f_i/2)(1 - f_j/2)$ play an important role here by enforcing Pauli principle in the course of fermion collisions. In the ground state, they correctly block all kinematically possible (and thus classically possible) collisions. At high excitation energy phase space opens up and two body collisions start to populate it in the course of thermalization.

2.3.4 The regime for a semi-classical approximation

A standard measure for the importance of quantum effects is provided by the de Broglie wavelength λ_B. Let us evaluate $\lambda_B = h/p = 2\pi/k$ where p $(= \hbar k)$ is a typical momentum of the system. The actual value of p depends on the dynamical scenario, but we first evaluate it in the ground state. The saturating nature of nuclei and metal clusters allows to adopt the Fermi gas picture where the average energy per particle is $\epsilon = 3\epsilon_{\rm F}/5$, delivering an average value of $k \simeq \sqrt{3/5}k_{\rm F}$. The Fermi momentum $k_{\rm F}$ is directly linked to the average density $\rho = {k_{\rm F}}^3/(3\pi^2)$ leading finally to $k_{\rm F} r_{0,s} = (9\pi/4)^{1/3} \simeq 2$, which provides typical value of λ_B in relation to the basic scale of the system $r_{0,s}$:

$$\lambda_B = \frac{2\pi}{\langle k \rangle} = \frac{2\pi}{\sqrt{3/5}k_{\rm F}} = \frac{2\pi}{\sqrt{3/5}(9\pi/4)^{1/3}} r_{0,s}.$$

We obtain $\lambda_B/r_{0,s} \simeq 4$, about $2 - 3$ times the typical distance between constituents. Nuclei and metal clusters in their ground state are thus deep in the quantal regime and a semi-classical description is only marginally acceptable.

Let us now consider dynamical scenarios, namely intermediate energy heavy ion collisions for nuclei and laser irradiations for metal clusters. In heavy-ion collisions, the typical Fermi gas average momentum $\langle k \rangle$ is to be complemented by the beam momentum $k_{\rm b}$ (with proper center of mass correction). In a symmetric system (projectile = target) half the beam energy $E_{\rm lab}/A$ is active in relative motion. The delivered momentum per nucleon is thus given by $(\hbar^2/2m)k_{\rm b}^2 = E_{\rm lab}/(2A)$, which leads to $k_{\rm b} \sim k_{\rm F}$ for $E_{\rm lab}/A \sim 80 - 100$ MeV$/A$. For such beam energies, the typical de Broglie wavelength is thus reduced by more than a factor 2 which makes the Vlasov equation acceptable.

In metal clusters, let us consider irradiation by "intense" lasers. Writing $p\omega = eE$ where E is the amplitude of the laser field and ω its frequency (typically in the optical domain) and expressing the amplitude as a function of the laser intensity ($I \propto E^2$) allows to relate typical values of the momentum to the laser intensity $\propto \sqrt{I}$. One recovers the Fermi momentum for $I \sim 10^{10}$ W/cm^2 for an optical photon ($\hbar\omega \sim 3$ eV). A semi-classical approach should be well justified above such laser intensities.

3 From Successes to New Questions

3.1 Some Successes

The use of the VUU approach in nuclear dynamics started in the mid 1980's and led to many satisfying results, especially in the study of the properties of hot nuclei [3]. The limitations of these approaches were rapidly reached when considering highly excited situations leading to fragmentation of the excited system. This led to the appearance of various, sometimes *ad hoc* approaches in order to in particular include the strong fluctuations associated to these highly dissipative dynamical scenarios. A schematic (but non exhaustive) picture of these theories is presented in Figure 3. While the extensions of nuclear time dependent mean-field (TDHF) were basically stalled since the early 1980's several so-called "Molecular Dynamics" (MD) approaches were developed. The most sound approaches were the so called AMD and FMD methods [12] which, while allowing fragmentation scenarios, preserve most of the crucial quantum mean-field. Dissipation is included by means of a VUU-like collision term which makes the overall theory a mixture of quantum and classical approaches.

The case of clusters has been much less investigated. A few VUU calcula-

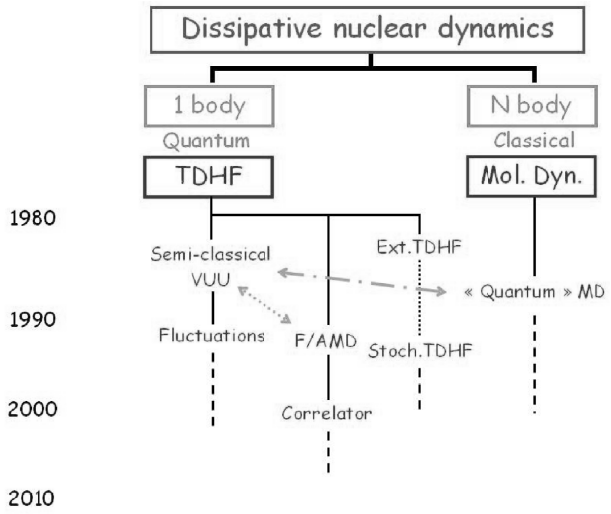

Figure 3. Sketch of theories of the nuclear many body problem in the time domain. In parallel to many-body dynamics (Molecular Dynamics approaches) mean-field is a major issue (TDHF) which needs to be extended to account for dissipation. A major way here was attained through semi-classical approaches [11]. Extended TDHF approaches were only little considered since the 1980's [9] but for isolated attempts such as Stochastic TDHF [14]. The AMD/FMD track provide an acceptable compromise in many cases between quantal features and practical issues [12].

tions were performed as early as the late 1990's with applications to high intensity laser excitations [5]. More recently, similar calculations were performed for various irradiation scenarios [13].

3.2 Need for Quantum Effects

The successes attained by VUU or AMD/FMD approaches in nuclear physics, and, to a lesser extent, by VUU in cluster dynamics should not lead to the conclusion that the problem is fully solved. On the one hand, such approaches are fully justified in the rather high energy domain. On the other hand, there also exist some fundamental restrictions at the side of the actual content of the theories. The major restriction of the most elaborate AMD/FMD approaches concern the fact that the effect of 2-body collisions is treated semi-classically. This raises formal questions and restrict the use of these theories, in principle, to rather energetic processes, even if pure mean-field calculations (at very low energies) are certainly valid in this approximate TDHF scheme. The case of electronic systems is even more plagued by the semi-classical approximation in the sense that all Vlasov/VUU calculations can be performed only in simple metals like Na or K. This singularity restricts the range of applications. An example such as C_{60} illustrated in Figure 2 cannot be in reach of such theories. This adds up to the fact, again, that dissipation is also accounted for via a semi-classical collision term which restricts its range of potential applications in terms of dynamical regimes. The electronic case thus somewhat paradocally doubly suffers from the semi-classical content of the underlying theories. This is all the more infortunate than dissipative dynamics is more and more explored in electron dynamics in clusters and molecules, while the nuclear case has been somewhat less explored during the last years.

3.3 Need for a (New?) Theory

The need for new theories is thus rather clear even if, depending on the field, their necessity is more or less urgent. The basic requirements are that i) one would recover standard time dependent mean-field at vanishing excitation and ii) one would like to account for quantum effects, as much as possible, at the side of dissipation, which would allow to treat low energy cases. Finally, it might also be worth accounting for fluctuations associated to dissipation and thus have an ensemble description rather than one based on a single Slater state. An example of such a theory was proposed two decades ago in the nuclear context but unfortunately not really tested on realistic cases [14]. The idea was to compute dynamical correlations perturbatively and implement them at the side of an ensemble of Slater states in a statistical manner. The implementation of this approach in the nuclear was considered on some test examples [15] using a semi-classical treatment of correlations in the spirit of AMD, but keeping a full description of the TDHF dynamics. It has nevertheless not been further explored since then. The new developments in low energy nuclear dynamics might

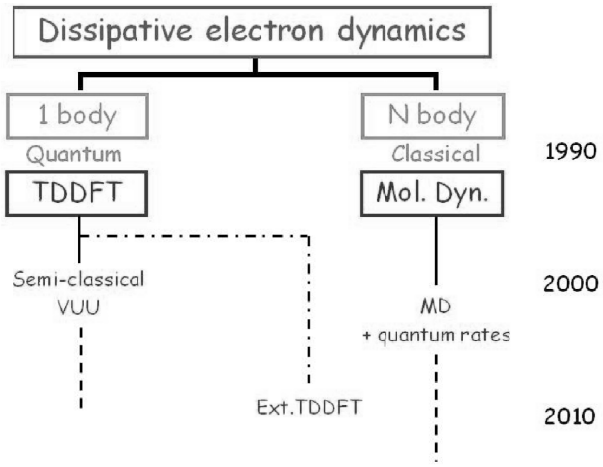

Figure 4. Same as Figure 3 but for electrons. Only few attempts do exist beyond mere TDDFT.

motivate some new investigations with this approach.

The electronic case is even less explored as illustrated in Figure 4. One should furthermore realize that the problem is complicated here by the presence of ions whose dynamics itself is to be taken into account. A whole class of approaches have been devoted to these studies and are known as Trajectory Surface Hopping ones [16]. The idea is to allow the system to hop from one potential energy surface to a neighbouring one when ionic motion brings two potential energy surface sufficiently close to each other. This does not directly address true dissipation as encountered in high energy phenomena, for example in laser irradiations. But it already covers some low energy aspects of the problem. Practically, the picture is limited to rather simple cases where only a few potential energy surfaces may come close to each other which singularly limits the range of applications of such theories. Furthermore, hopping algorithms are a bit heuristic and would certainly deserve close examination in order to be applied in a general "on the fly" manner. There is thus here a lot to be done before reaching a true account of dissipation in electronic dynamics.

4 Next Steps

The next steps to go have been a bit outlined in the previous sections. There admittedly exist a bunch of studies on this basic theoretical problem of account of dissipation in time-dependent quantum mean-field theories. Nuclear physics has provided a rich corpus of results within the semi-classical domain, even accounting for a sizable fraction of quantum effects at the mean-field side. Dissipation itself has nevertheless always been approached in a semi-classical manner. The

situation in electronic systems is even more open with only few tentative explorations following the now flourishing experiments in the domain as attainable with new laser facilities. In that respect, there is thus certainly a challenging problem to address.

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