Annals of Physics 355 (2015) 182–203

Contents lists available at ScienceDirect

Annals of Physics

journal homepage: www.elsevier.com/locate/aop

On the inclusion of collisional correlations in quantum dynamics

N. Slama [a], P.-G. Reinhard [b], E. Suraud [a,c,*]

[a] Laboratoire de Physique Théorique, Université Paul Sabatier, CNRS, F-31062 Toulouse Cédex, France
[b] Institut für Theoretische Physik, Universität Erlangen, D-91058 Erlangen, Germany
[c] Physics Department, University at Buffalo, The State University New York, Buffalo, NY 14260, USA

ARTICLE INFO

Article history:
Received 3 November 2014
Accepted 8 February 2015
Available online 17 February 2015

Keywords:
Collisional correlations
Time dependent mean field
Occupation numbers
Single particle entropy
Density matrices

ABSTRACT

We present a formalism to describe collisional correlations responsible for thermalization effects in finite quantum systems. The approach consists in a stochastic extension of time dependent mean field theory. Correlations are treated in time dependent perturbation theory and loss of coherence is assumed at some time intervals allowing a stochastic reduction of the correlated dynamics in terms of a stochastic ensemble of time dependent mean-fields. This theory was formulated long ago in terms of density matrices but never applied in practical cases because of its complexity. We propose here a reformulation of the theory in terms of wave functions and use a simplified 1D model of cluster and molecules allowing to test the theory in a schematic but realistic manner. We illustrate the performance in terms of several observables, in particular global moments of the density matrix and single particle entropy built on occupation numbers. The occupation numbers remain fixed in time dependent mean-field propagation and change when evaluating the correlations, then taking fractional values. They converge asymptotically towards Fermi distributions which is a clear indication of thermalization.

* Corresponding author at: Laboratoire de Physique Théorique, Université Paul Sabatier, CNRS, F-31062 Toulouse Cédex, France.
E-mail address: suraud@irsamc.ups-tlse.fr (E. Suraud).

http://dx.doi.org/10.1016/j.aop.2015.02.008
0003-4916/

1. Introduction

The dynamical description of thermalization in finite quantum systems, following their excitation, is a long standing question. It concerns various fields of physics. It occurs in excitations of clusters and molecules by intense laser fields [1–4] but also for ballistic electron transport in nano systems [5], as well as thermalization in trapped Fermi gases [6], to cite a few prominent examples. Recent advances in the analysis of electronic emission (energy-, angular-resolved distributions, etc.), through elaborate imaging techniques such as Velocity Map Imaging (VMI) [7,8], reveal for the first time crucial details on the dynamics of irradiation in such finite quantum systems [4] and will thus be of key importance for understanding, and ultimately controlling by light, nano systems. Understanding dissipation and thermalization is thus crucial to describe these experiments properly.

Thermalization effects have been explored since long in nuclear physics, especially in induced nuclear fission or nuclear collisions [9,10]. The nuclear case actually provides one of the earliest examples of such investigations, back to the seminal work of Bohr and Wheeler [11]. They pointed out that atomic nuclei can be "heated up" following neutron impact [11]. The generic scenario of such dynamical processes is there very neatly described: the initial energy deposit first provided by neutron hit is progressively redistributed among internal degrees of freedom leading to thermalization of the nucleons. The resulting "hot" nucleus then de-excites via thermal neutron emission and by radiative decay [11]. The example allows to identify the standard phases of the path to thermalization on the basis of "elementary collisional events" which we will from then on call "collisional correlations". The notion of "thermalization" should be taken with a grain of salt. Thermodynamical concepts are developed for infinite bulk. Their application to finite systems requires, in principle, additional consideration [12]. We take here the naive approach and employ standard thermodynamical terms. This is often found sufficient in finite systems if they are not too small, see the above mentioned applications in nuclear physics. The subtleties of finite-size thermodynamics are usually invisible amongst the large fluctuations of the results.

Nuclear theory devoted major efforts since 4 decades to describe thermalization in nuclear reactions, predominantly using semi-classical methods [13,14,10], in line with similar problems in quantum liquids [15,16]. There were attempts to develop improved molecular dynamics methods combining quantum features with a semi classical treatment of dynamical correlations [17,18]. Still, no clear-cut quantum approach is readily available yet, in spite of numerous formal attempts [19,20,10]. The field of clusters and nano structures is far younger but fast developing in relation to the ongoing developments of lasers and imaging techniques. Semiclassical approaches were also considered in the field to include some dynamical corrections [21,22] and could qualitatively describe dynamical processes. But such approaches are bound to simple metals with sufficiently delocalized wave functions, and thus smooth potentials justifying semiclassical approximations. The case of organic systems, in particular the much celebrated C_{60} [4,23], cannot be treated this way. Semi classical, and even classical approaches, can be used at very high excitations such as delivered by very intense laser pulses [2]. In such cases the system is blown up and details of its quantum mechanical features do not matter anymore. But for less violent scenarios, quantum shell effects cannot be ignored.

Although the classical approach is not directly transferable to the quantum mechanical world it is instructive to recall some of its basic aspects. The prototype model equation of non equilibrium dynamics is the Boltzmann equation which provides a microscope picture of the path to thermalization through elementary (local) collisional processes. It has been successfully applied to a wide variety of classical systems [24]. In quantum systems one needs to account for two additional key aspects. On the one hand the uncertainty principle inhibits the notion of local collisions, typical of Boltzmann picture. Furthermore Pauli principle hinders collisions in occupied states. Accounting for both aspects leads to highly involved quantum kinetic equations hardly applicable in realistic finite systems [15,25]. The Pauli principle can be included in the Boltzmann equation in the form proposed by Uehling and Uhlenbeck to deliver the Boltzmann–Uehling–Uhlenbeck (BUU) equation [26], also known as Vlasov–Uehling–Uhlenbeck (VUU) equation. This can be applied to Fermion systems where quantum shell effects are small such as homogeneous Fermion liquids (gases), electrons in solids [5], or nucleons in neutron stars [27]. Furthermore one can consider BUU as the semi classical limit of a quantum kinetic equation, thus applicable to finite Fermion systems under suitable conditions,