NUCLEAR STRUCTURE AND DYNAMICS WITH DENSITY FUNCTIONAL THEORY*

Ionel Stetcu

Theoretical Division, Los Alamos National Laboratory
Los Alamos, New Mexico 87545, USA

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The superfluid local density approximation (SLDA) is widely used to compute ground-state properties of heavy nuclei. In the same framework, the time-dependent (TD) SLDA can provide information about the excited states and can be used to investigate phenomena involving large amplitude collective motion such as nuclear reactions. Hence, the TDSLDA represents an alternative to the more traditional approaches to nuclear reactions, in which the static and dynamic properties are usually decoupled. In this consistent framework, I briefly discuss the main characteristics of the Coulomb excitation of a ^{238}U nucleus by a relativistic projectile.

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1. Introduction

In the absence of *ab initio* methods applicable to heavy nuclei without restrictions, one can obtain an *ab initio* description of ground-state properties by means of the density functional theory (DFT) [1], and its extension to superfluid systems in its local variant, the superfluid local density approximation (SLDA) [2, 3]. In such an approach, the need to compute a many-body wave function by solving a many-body Schrödinger equation is replaced by the mere minimization of a universal energy functional (EDF), which depends only upon a small number of one-body densities. No construction theorem exists for the EDF, which can be arbitrarily complicated and can contain non-local terms. In our investigations, we use a local approximation of the EDF [4], which simplifies considerably the equations that are solved. However, because in realistic situations the number of coupled three-dimensional equations that have to be solved is of the order of hundreds of thousands, the numerical effort is significant and requires the use of leadership-class computers.

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In addition to the ground-state properties, in a time-dependent (TD) DFT approach [5, 6] one can obtain information about excited states. TDSLDA appears formally as a time-dependent self-consistent local mean-field approximation, which preserves all symmetries of the underlying Hamiltonian. In the small amplitude limit, the same description can be obtained within QRPA. A first application of the TDSLDA to the description of the isovector giant dipole resonance (IVGDR) in deformed nuclei (including triaxial deformation) was presented in Ref. [7]. However, TDSLDA is more powerful because it can be extended beyond linear response. Thus, unlike other approaches in which the nuclear structure information is used as a separate input into reaction models, TDSLDA treats on the same footing the nuclear structure and dynamics [6], and is well suited to provide more reliable description for a large number of processes involving heavy nuclei, from the nuclear response to electroweak probes, to nuclear reactions, such as neutron-induced reactions, or nuclear fusion [8] and fission.

TDSLDA has also limitations. First, only one-body densities and currents, and quantities that can be calculated from these, can be accurately described. In order to compute two-body observables, extensions to the formalism are necessary. Second, the results depend on the accuracy of the EDF. Here, we use the SLy4 parametrization [4], but the code is very flexible and any local EDF can be easily adopted. Finally, the time evolution of the system needs significant computational resources [9], while an extension to the stochastic TDSLDA requires exascale facilities.

2. Relativistic Coulomb excitation

We have studied the response of a ^{238}U nucleus to the electromagnetic field produced by another U nucleus moving at relativistic speed $v = 0.7c$. This allows us to investigate microscopically how much energy is absorbed into the target (excluding the acquired translational motion), compare it against the semiclassical model of Goldhaber and Teller (GT) [10]. In addition, by performing a multipole expansion of the energy spectrum (*i.e.*, $dE/d\hbar\omega$, where E is the emitted energy and ω is the radiation frequency) of the classical electromagnetic radiation produced by the protons in the target nucleus [11], one can identify the main modes of excitation. For our implementation of the GT approach, see the online supplement to Ref. [11].

In our simulations, we place the nucleus on a rectangular lattice, with 1 to 1.25 fm spacing between the lattice points. The derivatives are evaluated using Fourier transforms. The initial solution is obtained by minimizing the energy functional via successive large-scale diagonalizations. Then, the time evolution is realized [9] with the multistep predictor–modifier–corrector Adams–Bashford–Milne. At impact parameters larger than the size of the nuclei, the nuclear interaction can be neglected and the effect of the projectile can be replaced by the electromagnetic (EM) field produced by the moving charge. We neglect the deflection and assume the projectile on a linear trajectory that produces the EM field described by scalar and vector Lienard–Wiechert potentials $(\boldsymbol{A}(\boldsymbol{r},t), \Phi(\mathrm{r},t))$. In their presence, we modify the derivative operator in the density functional to allow minimal gauge coupling, *i.e.*, $\boldsymbol{\nabla}_A = \boldsymbol{\nabla} - ie\boldsymbol{A}/\hbar c$ [11].

Numerical stability does not allow us to follow the response over a very long period of time. Here, we consider trajectories of about 2500 fm/c. In such a time interval, only pre-equilibrium neutrons and γ rays can be observed. We have studied the properties of the EM radiation emitted classically by the protons in the target nucleus. This allowed us to identify the modes of excitation for the target by performing a multipole decomposition of the radiation spectrum. In Fig. 1, we show the dipole and quadrupole contribution to the EM spectrum, microscopically confirming that the main mode of excitation is dipole, as assumed in the GT model. The peak is associated with the IVGDR. In Table I, we show that significantly more energy

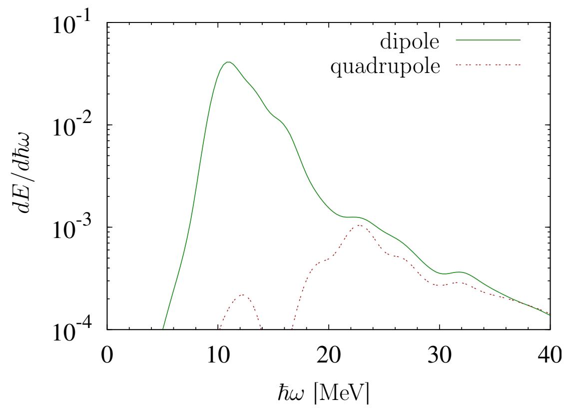

Fig. 1. Dipole and quadrupole contributions to the total spectrum of the emitted EM radiation as a function of the radiation frequency ω, for $b = 14.6$ fm.

TABLE I

Internal excitation energy in TDSLDA (E_{int}), which excludes the energy of the translational motion, and in the Goldhaber–Teller model (E_{GT}) for three values of the impact parameter b. Even if $b = 14.6$ fm could be considered too small, we are mostly interested in trends and, in principle, can exclude small impact parameters.

b [fm]	14.6	16.2	20.2
E_{int} [MeV]	14.98	10.11	4.24
E_{GT} [MeV]	8.06	5.64	2.46

is deposited by the projectile within the TDSLDA than in the GT model, which is the equivalent of a linear response calculation. The difference arises from the non-linear terms, appropriately described in TDSLDA. This fact implies that a QRPA calculation would be subject to large errors, as it only computes the linear response.

3. Conclusions and outlook

We have briefly discussed here an application of the TDSLDA to a simple nuclear reaction: the Coulomb excitation of a ^{238}U nucleus by a relativistic projectile. By studying the multipole decomposition of the classical radiation emitted by the target, we can show that the main mode of excitation is dipole. In addition, our comparison between the TDSLDA and GT model clearly shows the non-linear character of the process [11].

The lack of space does not allow us to discuss other dynamical properties of the nuclear response. However, the main message of this contribution is that TDSLDA can be used to investigate other processes beyond linear response. For example, nuclear fission beyond the barrier is particularly suited TDSLDA. It requires a considerable amount of computational power, but it is achievable with capabilities available today.

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