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Towards quantum transport for nuclear reactions

Pawel Danielewicz *, Arnau Rios, Brent Barker

National Superconducting Cyclotron Laboratory, Department of Physics and Astronomy, Michigan State University, East Lansing, MI 48824-1321, USA

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ABSTRACT

Nonequilibrium Green's functions represent a promising tool for describing central nuclear reactions. Even at the single-particle level, though, Green's functions contain more information that computers may handle in the foreseeable future. In this study, we investigate whether all the information contained in Green's functions is necessarily relevant when describing the time evolution of nuclear reactions. For this, we carry out mean-field calculations of slab collisions in one dimension.

1. Simulations of nuclear reactions

Historically, the description of central nuclear reactions has involved a handful of methods. On the one hand, the time-dependent Hartree–Fock (TDHF) approach has been used to study low-energy reactions [1–3]. On the other hand, the semiclassical Boltzmann equation (BE) has been applied to the reactions at intermediate and high-energies [4]. Molecular dynamics approaches, sharing elements of both TDHF and BE, have also been employed [5,6]. Either TDHF or BE have some serious limitations that are principally remedied within the nonequilibrium Green's function method [7,8], as will be indicated in the following. Even at the basic single-particle level, however, Green's functions method involves the handling of a vast amount of information, likely to overwhelm the capabilities of computing systems. Here, we investigate whether all the information in Green's functions is equally important for the reaction dynamics. To this end, we study the dynamics in one dimension in the absence of correlations. These results are principally equivalent to one-dimensional TDHF calculations, but are performed in terms of Green's functions rather than single-particle wavefunctions.

Within the TDHF method, the system wavefunction Φ is approximated in terms of one Slater determinant of single-nucleon wavefunctions, $\{\phi_j\}_{j=1}^{A}$:

$$\Phi(\{\mathbf{r}_j\}_{j=1}^{A},t)=\frac{1}{A!}\sum_{\sigma}\prod_{k=1}^{A}(-1)^{\mathrm{sgn}\,\sigma}\phi_k(\mathbf{r}_{\sigma(k)},t). \tag{1}$$

The single-nucleon wavefunctions follow wave equations in terms of a self-consistent mean field U:

$$i\frac{\partial}{\partial t}\phi_j=\left(-\frac{\nabla^2}{2m}+U(\{\phi_k\})\right)\phi_j. \tag{2}$$

The first applications of TDHF in the nuclear field have included fusion reactions. An example of the head-on reaction of $^{16}O+{}^{22}Ne$, at $E_{cm}=95\,\mathrm{MeV}$, from a calculation by Umar and Oberacker [3], is shown in Fig. 1. In this particular collision, the nuclei form a compound object that subsequently breaks up, i.e. no fusion occurs. TDHF calculations, in fact, predict a so-called low-ℓ window, regarding fusion reactions, that develops at high collision energies [2,9], see Fig. 2. While nuclei fuse in the more peripheral reactions (at high angular momenta), they fail to do so in the more central reactions (at low angular momenta). No evidence of such a low-ℓ window has been found experimentally [10]. The failure of TDHF with that respect has been attributed to the lack of dissipation, associated to the missing correlations in a mean-field description. In this particular context, the interest in TDHF as a general theoretical method for addressing central reactions has seriously waned.

Higher-energy central nuclear reactions have been commonly described [4,11] in terms of the BE for the evolution of the phase-space distribution functions, $f(\mathbf{r},\mathbf{p},t)$, of nucleons and other particles:

$$\frac{\partial f}{\partial t}+\frac{\partial\omega_{\mathbf{p}}}{\partial\mathbf{p}}\frac{\partial f}{\partial\mathbf{r}}-\frac{\partial\omega_{\mathbf{p}}}{\partial\mathbf{p}}\frac{\partial f}{\partial\mathbf{p}}=I\{f\}. \tag{3}$$

Here, $\omega_{\mathbf{p}}(\mathbf{r},t)$ is the quasiparticle energy for a nucleon with momentum $\mathbf{p}$, at location $\mathbf{r}$, and I is a collision integral. BE may be solved following test-particle method, where the phase-space

* Corresponding author.
E-mail address: danielewicz@nscl.msu.edu (P. Danielewicz).

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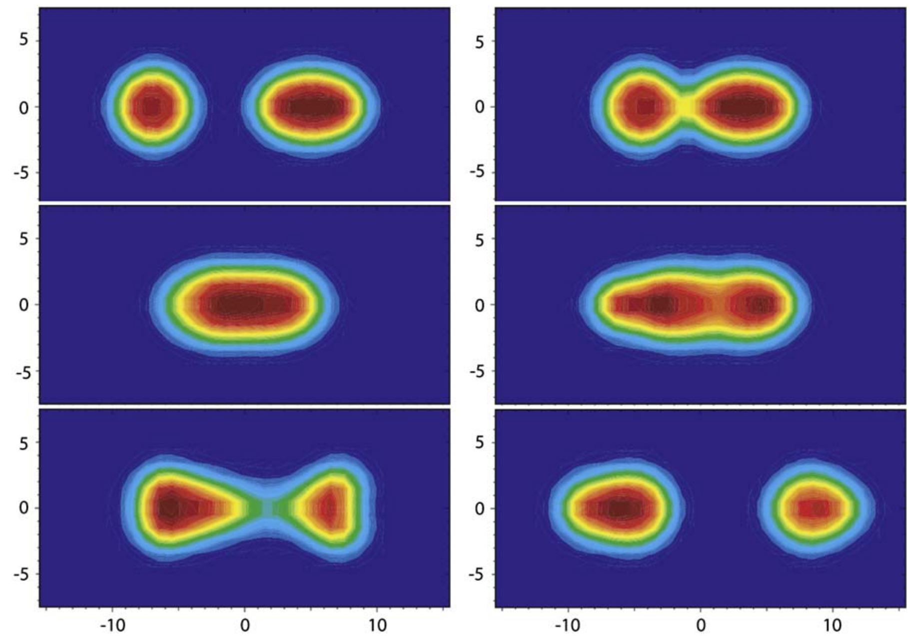

Fig. 1. Contour plots for nucleon density in a head-on collision of $^{16}O+^{22}Ne$ at $E_{cm}=95\,\text{MeV}$, from TDHF calculations of Ref. [3].

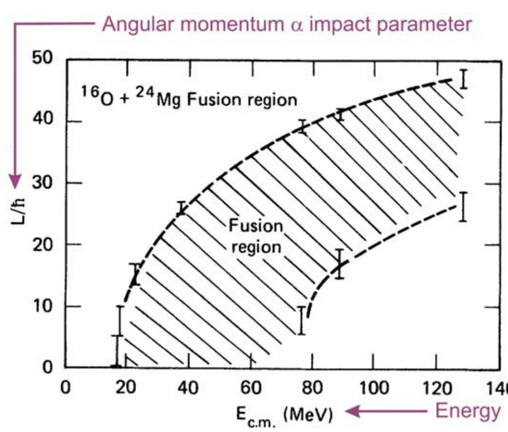

Fig. 2. Fusion region in the plane of angular momentum vs. center-of-mass energy for a $^{16}O+^{24}Mg$ reaction, from the TDHF calculations of Ref. [9]. The outer boundary of the region is associated with the fact that nuclei, in their relative motion, must overcome combined Coulomb and centrifugal barriers.

distribution is represented in terms of test-particles at phase-space locations $(\boldsymbol{r}_i(t),\boldsymbol{p}_i(t))$,

$$f(\boldsymbol{r},\boldsymbol{p},t)\simeq\mathscr{W}\sum_i\delta(\boldsymbol{r}-\boldsymbol{r}_i(t))\delta(\boldsymbol{p}-\boldsymbol{p}_i(t)). \tag{4}$$

The test-particle locations obey Hamilton-type equations that follow from integrating the l.h.s. of Eq. (3),

$$\dot{\boldsymbol{r}}_i=\frac{\partial\omega_{\boldsymbol{p}}}{\partial\boldsymbol{p}},\quad \dot{\boldsymbol{p}}_i=-\frac{\partial\omega_{\boldsymbol{p}}}{\partial\boldsymbol{r}}. \tag{5}$$

Moreover, the test-particles undergo collisions which accomplish a Monte-Carlo integration of the collision integral I [4,11].

BE has been fairly successful in describing many aspects of higher-energy reactions, see e.g. Fig. 3. However, the use of BE in reactions has been criticized on theoretical grounds. Thus, BE relies on the quasiparticle picture and simple estimates [8] indicate that particle scattering rates are comparable to particle energies, which undermines that picture. In addition, in this context it is theoretically difficult [12] to separate collisional

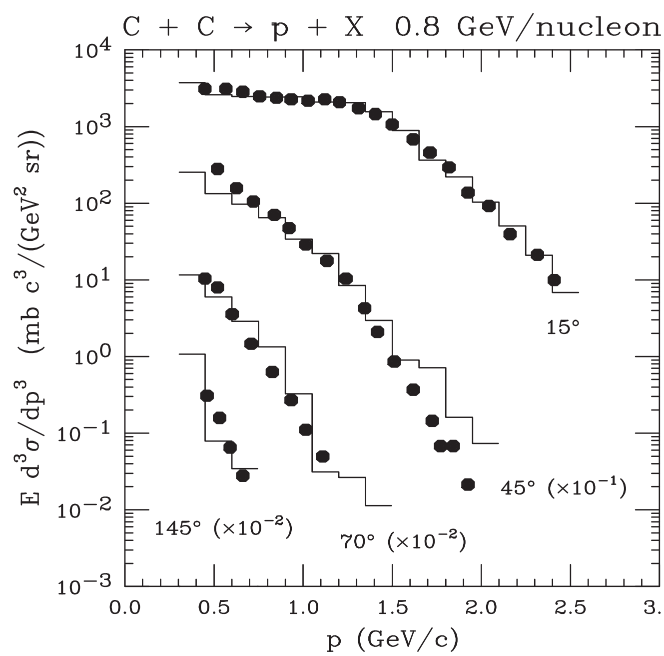

Fig. 3. Proton spectra from an 800 MeV/nucleon $^{12}C+^{12}C$ reaction. Dots represent data of Ref. [13] and histograms represent BE calculations of Ref. [11].

effects, described with cross-sections and entering the integral I, from mean-field effects entering the quasiparticle energies, such as in $\omega_{\boldsymbol{p}}=p^2/2m+U$.

2. Kadanoff–Baym equations

With quantum nonequilibrium many-body theory, the dynamics of a system, starting from an initial state $|\Phi\rangle$, may be described, in a self-contained manner, in terms of a generalized single-particle Green's function

$$iG(1,1')=\langle\Phi|T\{\psi(1)\psi^{\dagger}(1')\}|\Phi\rangle. \tag{6}$$