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Heavy-ion interaction potential deduced from density-constrained time-dependent Hartree-Fock calculation

A. S. Umar and V. E. Oberacker
Department of Physics and Astronomy, Vanderbilt University, Nashville, Tennessee 37235, USA
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We present a new method for calculating the heavy-ion interaction potential from a density-constrained time-dependent Hartree-Fock calculation.

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The study of internuclear potentials for heavy-ion collisions is of fundamental importance for the formation of superheavy elements and nuclei far from stability. While asymptotically such potentials are determined from Coulomb and centrifugal interactions, the short distance behavior strongly depends on the nuclear surface properties and the readjustments of the combined nuclear system, resulting in potential pockets, which determine the characteristics of the compound nuclear system.

Among the various approaches for calculating ion-ion potentials are: (1) Phenomenological models such as the Bass model [1,2], the proximity potential [3–6], and potentials obtained via the double-folding method [7–10]. Some of these potentials have been fitted to experimental fusion barrier heights and have been remarkably successful in describing scattering data. (2) Semimicroscopic and full microscopic calculations such as the macroscopic-microscopic method [11–13], the asymmetric two-center shell-model [14], constrained Hartree-Fock (CHF) with a constraint on the quadrupole moment or some other definition of the internuclear distance [15,16], and other mean-field-based calculations [17–19].

One common physical assumption used in many of the semimicroscopic calculations is the use of the *frozen density* or the *sudden* approximation. As the name suggests, in this approximation the nuclear densities are unchanged during the computation of the ion-ion potential as a function of the internuclear distance. On the other hand, the microscopic calculations follow a minimum energy path and allow for the rearrangement of the nuclear densities as the relevant collective parameter changes. As it was pointed out in Ref. [12], CHF calculations seldom produce the correct saddle-point since the system can follow any one of the minimum potential valleys in the multidimensional potential energy surface. In this article we call this the *static adiabatic approximation* since a real adiabatic calculation would involve a fully dynamical calculation, thus also including the effects of dynamical rearrangements.

One conclusion that may be reached from the discussion above is that ultimately we would like to have an approach for calculating internuclear potentials that is time-dependent and is unrestricted in the choice of collective variables. In this paper we provide such an approach in which time-dependent Hartree-Fock (TDHF) is used for the nuclear dynamics and the potential energy is calculated by constraining the time-dependent density.

The *density constraint* is a novel numerical method that was developed in the mid 1980s [20,21] and was used to provide a microscopic description of the formation of shape resonances in light systems [21]. In this approach the TDHF time evolution takes place with no restrictions. At certain times during the evolution the instantaneous density is used to perform a static Hartree-Fock minimization while holding the total density constrained to be the instantaneous TDHF density. In essence, this provides us with the TDHF dynamical path in relation to the multidimensional static energy surface of the combined nuclear system. Since we are constraining the total density all moments are simultaneously constrained. In the traditional CHF notation this corresponds to the replacement

$$\lambda \hat{Q} \longrightarrow \lambda \hat{\rho}. \tag{1}$$

The numerical procedure for implementing this constraint and the method for steering the solution to $\rho_{\mathrm{TDHF}}(\mathbf{r}, t)$ is discussed in Refs. [20,21]. The convergence property is as good if not better than in the traditional CHF calculations with a constraint on a single collective degree of freedom. Although the self-consistent minimization produces the lowest state consistent with the prescribed density, that density itself may contain some degree of excitation, not because of motion but rather, for example, because of the flexibility of the system to change the proton and neutron radii while keeping the total radius constant.

In this article, we shall call the energy of the system obtained by the density constraint method $E_{\mathrm{DC}}(R)$, where the dependence is on the instantaneous internuclear separation, $R(t)$. Because this quantity contains no translational kinetic energy (taken out by the static minimization), it is actually a potential as we show below. We define the excitation energy of the system as

$$E^*(R) = E_{\mathrm{TDHF}} - T_R - E_{\mathrm{DC}}(R), \tag{2}$$

where E_{TDHF} is the total TDHF energy

$$E_{\mathrm{TDHF}} = \int d^3r\, \mathcal{H}(\mathbf{r}, t), \tag{3}$$

which is conserved throughout the calculation, and T_R is the instantaneous translational energy between the two nuclei

$$T_R = \tfrac{1}{2}\mu \dot{R}^2, \tag{4}$$

with μ being the reduced mass of the system and $\dot{R}$ the velocity associated with the internuclear separation coordinate $R(t)$. At the same time the total TDHF energy can be written in terms

of the excitation energy as

$$E_{\rm TDHF} = T_R + V(R) + E^*(R), \tag{5}$$

such that when combined with Eq. (2) it shows that $V(R) = E_{\rm DC}(R)$. However, the density constrained potential still contains the binding energies of individual nuclei, which should be subtracted out;

$$V(R) \to V(R) = E_{\rm DC}(R) - E_{A_1} - E_{A_2}. \tag{6}$$

Equation (6) is the internuclear potential and contains *no free parameters*. Given an effective nuclear interaction, such as the Skyrme force, $V(R)$ can be constructed by performing a TDHF evolution and minimizing the energy at certain times to obtain $E_{\rm DC}(R)$, while E_{A_1} and E_{A_2} are the results of a static Hartree-Fock calculation with the same effective interaction. One can see that the expression also has the correct asymptotic behavior since numerically for large R we exactly get

$$E_{\rm DC}(R_{\rm max}) = E_{A_1} + E_{A_2} + \frac{Z_1 Z_2 e^2}{R_{\rm max}}, \tag{7}$$

such that

$$V(R_{\rm max}) = \frac{Z_1 Z_2 e^2}{R_{\rm max}}, \tag{8}$$

so that normalization of $V(R)$ is not necessary.

We have carried out a number of TDHF calculations with accompanying density constraint calculations to compute $V(R)$ given by Eq. (6). A detailed description of our new three-dimensional unrestricted TDHF code was recently published in Ref. [22]. For the effective interaction we have used the Skyrme SLy5 force [23] including all of the time-odd terms. In Fig. 1 we show the result of our calculation for the head-on (zero impact parameter) collision of ^{16}O+^{16}O at $E_{\rm c.m.} = 34$ MeV. Also shown in Fig. 1 are two widely used phenomenological potentials, the standard proximity potential for two spherical nuclei [3–5] and the double-folding potential with M3Y effective NN interaction [7–10]. We evaluate the double-folding integral for the strong nuclear and Coulomb interaction in momentum space [10]. For the charge and matter densities we utilized generalized Fermi distributions whose parameters were determined from electron scattering experiments [24]. The double-folding potential agrees almost perfectly with the DC-TDHF approach for distances $R \geqslant 6$ fm. At smaller distances, the double-folding potential tends to overestimate the nuclear interaction as a result of the (unphysical) frozen density approximation. The classical TDHF curve corresponds to the older definition

$$V(R) = E_{\rm c.m.} - T_R, \tag{9}$$

used in Ref. [25].

We also repeated the above calculations for different center-of-mass energies. In this case, we find that the results at the barrier do not appreciably change but the depth of the potential increases for lower energies. For $E_{\rm c.m.} = 12$ MeV the potential is about 1.5 MeV deeper than the one at 34 MeV. One comment is required regarding the calculation of the internuclear separation R. As usual, this quantity becomes somewhat unclear for a strongly overlapping system. In our case we use the standard TDHF approach of finding left and right dividing planes and computing the centers of the density in these two halves and thus the separation.

In TDHF, fusion occurs when the relative kinetic energy in the entrance channel is entirely converted into internal excitations of a single well-defined compound nucleus. The dissipation of the relative kinetic energy into internal excitations is due to the collisions of the nucleons with the "walls" of the self-consistent mean-field potential. TDHF studies demonstrate that the randomization of the single-particle motion occurs through repeated exchange of nucleons from one nucleus into the other. Consequently, the equilibration of excitations is very slow and it is sensitive to the details of the evolution of the shape of the composite system. This is in contrast to most classical pictures of nuclear fusion, which generally assume near instantaneous, isotropic equilibration. This equilibration can be observed in the DC-TDHF approach by tracking the evolution of the excitation energy in time for a system on the way to fusion, or alternately one can examine the change in the internuclear potential for the compound system. In Fig. 2 we show this for the ^{16}O+^{16}O system corresponding to the case shown in Fig. 1. After passing the first minimum the system falls back to a second minimum and climbs

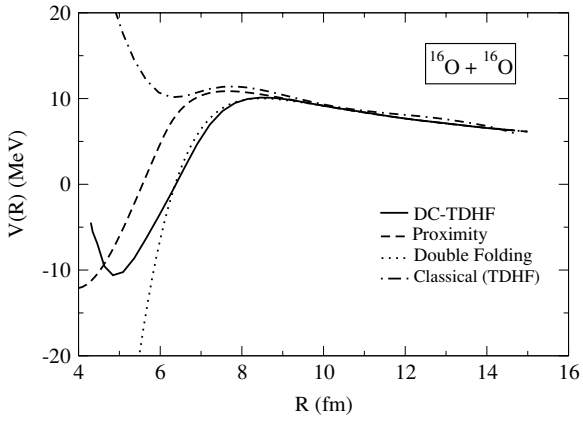

FIG. 1. Internuclear potential obtained from Eq. (6) and various model calculations for the head-on collision of the ^{16}O+^{16}O system at $E_{\rm c.m.} = 34$ MeV.

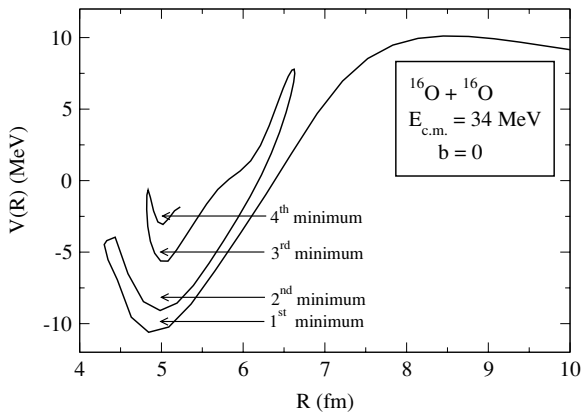

FIG. 2. Internuclear potential obtained from Eq. (6) shown for the entire time evolution of the ^{16}O+^{16}O system at $E_{\rm c.m.} = 34$ MeV.

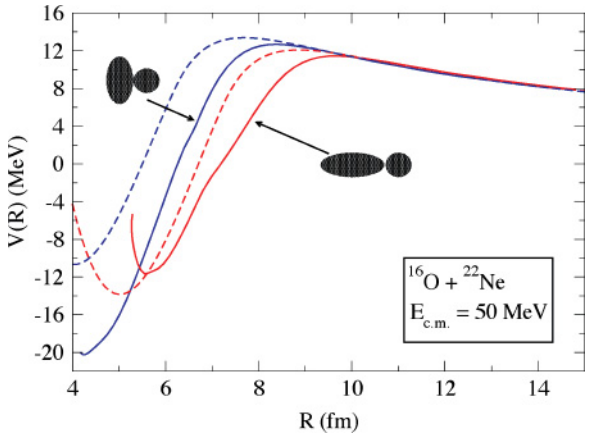

FIG. 3. (Color online) Internuclear potentials obtained from Eq. (6) shown for the evolution of the $^{16}O+^{22}Ne$ system at $E_{c.m.} = 50$ MeV (solid curves). The two curves correspond to different orientations of the Ne nucleus. The corresponding proximity potential curves are also shown (dashed curves).

up the potential barrier, but it cannot overcome the barrier because of some of the energy being converted into internal excitations; consequently it falls back to a third minimum, fourth minimum, and so on, until complete equilibration. This *potential ladder* effect is characteristic for all fusing systems.

Finally, we have performed calculations for the $^{16}O+^{22}Ne$ system at $E_{c.m.} = 50$ MeV. In this case the ^{22}Ne nucleus shows a strong axial deformation, which can have different orientations with respect to the collision axis. We have recently reported a procedure for doing such calculations within the TDHF framework in Ref. [26]. Here, we show the result of our potential calculations for two orientations of the ^{22}Ne nucleus, one in which the symmetry axis of the Ne is aligned with the collision axis and the other in which the symmetry axis is perpendicular to the collision axis. In TDHF, for the first case (aligned with the collision axis), we see no fusion at this energy, whereas for the perpendicular alignment the system fuses. In Fig. 3 we show the results of our potential calculations. We observe that the barrier height and its position in R space and the potential minimum and its position are considerably different for the two orientations. For comparison we have also added the corresponding curves for the proximity potential.

In summary, we have presented a method for calculating internuclear potentials directly from the TDHF time evolution of the colliding system. The method uses the *density constraint* to trace the TDHF trajectory in relation to the static multidimensional energy surface of the combined system. Because the TDHF evolution is unhindered, all of the collective dynamics associated with the evolution are included in the calculations. We believe this provides a unique way to calculate ion-ion potentials from mean-field calculations. Of course, we can only perform such calculations for energies above the barrier because TDHF is a semiclassical theory in this regard. Finally, the results are expected to be only as good as the TDHF description of the particular system under study.

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[1] R. Bass, Nucl. Phys. **A231**, 45 (1974).
[2] R. Bass, *Nuclear Reactions with Heavy Ions* (Springer-Verlag, New York, 1980).
[3] J. Blocki, J. Randrup, W. J. Swiatecki, and C. F. Tsang, Ann. Phys. (NY) **105**, 427 (1977).
[4] J. Randrup and J. S. Vaagen, Phys. Lett. **B77**, 170 (1978).
[5] M. Seiwert, W. Greiner, V. Oberacker, and M. J. Rhoades-Brown, Phys. Rev. C **29**, 477 (1984).
[6] J. R. Birkelund and J. R. Huizenga, Phys. Rev. C **17**, 126 (1978).
[7] G. R. Satchler and W. G. Love, Phys. Rep. **55**, 183 (1979).
[8] G. Bertsch, J. Borysowicz, H. McManus, and W. G. Love, Nucl. Phys. **A284**, 399 (1977).
[9] M. J. Rhoades-Brown and V. E. Oberacker, Phys. Rev. Lett. **50**, 1435 (1983).
[10] M. J. Rhoades-Brown, V. E. Oberacker, M. Seiwert, and W. Greiner, Z. Phys. A **310**, 287 (1983).
[11] H. J. Krappe, J. R. Nix, and A. J. Sierk, Phys. Rev. C **20**, 992 (1979).
[12] P. Möller, A. J. Sierk, and A. Iwamoto, Phys. Rev. Lett. **92**, 072501 (2004).
[13] T. Ichikawa, A. Iwamoto, P. Möller, and A. J. Sierk, Phys. Rev. C **71**, 044608 (2005).
[14] J. Maruhn and W. Greiner, Z. Phys. **251**, 431 (1972).
[15] P. G. Zint and U. Mosel, Phys. Rev. C **14**, 1488 (1976).
[16] T. Bürvenich, M. Bender, J. A. Maruhn, and P.-G. Reinhard, Phys. Rev. C **69**, 014307 (2004).
[17] V. Yu. Denisov and W. Nörenberg, Eur. Phys. J. A **15**, 375 (2002).
[18] A. Dobrowolski, K. Pomorski, and J. Bartel, Nucl. Phys. **A729**, 713 (2003).
[19] H. Goutte, J. F. Berger, P. Casoli, and D. Gogny, Phys. Rev. C **71**, 024316 (2005).
[20] R. Y. Cusson, P.-G. Reinhard, M. R. Strayer, J. A. Maruhn, and W. Greiner, Z. Phys. A **320**, 475 (1985).
[21] A. S. Umar, M. R. Strayer, R. Y. Cusson, P.-G. Reinhard, and D. A. Bromley, Phys. Rev. C **32**, 172 (1985).
[22] A. S. Umar and V. E. Oberacker, Phys. Rev. C **73**, 054607 (2006).
[23] E. Chabanat, P. Bonche, P. Haensel, J. Meyer, and R. Schaeffer, Nucl. Phys. **A635**, 231 (1998); **A643**, 441(E) (1998).
[24] I. Sick and J. S. McCarthy, Nucl. Phys. **A150**, 631 (1970).
[25] S. E. Koonin, K. T. R. Davies, V. Maruhn-Rezwani, H. Feldmeier, S. J. Krieger, and J. W. Negele, Phys. Rev. C **15**, 1359 (1977).
[26] A. S. Umar and V. E. Oberacker, Phys. Rev. C **74**, 024606 (2006); http://arxiv.org/abs/nucl-th/0604010.