Approximate treatment of particle collisions in the time-dependent mean-field theory

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In order to study the gross effects of particle collisions, we formulate a model to include particle collisions in the time-dependent mean-field theory. The model consists of the time-dependent Hartree-Fock equation for the single-particle states and a linearized but truncated equation for the occupation numbers, with the H-theorem and the conservation laws properly satisfied. Numerical calculations are performed with a "conventional" set of basis states in which the occupied and the unoccupied static Hartree-Fock states are boosted in the same way. They are carried out for the head-on collisions of ^{16}O on ^{40}Ca and ^{28}Si on ^{28}Si at 100 MeV per nucleon. It is found that the dynamics of the reaction is affected in only a minor way when particle collisions are included. The projectile and the target nuclear matter appear to interpenetrate each other, with only a 20% reduction in the center-of-mass kinetic energies, just as in mean-field calculations with no particle collisions. This result reinforces the idea that the conventional basis states do not include some important degrees of freedom. It is suggested that in future work one should modify the basis in order to allow for ample wave propagation in the direction normal to the collision axis.

NUCLEAR REACTIONS Extended time-dependent Hartree-Fock theory. Particle collision models. Numerical calculations for $^{16}O + ^{40}Ca$ and $^{28}Si + ^{28}Si$ at $E_{lab} = 100$ MeV per nucleon.

I. INTRODUCTION

In the time-dependent Hartree-Fock (TDHF) approximation, particles interact only through the mean field and the collisions between particles are not taken into account.[1,2] This may be a good approximation for low-energy nuclear phenomena where particle collisions are inhibited by the Pauli exclusion principle. For intermediate-energy heavy-ion collisions (with $E_{lab}/A \sim$ fermi energy ~ 35 MeV), the Pauli exclusion principle may not be effective in preventing particle collisions. It becomes important to consider both the mean-field and particle collisions. Particle collisions are also important in the study of the approach to equilibrium.[3–9]

Previously, we incorporated particle collisions into the mean-field theory.[3,4] Starting with the equations of motion for the Green's function, we obtained the extended time-dependent Hartree-Fock (ETHF) approximation. It consists of an equation of motion for the single-particle wave function which is the same as the TDHF equation, and a master equation for the occupation numbers. Subsequent investigations by other workers led to similar results.[10,11] The collision term has also been examined from a random matrix model[12] and by using a projection method.[13] In addition, it has been conjectured that particle collisions may be responsible for the time smoothing leading to dissipation in a time-dependent and time-smoothed mean-field theory.[14] Other phenomenological ways to introduce the collision term have been presented,[15,16] and numerical ETDHF calculations were performed for simple systems.[17] The complete set of non-Markovian equations involving the one-body Green's function has recently been solved for nonequilibrium nuclear matter.[18] Also, the effects of particle collisions on the mean-field potential and the procedures for maintaining a diagonal occupation matrix have been investigated.[19]

As is well known, the TDHF approximation involves rather time-consuming calculations.[2] The ETDHF approximation is even more complicated as it requires the evaluation of the two-body matrix elements between all the pairs of single-particle states at each time step. The suggested refinements[19] only increase the complexity of the problem. It is desirable to approximate the ETDHF theory. We call the resultant approximations the collision model, in analogy with the collision models used to approximate the Boltzmann equations.[20,21] As in the Bhatnagar, Krook, and Gross (BKG) collision model,[21] which first introduced the relaxation ansatz, we have simplified the ETDHF theory so that it has the form of a relaxation approximation. This (particle) collision model allows one to study the gross features of the dynamical process. Then, from such studies, one may be able to single out important degrees of freedom for use in future collision calculations.

In our description, we have a complete set of time-dependent self-consistent single-particle states, each satisfying the TDHF equation. The occupation numbers of the single-particle states change with time due to particle collisions. The collision model is obtained from the ETDHF approximation by linearizing and truncating the

master equation in order to include only the dominant term, with the H theorem and the conservation laws appropriately satisfied.

When we apply the collision model to specific problems, it is necessary to choose a truncated set of basis states. In line with conventional TDHF calculations, the simplest basis is the set of static Hartree-Fock states (some of which are unoccupied), all initially boosted with the appropriate momenta. Thus, the occupied and unoccupied states in each nucleus are treated in exactly the same way. We shall first report on the results using such a conventional set of basis states for the collision of ^{16}O on ^{40}Ca and ^{28}Si on ^{28}Si at 100 MeV per nucleon. These results are then analyzed to determine whether important degrees of freedom are properly being included in the conventional set of basis states.

This paper is organized as follows. We first summarize the ETDHF approximation in Sec. II in order to introduce model equations for the mean-field theory with particle collisions. In Sec. III, we use the H theorem and the conservation laws to determine a class of collision models with different degrees of nonlinearity in the occupation numbers. Then in Sec. VI, specializing to a linear approximation, we discuss numerical details for calculations of $^{16}O+{}^{40}Ca$ and $^{28}Si+{}^{28}Si$. The results for head-on collisions at 100 MeV/nucleon are presented in Sec. V. Finally, in Sec. IV we suggest that various deficiencies in the implementation of the present collision model may be remedied in future studies by including additional degrees of freedom in the single-particle wave functions.

II. APPROXIMATE COLLISION MODELS

We first summarize the ETDHF approximation which forms the basis for the particle collision models in the mean-field theory. The ETDHF equations of motion consist of an equation for ψ_λ,

$$i\hbar\partial_t\psi_\lambda = h\psi_\lambda = \left[-\frac{\hbar^2}{2m}\nabla^2+\mathscr{V}_{\rm HF}(\rho)\right]\psi_\lambda, \quad \lambda=1,2,\cdots, \tag{2.1}$$

where h is the single-particle Hamiltonian and $\mathscr{V}_{\rm HF}(\rho)$ is the mean-field density-dependent potential defined in the usual way.[1,2] The density ρ in (2.1) is defined as

$$\rho(\vec{r})=\sum_{\lambda=1}^{\infty} n_\lambda\psi_\lambda(\vec{r})\psi_\lambda^*(\vec{r}) . \tag{2.2}$$

The occupation number n_λ satisfies the master equation

$$\frac{\partial n_\lambda}{\partial t}=F_\lambda(\{n_\lambda\}) , \tag{2.3}$$

where

$$F_\lambda(\{n_\lambda\})=\frac{\pi}{\hbar}\sum_{2,3,4}^{\infty}[n_3n_4(1-n_\lambda)(1-n_2)-n_\lambda n_2(1-n_3)(1-n_4)]D(\epsilon_\lambda+\epsilon_2-\epsilon_3-\epsilon_4)\,|\,\langle\lambda2\,|\,v'\,|\,34\rangle_A\,|^2 . \tag{2.4}$$

The quantity ϵ_λ is given by

$$\epsilon_\lambda=\left\langle\lambda\left|-\frac{\hbar^2}{2m}\nabla^2+\mathscr{V}_{\rm HF}(\rho)\right|\lambda\right\rangle , \tag{2.5}$$

$\langle\lambda2\,|\,v'\,|\,34\rangle_A$ is an antisymmetrized two-body matrix element of the residual interaction v', and $D(\epsilon_\lambda+\epsilon_2-\epsilon_3-\epsilon_4)$ is defined by

$$D(\epsilon_\lambda+\epsilon_2-\epsilon_3-\epsilon_4)=\frac{\Gamma_{\lambda234}/2}{2\pi[(\epsilon_\lambda+\epsilon_2-\epsilon_3-\epsilon_4)^2+(\Gamma_{\lambda234}/2)^2]} , \tag{2.6}$$

where $\Gamma_{\lambda234}$ is the sum of the single-particle widths of the states λ, 2, 3, and 4.

We now construct linearized collision models in the following way. We first assume that at every time step, it is possible to find a set of equilibrium occupation numbers $n_\lambda^{(e)}$, $\lambda=1,2,\cdots$, satisfying

$$F_\lambda(\{n_\lambda^{(e)}\})=0 . \tag{2.7}$$

We next define the difference

$$\delta n_\lambda=n_\lambda-n_\lambda^{(e)} , \tag{2.8}$$

and expand $F_\lambda(\{n_\lambda\})$ with respect to δn_λ. If δn_λ is small so that higher-order terms can be neglected, we obtain the linearized equation

$$\begin{aligned}\frac{\partial n_\lambda}{\partial t}=\frac{\pi}{\hbar}\sum_{2,3,4}\,&|\,\langle\lambda2\,|\,v'\,|\,34\rangle_A\,|^2D(\epsilon_\lambda+\epsilon_2-\epsilon_3-\epsilon_4)\\ &\times\{-\delta n_\lambda[n_2^{(e)}(1-n_3^{(e)})(1-n_4^{(e)})+n_3^{(e)}n_4^{(e)}(1-n_2^{(e)})]-\delta n_2[n_\lambda^{(e)}(1-n_3^{(e)})(1-n_4^{(e)})+n_3^{(e)}n_4^{(e)}(1-n_\lambda^{(e)})]\\ &+\delta n_3[n_\lambda^{(e)}n_2^{(e)}(1-n_4^{(e)})+(1-n_\lambda^{(e)})(1-n_2^{(e)})n_4^{(e)}]\\ &+\delta n_4[n_\lambda^{(e)}n_2^{(e)}(1-n_3^{(e)})+(1-n_\lambda^{(e)})(1-n_2^{(e)})n_3^{(e)}]\},\quad \lambda=1,2,\cdots,\end{aligned} \tag{2.9}$$

We rewrite this equation as

$$\frac{\partial n_\lambda}{\partial t}=-\frac{\delta n_\lambda}{\tau_\lambda}-\sum_2\frac{\delta n_2}{\tau_2}+\sum_3\frac{\delta n_3}{\tau_3}+\sum_4\frac{\delta n_4}{\tau_4}\ , \tag{2.10}$$

where

$$\frac{1}{\tau_\lambda}=\frac{\pi}{\hbar}\sum_{2,3,4}|\langle\lambda 2\,|\,v'\,|\,34\rangle_A|^2D(\epsilon_\lambda+\epsilon_2-\epsilon_3-\epsilon_4)[n_2^{(e)}(1-n_3^{(e)})(1-n_4^{(e)})+n_3^{(e)}n_4^{(e)}(1-n_2^{(e)})]\ , \tag{2.11}$$

$$\frac{1}{\tau_2}=\frac{\pi}{\hbar}\sum_{3,4}|\langle\lambda 2\,|\,v'\,|\,34\rangle_A|^2D(\epsilon_\lambda+\epsilon_2-\epsilon_3-\epsilon_4)[n_\lambda^{(e)}(1-n_3^{(e)})(1-n_4^{(e)})+n_3^{(e)}n_4^{(e)}(1-n_\lambda^{(e)})]\ , \tag{2.12}$$

$$\frac{1}{\tau_3}=\frac{\pi}{\hbar}\sum_{2,4}|\langle\lambda 2\,|\,v'\,|\,34\rangle_A|^2D(\epsilon_\lambda+\epsilon_2-\epsilon_3-\epsilon_4)[n_\lambda^{(e)}n_2^{(e)}(1-n_4^{(e)})+(1-n_\lambda^{(e)})(1-n_2^{(e)})n_4^{(e)}]\ , \tag{2.13}$$

and

$$\frac{1}{\tau_4}=\frac{\pi}{\hbar}\sum_{2,3}|\langle\lambda 2\,|\,v'\,|\,34\rangle_A|^2D(\epsilon_\lambda+\epsilon_2-\epsilon_3-\epsilon_4)[n_\lambda^{(e)}n_2^{(e)}(1-n_3^{(e)})+(1-n_\lambda^{(e)})(1-n_2^{(e)})n_3^{(e)}]\ . \tag{2.14}$$

Note that, from symmetry, the last two terms in Eq. (2.10) are equal. By assuming constant matrix elements and a uniform density of states, one can obtain the following very crude estimates:

$$\left[\frac{1}{\tau_j}\Big/\frac{1}{\tau_\lambda}\right]\lesssim\frac{1}{N_t},\quad j=2,3,4, \tag{2.15}$$

where N_t is the (arbitrarily large) number of states in the system. Furthermore, if $1/\tau_2, 1/\tau_3$, and $1/\tau_4$ are constant, we have

$$\sum_2\delta n_2=\sum_3\delta n_3=\sum_4\delta n_4=0\ ,$$

indicating that there are likely cancellation effects in the last three terms of Eq. (2.10) which tend to make them small compared to the first term. Thus, we assume that we can neglect the last three terms in Eq. (2.10) and that a reasonable approximation is given by

$$\frac{\partial n_\lambda}{\partial t}=-\frac{\delta n_\lambda}{\tau_\lambda}\ . \tag{2.16}$$

The change of the occupation numbers is the most drastic for those states for which δn_λ is large. For states having a small deviation from equilibrium, the values of τ_λ do not affect much the time rate of change of occupation numbers. Therefore, it is convenient to make the further approximation for Eq. (2.16)

$$\frac{\partial n_\lambda}{\partial t}=-\frac{n_\lambda-n_\lambda^{(e)}}{\tau}\ , \tag{2.17}$$

where τ is a constant. Equation (2.17) is probably a reasonable approximation for a large system in which the dynamics will not depend critically on the values of $1/\tau_\lambda$ for one or two states, but only on the average of $1/\tau_\lambda$ for a large number of states.

It is important to distinguish the physical meanings of the sets of occupation numbers $\{n_\lambda\}$ and $\{n_\lambda^{(e)}\}$. The time-dependent occupation numbers $\{n_\lambda(t)\}$ and wave functions $\{\psi_\lambda(t)\}$ describe the dynamics of the system. However, $\{n_\lambda^{(e)}(t)\}$ is also time dependent and is the set of occupation numbers towards which the true occupation numbers $\{n_\lambda(t)\}$ tend to approach at time t. When thermal equilibrium has not been achieved, the set $\{n_\lambda(t)\}$ is different from $\{n_\lambda^{(e)}(t)\}$. The two sets are equal only when the system attains true thermal equilibrium.

Equation (2.17) is a linearized and truncated approximation of the original master equation. It is essential that it preserves the H theorem and the conservation laws. We show in the next section how these requirements can be satisfied.

It is instructive to rewrite Eqs. (2.1) and (2.17) in density matrix form by introducing the density matrix $\rho(\vec{r},\vec{r}')$ as follows:

$$\rho(\vec{r},\vec{r}')=\sum_\lambda n_\lambda\psi_\lambda(\vec{r})\psi_\lambda^*(\vec{r}')\ . \tag{2.18}$$

Then, Eqs. (2.1) and (2.17) can be rewritten as

$$i\hbar\partial_t\rho(\vec{r},\vec{r}')=[h,\rho]-i\hbar\frac{\rho(\vec{r},\vec{r}')-\rho^{(e)}(\vec{r},\vec{r}')}{\tau}\ . \tag{2.19}$$

Here, $[h,\rho]$ is the usual TDHF commutator. For the case of velocity-independent two-body interactions, the commutator, after averaging over spin and isospin, becomes

$$[h,\rho]=\left\{-\frac{\hbar^2}{2m}(\nabla_r^2-\nabla_{r'}^2)+\mathscr{V}_{\rm HF}[\rho(r)]-\mathscr{V}_{\rm HF}[\rho(r')]\right\}\rho(\vec{r},\vec{r}')\ , \tag{2.20}$$

In Eq. (2.19), the quantity $\rho^{(e)}$ is the equilibrium density matrix given by

$$\rho^{(e)}(\vec{r},\vec{r}')=\sum_\lambda n_\lambda^{(e)}\psi_\lambda(\vec{r})\psi_\lambda^*(\vec{r}')\ . \tag{2.21}$$

The approximate equation (2.17) is explicitly linear in n_λ (but is implicitly nonlinear since $n_\lambda^{(e)}$ depends on the set of $\{n_\lambda\}$ through the conservation laws). However, we note that the original master equation (2.3) for $\partial n_\lambda/\partial t$ is cubical in the occupation numbers. Thus, it is of interest to write down approximate equations which are explicitly nonlinear in δn_λ. As a matter of fact, we show in the next section that a general equation satisfying the H theorem and the conservation laws is of the form

$$\frac{\partial n_\lambda}{\partial t}=-\frac{f(\delta n_\lambda)}{\tau}\ , \tag{2.22}$$

where $f(\delta n_\lambda)$ is a function of δn_λ which has the same sign as δn_λ and vanishes if and only if $\delta n_\lambda = 0$.

The collision model presented here consists of Eqs. (2.1) and (2.17) [or (2.19)]. It is analogous to the BKG (Bhatnagar, Krook, and Gross) collision model[20,21] (which first introduced the relaxation ansatz), the model proposed by Köhler,[15] and the model proposed by Nörenberg.[22] However, our treatment differs from Refs. 15, 20, 21, and 22 in the following ways. Here, the mean-field, single-particle states and their associated occupation numbers are all basic dynamical variables. Then, the approach to equilibrium is described in terms of the relaxation of $\{n_\lambda\}$ towards $\{n_\lambda^{(e)}\}$. In contrast, in both the BKG model[20,21] and the model of Köhler,[15] the basic variable $f(\vec{R},\vec{p})$ is a function of the space coordinate $\vec{p}$, with the equilibrium distribution $f^{(0)}(\vec{R},\vec{p})$ defined in terms of local parameters $\mu(\vec{R})$, $\vec{j}(\vec{R})$, and $kT(\vec{R})$. Specifically, in the model of Köhler, $f^{(0)}(\vec{R},\vec{p})$ is assumed to be of a Fermi-Dirac distribution whose parameters depend on the space coordinate $\vec{R}$. In terms of the density matrix, the equation proposed by Köhler is

$$i\hbar\frac{\partial}{\partial t}\rho(\vec{r},\vec{r}')=[h,\rho]-i\hbar\frac{\rho(\vec{r},\vec{r}')-\rho^{(0)}(\vec{r},\vec{r}')}{\tau}\ , \tag{2.23}$$

where

$$\rho^{(0)}(\vec{r},\vec{r}')=\int\frac{e^{i\vec{p}\cdot(\vec{r}-\vec{r}')}}{1+\exp\{[\epsilon-\mu(\vec{R})]/kT(\vec{R})\}}d\vec{p}\ , \tag{2.24}$$

$$\epsilon=\frac{\hbar^2}{2m}\{\vec{p}-[m\,\vec{j}(\vec{R})/\rho(\vec{R})]\}^2\ , \tag{2.25}$$

and

$$\vec{R}=(\vec{r}+\vec{r}')/2\ . \tag{2.26}$$

Although Eqs. (2.19) and (2.23) are similar in form, $\rho^{(e)}(\vec{r},\vec{r}')$ of our model is very different from $\rho^{(0)}(\vec{r},\vec{r}')$ used by Köhler. Also, the single-particle states used here are completely self-consistent, in contrast to the diabatic or adiabatic orbitals generated by a non—self-consistent potential well and considered by Nörenberg.[22] Finally, we mention that a collision model based on mean-field dynamics has recently been proposed by Cusson and Wolchin.[23]

III. CONSERVATION LAWS AND THE H THEOREM

The H theorem is a central concept in the discussion of nonequilibrium dynamical systems. It states that the entropy of a dynamical system never decreases and becomes stationary when thermal equilibrium is reached. The collision models we propose must satisfy the H theorem so that the approach to equilibrium is an irreversible process. In addition, for the total system we demand conservation of energy, linear momentum, proton number, and neutron number.

The gross features of the dynamics are expected to depend less on the exact shape of $n_\lambda^{(e)}$ than on the speed with which the equilibrium distribution is approached and on other important factors to be discussed in later sections. It is sufficient to consider approximate forms of $n_\lambda^{(e)}$ which are simple and manageable. Accordingly, when the single-particle widths vanish, the function $D(x)$, Eq. (2.6), becomes a delta function and the equilibrium distribution satisfying Eq. (2.7) can be shown to be of the form[4]

$$\eta_\lambda^{(e)}=1/(1+\{[\epsilon_\lambda-\mu]\}/kT$$

for equal mass collisions. For unequal masses, it is reasonable to assume a form of the equilibrium distribution given by

$$n_\lambda^{(e)}=1/(1+\exp\{[\epsilon_\lambda-(\vec{p}_\lambda\cdot\vec{p}_0/m)-\mu]\}/kT)\ , \tag{3.1}$$

where

$$\vec{p}_\lambda=\left\langle\lambda\left|\frac{\hbar}{i}\nabla\right|\lambda\right\rangle\ ,$$

and the quantities μ, $\vec{p}_0$, and kT are parameters to be determined. As the neutron and proton single-particle energies are different, it is necessary to introduce μ_p and μ_n for protons and neutrons separately. The parameters μ_p, μ_n, $\vec{p}_0$, and kT must be chosen so that the equations of motion Eqs. (2.1) and (2.17) [or (2.19)] will satisfy the conservation laws. It should be noted that this condition is distinctly different from requiring that $\{n_\lambda^{(e)}\}$ and $\{\psi_\lambda\}$ lead directly to spatial densities and currents which conserve total energy, linear momentum, and neutron and proton numbers. With the former condition, the system, as described by n_λ and ψ_λ, conserves all the relevant physical quantities at all times, which need not be true with the latter condition.

To formulate the conservation laws, we define the total proton number Z as

$$Z=\sum_{\lambda=1}^{\infty}n_\lambda\delta(\tau_{\lambda Z},\tfrac{1}{2})\ , \tag{3.2}$$

the total neutron number N as

$$N=\sum_{\lambda=1}^{\infty}n_\lambda\delta(\tau_{\lambda Z},-\tfrac{1}{2})\ , \tag{3.3}$$

and the total momentum $\vec{P}$ as

$$\vec{P}=\sum_{\lambda=1}^{\infty}n_\lambda\vec{p}_\lambda\ . \tag{3.4}$$

Our present description, based on partial occupations of single-particle states, is essentially an independent-particle description. It is appropriate to define the total energy in this self-consistent, independent-particle model in the usual way:

$$E=\int d\vec{r}\,T(\vec{r})+\frac{i^2}{2}\int d1\,d2\,v(12)g_{20}(12,1^+2^+)\ , \tag{3.5}$$

where $T(\vec{r})$ is the kinetic energy density

$$T(\vec{r})=\sum_{\lambda=1}^{\infty}n_\lambda\psi_\lambda^*(\vec{r})\left[-\frac{\hbar^2}{2m}\nabla^2\right]\psi_\lambda(\vec{r})\ , \tag{3.6}$$

$v(12)$ is the effective interaction, $g_{20}(12,1^+2^+)$ is the uncorrelated two-body Green's function, and the symbol 1^+ denotes $t_1^+=t_1+\epsilon$ (with $\epsilon\to 0$). The two-body Green's function is the antisymmetrized product of the one-body Green's functions

$$g_{20}(12,1^+2^+)=\mathscr{A}[g^<(11^+)g^<(22^+)]\ . \tag{3.7}$$

In terms of n_λ and ψ_λ, the one-body Green's function $g^<(1,1^+)$ is given by

$$-ig^<(1,1^+)=\sum_{\lambda=1}^{\infty} n_\lambda \psi_\lambda(1)\psi_\lambda^*(1^+) . \tag{3.8}$$

We are now in a position to write down the conservation laws. The conservation of proton and neutron numbers leads to

$$\frac{\partial Z}{\partial t}=\sum_{\lambda=1}^{\infty}\frac{\partial n_\lambda}{\partial t}\delta(\tau_{\lambda Z},\tfrac{1}{2})=0 \tag{3.9}$$

and

$$\frac{\partial N}{\partial t}=\sum_{\lambda=1}^{\infty}\frac{\partial n_\lambda}{\partial t}\delta(\tau_{\lambda Z},-\tfrac{1}{2})=0 . \tag{3.10}$$

Conservation of momentum gives

$$\frac{\partial \vec{\mathrm{P}}}{\partial t}=\sum_{\lambda=1}^{\infty}\frac{\partial n_\lambda}{\partial t}\vec{\mathrm{P}}_\lambda+\sum_{\lambda=1}^{\infty} n_\lambda\frac{\partial \vec{\mathrm{p}}_\lambda}{\partial t}=0 . \tag{3.11}$$

The second term of the above equation is, however, zero because of the translational invariance of the two-body effective interaction $v(12)$. Therefore, we find that

$$\frac{\partial \vec{\mathrm{P}}}{\partial t}=\sum_{\lambda=1}^{\infty}\frac{\partial n_\lambda}{\partial t}\vec{\mathrm{P}}_\lambda=0 . \tag{3.12}$$

Conservation of energy is expressed as

$$\frac{\partial E}{\partial t}=\sum_{\lambda=1}^{\infty}\frac{\partial n_\lambda}{\partial t}\epsilon_\lambda+\left.\frac{\partial E}{\partial t}\right|_{\{n_\lambda\}}=0 . \tag{3.13}$$

The second term in (3.13) is evaluated by fixing the occupation numbers and is identically zero, since the single-particle states satisfy the TDHF equation (2.1), so that

$$\frac{\partial E}{\partial t}=\sum_{\lambda=1}^{\infty}\frac{\partial n_\lambda}{\partial t}\epsilon_\lambda=0 . \tag{3.14}$$

The equation of motion $\partial n_\lambda/\partial t$ must satisfy the conservation laws as given by Eqs. (3.9), (3.10), (3.12), and (3.14). Then, from Eq. (2.17) [or (2.22)] the equation for the conservation laws can be written as

$$\sum_{\lambda=1}^{\infty} f(\delta n_\lambda)\begin{Bmatrix}\delta(\tau_{\lambda z},\frac{1}{2})\\ \delta(\tau_{\lambda z},-\frac{1}{2})\\ \vec{\mathrm{p}}_\lambda\\ \epsilon_\lambda\end{Bmatrix}=0 . \tag{3.15}$$

In the above equation, the only unknown quantities for a given form of $f(\delta n_\lambda)$ are the parameters μ_p, μ_n, $\vec{\mathrm{p}}_0$, and kT which specify the equilibrium distribution $n_\lambda^{(e)}$ [Eq. (3.1)]. These parameters can be chosen so that the conservation laws are satisfied.

We are now in a position to discuss the H theorem. In our description in terms of partial occupation of self-consistent, single-particle states, the entropy of a system S can be defined in the usual way,[24]

$$S=-k\sum_\lambda[n_\lambda\ln n_\lambda+(1-n_\lambda)\ln(1-n_\lambda)] , \tag{3.16}$$

where k is the Boltzmann constant. Therefore, we have

$$\frac{\partial S}{\partial t}=-k\sum_\lambda\frac{\partial n_\lambda}{\partial t}\ln\left[\frac{n_\lambda}{1-n_\lambda}\right] . \tag{3.17}$$

On the other hand, from Eq. (3.1) and the conservation laws, Eqs. (3.9), (3.10), (3.12), and (3.14), one can show that

$$\sum_\lambda\frac{\partial n_\lambda}{\partial t}\ln\left[\frac{n_\lambda^{(e)}}{1-n_\lambda^{(e)}}\right]=0 . \tag{3.18}$$

Combining Eqs. (3.17) and (3.18), we obtain

$$\frac{\partial S}{\partial t}=-k\sum_\lambda\frac{\partial n_\lambda}{\partial t}\left[\ln\left[\frac{n_\lambda}{n_\lambda^{(e)}}\right]-\ln\left[\frac{1-n_\lambda}{1-n_\lambda^{(e)}}\right]\right] . \tag{3.19}$$

We next prove that the H theorem can be satisfied by introducing a general collision model

$$\frac{\partial n_\lambda}{\partial t}=-\frac{f(\delta n_\lambda)}{\tau} , \tag{3.20}$$

where $\tau>0$ and $\delta n_\lambda=n_\lambda-n_\lambda^{(e)}$; $n_\lambda^{(e)}$ is given by Eq. (3.1) and satisfies the conservation laws of Eq. (3.15). Furthermore, we demand that the function $f(\delta n_\lambda)$ have the same sign as δn_λ, i.e.,

$$\begin{aligned} &f(\delta n_\lambda)>0 \quad \text{for } \delta n_\lambda>0,\\ &f(\delta n_\lambda)<0 \quad \text{for } \delta n_\lambda<0 , \end{aligned} \tag{3.21}$$

and also

$$f(\delta n_\lambda)=0 \quad \text{for } \delta n_\lambda=0 .$$

It then follows from Eq. (3.19) that

$$\frac{\partial S}{\partial t}\geq 0 , \tag{3.22}$$

i.e., the H theorem is satisfied. The equal sign in (3.22) holds only for $n_\lambda=n_\lambda^{(e)}$.

Equation (3.21) implies that $f(\delta n_\lambda)$ be an odd function of δn_λ, e.g.,

$$f(\delta n_\lambda)=n_\lambda-n_\lambda^{(e)} , \tag{3.23}$$

or

$$f(\delta n_\lambda)=(n_\lambda-n_\lambda^{(e)})+a(n_\lambda-n_\lambda^{(e)})^3 . \tag{3.24}$$

Since the original master equation (2.3) is cubic in δn_λ, Eq. (3.24) may lead to more adequate results. However, for the present exploratory calculations, we shall limit ourselves to the linear approximation, Eq. (3.23).

IV. CALCULATIONAL DETAILS

We have performed numerical calculations for head-on collisions of ^{16}O on ^{40}Ca and ^{28}Si on ^{28}Si at an energy of 100 MeV per nucleon. The first case was chosen in order to compare our results with previous calculations where particle collisions were not included.[25] The second case was chosen to examine whether the single-particle shell gap is an important feature of the dynamics.

The collision model consists of the TDHF equation (2.1) for the single-particle states and the equation of motion (2.17) for the occupation numbers. We performed our calculations by modifying the axially symmetric

TDHF code.[26] The set of single-particle wave functions $\{\psi_\lambda\}$ are evolved in time according to the methods of Ref. 26. Also, the calculations are performed in the center-of-mass system and the two-body effective interaction is the Skyrme II force, which was the interaction used in Ref. 25.

For the ^{16}O nucleus, we choose the Hartree-Fock states in the s, p, and s-d shells as the basis states, and for the ^{40}Ca and ^{28}Si nuclei we choose the states in the s,p, s-d, and p-f shells as the basis. As in the conventional TDHF calculations,[26] all these states are boosted initially by velocities appropriate to the given reaction. We emphasize that the occupied and unoccupied states are boosted in exactly the same manner. These two types of states differ only in their initial occupancy. Thus, at $t=0$ for ^{16}O, $n_\lambda=1$ for the $1s$ and $1p$ states, and $n_\lambda=0$ for the states in the s-d shell. Similarly, for ^{40}Ca, $n_\lambda=1$ for the s, p, and s-d shells, and $n_\lambda=0$ for the p-f shell, while for the ^{28}Si nucleus, $n_\lambda=1$ for the ls and $1p$ states, $n_\lambda=0.6$ for the $1d$ states, and $n_\lambda=0$ for the $2s$, $2p$ and $1f$ states. We shall refer to these sets of basis states as the conventional sets.

The quantity τ is the time required for a nuclear system to relax its occupation distribution to thermal equilibrium. It depends on the collision energy and the degree of Pauli blocking. Its value is not well determined, although there have been various estimates of its magnitude.[5-7] In a previous calculation, based on the relaxation of nucleons in nuclear matter, we obtained[5]

$$\tau\approx\frac{300\text{ fm}/c}{(E_{\rm lab}/A_p\text{ in MeV})} \tag{4.1}$$

where A_p is the projectile mass number. Based on this estimate for $E_{\rm lab}/A_p=100$ MeV per nucleon we have

$$\tau=3\text{ fm}/c\ =0.01\times10^{-21}\text{ sec}\ . \tag{4.2}$$

As a comparison, the high-energy interaction time for reactions of nuclei with radii R_1 and R_2 is approximately

$$T\sim\frac{2(R_1+R_2)}{v_{\rm rel}}\ . \tag{4.3}$$

For the cases considered here, $T\sim31$ fm/c so that $T\gg\tau$. In our exploratory investigations, we use $\tau=3$ fm/c and also $\tau=0.3$ fm/c. The smaller value has been chosen in order to ensure that particle collision effects, if sufficiently important, would manifest themselves in an obvious manner. As it has turned out, the results from using the two different values of τ are not very different (partially because $T\gg\tau$ and also for reasons to be discussed later). It is sufficient to discuss the results for one case which we choose to be

$$\tau=0.01\times10^{-21}\text{ sec}\ .$$

At each time step, we evaluate the equilibrium occupation numbers $\{n_\lambda^{(e)}\}$ at the middle of each time interval by solving the four conservation equations in Eq. (3.15). Then, the parameters $\mu_{\rm p}$, $\mu_{\rm n}$, $\vec{\rm p}_0$, and kT in Eq. (3.1) can be determined by Newton's method using values of these parameters at the previous time step as initial guesses. The detailed method is outlined in the Appendix.

It is clear that, before the two nuclei interact, there is no collision between nucleons in different nuclei and the occupation numbers do not change. After the two nuclei collide and separate, the relaxation of the two separated fragments involves a very long relaxation time and the occupation numbers are assumed to be unchanged. Accordingly, $\partial n_\lambda/\partial t$ is always equal to zero when the two nuclei do not interact. Operationally, we assume that the two nuclei interact when the density at an appropriate midpoint between them[26] reaches a "clutching" value of 0.075 nucleons/fm^3. When the two nuclei interact by turning on the residual nuclear interaction, the occupation numbers can relax to the equilibrium values and the equation of motion (2.17) is used. Since $n_\lambda^{(e)}$ is evaluated at the midpoint $t+\Delta t/2$ of the time interval $[t,t+\Delta t]$ and can be taken as constant within the interval, we integrate Eq. (2.17) to obtain explicitly the occupation number in the interval $t\le t'\le t+\Delta t$:

$$n_\lambda(t')=n_\lambda(t)e^{-(t'-t)/\tau}+n_\lambda^{(e)}\left[t+\frac{\Delta t}{2}\right](1-e^{-(t'-t)/\tau})\ . \tag{4.4}$$

The change in occupation numbers alters the spatial density which in turn changes the single-particle wave functions $\{\psi_\lambda\}$, the energies $\{\epsilon_\lambda\}$, and the momenta $\{\vec{\rm p}_\lambda\}$. The equilibrium distribution $\{n_\lambda^{(e)}\}$ is then altered. We continue this procedure, in stepwise fashion, until the two nuclei are well separated from each other.

V. RESULTS OF CALCULATIONS

As we show in the Appendix, we use $\{\epsilon_\lambda\}$ and $\{\vec{\rm p}_\lambda\}$ to calculate the equilibrium occupation numbers $\{n_\lambda^{(e)}\}$. They are characterized by four parameters: $\mu_{\rm p}$, $\mu_{\rm n}$, p_0, and kT, which are displayed in Fig. 1 for the head-on collision of ^{16}O + ^{40}Ca at an energy of 100 MeV per nucleon, with

$$\tau=0.01\times10^{-21}\text{ sec}\ .$$

The behavior of $\mu_{\rm p}$ and $\mu_{\rm n}$ reflects the rapid rise of the single-particle energies when the spatial density in the overlapping region of the two nuclei is large. (See Fig. 2).

In order to interpret the parameter p_0, we examine the initial TDHF wave functions. These are obtained by boosting the static Hartree-Fock states u_λ by the function $e^{i\vec{\rm k}\cdot\vec{\rm r}}$, corresponding to a velocity of $\hbar\vec{\rm k}/m$ in the center-of-mass system. The single-particle energy ϵ_λ for the simple case of a velocity-independent effective two-body interaction is given by

$$\epsilon_\lambda=\epsilon_\lambda^{(0)}+\frac{\hbar^2k^2}{2m}\ , \tag{5.1}$$

where $\epsilon_\lambda^{(0)}$ is the static Hartree-Fock energy. In addition, we have

$$\vec{\rm p}_\lambda=\hbar\vec{\rm k}\ . \tag{5.2}$$

From Eq. (3.1), the occupation numbers n_λ are determined by a combination of ϵ_λ and $\vec{\rm p}_\lambda$ which we call the effective (single-particle) energy ϵ_λ(eff),

$$\epsilon_\lambda(\text{eff})\equiv\epsilon_\lambda-\vec{\rm p}_\lambda\cdot\vec{\rm p}_0/m\ . \tag{5.3}$$

For the initial wave functions ϵ_λ(eff) becomes

$$\epsilon_\lambda(\text{eff})=\epsilon_\lambda^{(0)}+\frac{(\vec{\rm p}_\lambda-\vec{\rm p}_0)^2}{2m}-\frac{p_0^2}{2m}\ . \tag{5.4}$$

The sum of the first two terms of the above equation is just the value of ϵ_λ for the frame in which the center of mass is boosted by a velocity of $\vec{p}_0/m$ and this value differs from ϵ_λ(eff) by a constant. Thus, the frame in which the center of mass is boosted by a velocity of $\vec{p}_0/m$ is the natural frame for describing the equilibrium distribution. After the two nuclei interact with each other, the above equations are not strictly valid. However, in order to roughly understand the dynamics, we can interpret $\vec{p}_0$ as representing the frame in which the expectation value of ϵ_λ directly describes the equilibrium distribution. For the collision of ^{16}O on ^{40}Ca at 100 MeV per nucleon, the momentum of the ^{16}O nucleons in the center-of-mass system is initially $\sim 0.94\times10^{-21}$ MeV sec/fm, while the momentum of the ^{40}Ca nucleus is initially $\sim -0.39\times10^{-21}$ MeV sec/fm. From Fig. 1, we note that the value of p_0 is $\sim 0.33\times10^{-21}$ MeV sec/fm at $t=0$. Thus, the best frame to describe the initial equilibrium distribution is roughly the frame in which the speed of the ^{16}O nucleons and the ^{40}Ca nucleons are nearly equal. After the two nuclei interact, the preferred frame is one in which the average speed of the ^{16}O nucleons is slightly smaller than that of ^{40}Ca nucleons.

In Fig. 2 the occupation numbers at $t=0$ and at

$t=0.14\times10^{-21}$ sec

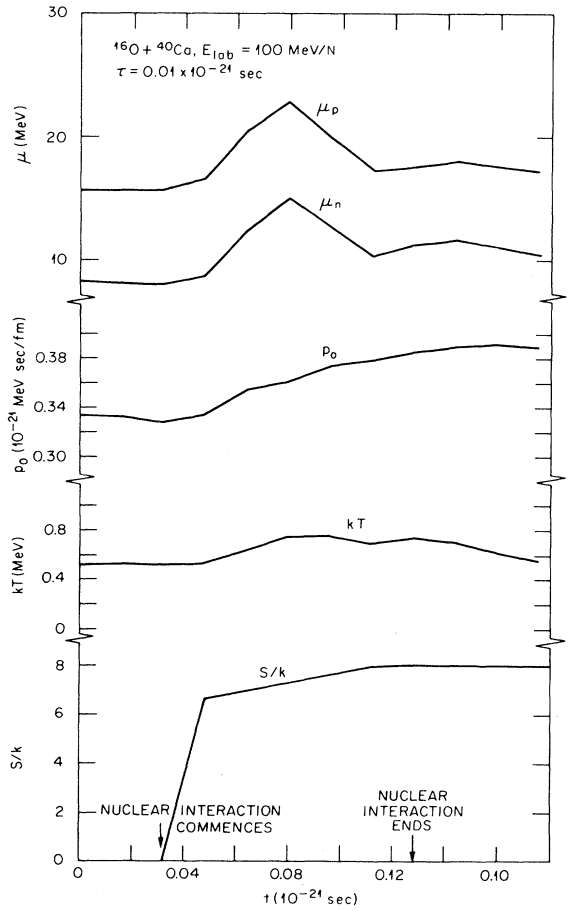

FIG. 1. The parameters μ_p, μ_n, p_0, and kT and the entropy S/k, as functions of time for the head-on collision of ^{16}O on ^{40}Ca at a laboratory bombarding energy of 100 MeV per nucleon. The parameter τ is 0.01×10^{-21} sec. The arrows indicate the times at which the residual nuclear interactions responsible for changing the occupation numbers are turned on or off.

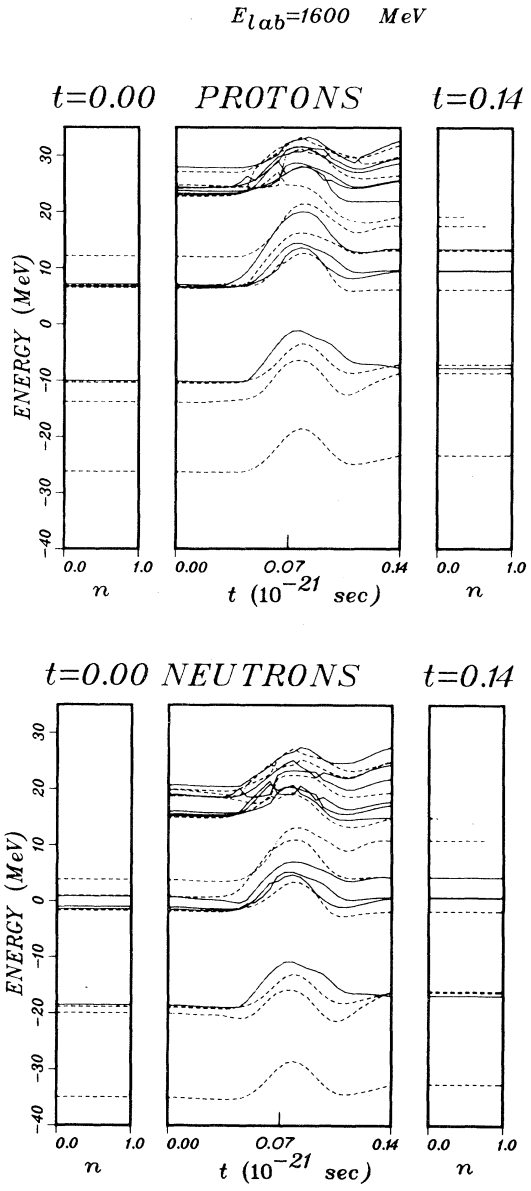

FIG. 2. Occupation numbers and effective energies for the head-on collision of ^{16}O on ^{40}Ca at 100 MeV per nucleon. The top pictures are for protons and the bottom pictures, for neutrons. The left and the right panels in each picture give the occupation numbers at $t=0$ and $t=0.14\times10^{-21}$ sec, respectively. The middle panel in each picture shows the variation of the single-particle effective energy ϵ_λ(eff) as a function of time. Solid curves are for states with degeneracy 4, while the dashed curves are for states with degeneracy 2. The parameter τ is 0.01×10^{-21} sec.

are shown on the left and the right panels, respectively. In the middle panel, we show ϵ_λ(eff) as a function of t. These results are obtained for

$$\tau=0.01\times10^{-21}\ \text{sec}\ .$$

It should be noted that there is a gap between the occupied states and the unoccupied states. Because p_0/m is approximately the velocity in the equal velocity frame, ϵ_λ(eff) is roughly the expectation value of the single-particle Hamiltonian in this frame. We note that the single-particle states of ^{16}O and ^{40}Ca gain about the same increase in kinetic energy and that the Fermi levels of the two nuclei are not too different. However, there is a shell gap which originates from the gaps in the ^{16}O and ^{40}Ca static ground states. The presence of this gap makes the results of the calculation insensitive to the choice of τ.

In Fig. 3 we show density contours for the head-on collision of ^{16}O + ^{40}Ca at 100 MeV per nucleon. We see that the two nuclei interpenetrate each other and separate after

$$t\gtrsim0.128\times10^{-21}\ \text{sec}\ .$$

The dynamics is almost identical to that of previous TDHF calculations at the same energy.[25] At

$$t\sim0.072\times10^{-21}\ \text{sec}\ ,$$

the overlapping region has a very high density ($\rho\sim0.20$ nucleons/fm^3), which produces a repulsive mean-field potential. As a result, streaming nucleons are deflected away from the symmetry axis. After the encounter, the ^{16}O nucleus has a very low density and is unlikely to remain stable while the ^{40}Ca nucleus has a density not very different from that of its ground-state configuration.

In order to provide a quantitative comparison between the TDHF results and the present calculation, we calculate the relative kinetic energies at $t=0$ and after separation of the two nuclei at

$$t=0.176\times10^{-21}\ \text{sec}\ .$$

We list in Table I the ratio of KE (final)/KE (initial). We find that, using the conventional set of basis states, the presence of particle collisions in our model does not lead to an additional damping of the relative collective motion. In fact, compared to the TDHF results,[25] there is even an increase of the relative kinetic energy, a result which contradicts our intuitive understanding of particle collisions. However, one does not know whether the absence of additional damping in our calculations is due to the single-particle shell gap or to other factors. It is therefore of interest to consider reactions of nonclosed shell nuclei for which there are no pronounced shell gaps at the top of the Fermi level.

As an example of such a system, we study the head-on collision of ^{28}Si on ^{28}Si at 100 MeV per nucleon. The initial occupation of ^{28}Si is as follows: the $1s$ and the $1p$ states are fully occupied; the $1d$ states have an occupation number of 0.6; and the $2s$, the $1f$, and the $2p$ states are all empty. The unoccupied states are boosted by the same velocity used for the occupied states. Calculations have been performed for

$$\tau=0.01\times10^{-21}\ \text{sec}$$

and for

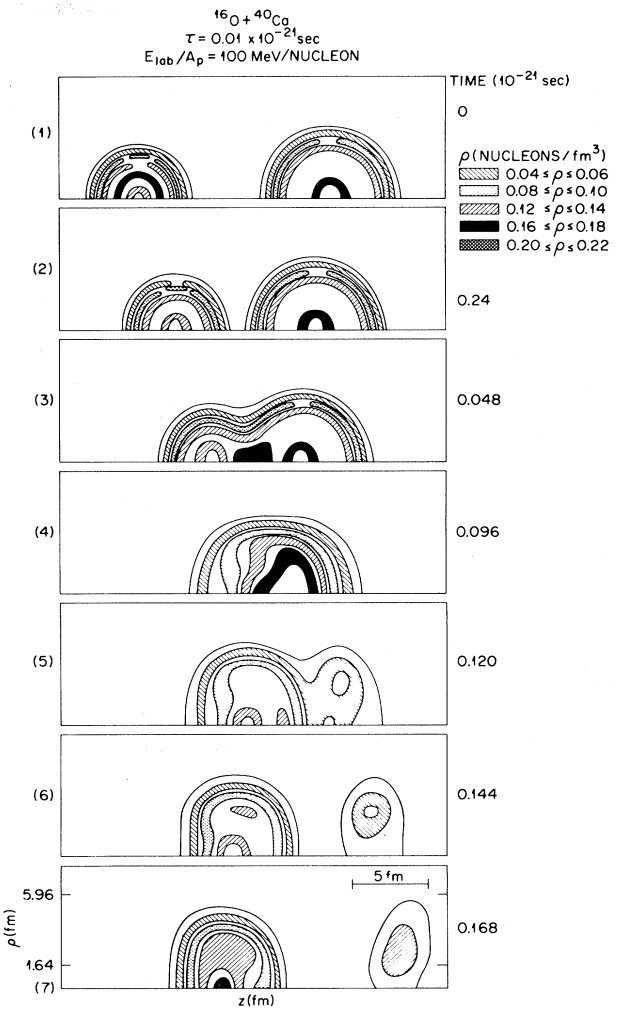

FIG. 3. Density contours for the head-on collision of ^{16}O on ^{40}Ca at 100 MeV per nucleon. The parameter τ is 0.01×10^{-21} sec.

$$\tau=10^8\times10^{-21}\ \text{sec}.$$

The latter leads to no change of the occupation numbers with time and is essentially a TDHF calculation.

The calculation with

TABLE I. Ratio of the final kinetic energy after separation, KE (final), to the initial kinetic energy before the collision, KE (initial), for various cases.

	Case	KE (final) / KE (initial)
^{16}O + ^{40}Ca	TDHF (Ref. 25)	0.816
	Collision model:	
	$\tau=0.01\times10^{-21}$ sec	0.823
	$\tau=0.001\times10^{-21}$ sec	0.823
^{28}Si + ^{28}Si	TDHF	0.793
	Collision model:	
	$\tau=0.01\times10^{-21}$ sec	0.821

$\tau=0.01\times10^{-21}$ sec

shows a substantial redistribution of the occupation numbers and represents a case with a large rearrangement of $\{n_\lambda\}$. The results for $^{28}Si+^{28}Si$ are presented in Figs. 4–7.

In Fig. 4 we show the parameters which characterize the equilibrium occupation number distributions and the entropy S/k. As before, the rapid rise and subsequent decrease of μ_p and μ_n are due to the high density of the overlapping region which gives rise to a strong repulsion that subsides after the reaction. For symmetric systems, p_0 is identically zero and is not exhibited. The equilibrium temperature kT decreases when the two nuclei begin to interact, while the entropy always increases.

We display in Fig. 5 the occupation numbers and effective energies ϵ_λ(eff) for the $^{28}Si+^{28}Si$ reaction. One observes that there is a substantial rearrangement of the occupation probabilities. This rearrangement gives rise to different final density distributions. We show in Fig. 6 and Fig. 7 the density contours for the TDHF case and for

$\tau=0.01\times10^{-21}$ sec .

Note that in the latter case, there is a pronounced ring with a density of $\rho\sim0.08$ nucleons/fm^3. Although the density distributions are different, the degree of damping of the relative collective motion is nearly the same for the two cases. We list in Table I the ratios of KE (final)/KE (initial) evaluated at

$t(\text{final})=0.192\times10^{-21}$ sec .

As one observes, the ratios are nearly the same. In fact, just as in the $^{16}O+^{40}Ca$ case, there is less damping of the relative kinetic energy in the collision model than in TDHF, in contradiction to what one intuitively expects.

VI. DISCUSSION

With the conventional basis states, the present particle-model studies give no more damping than the ordinary

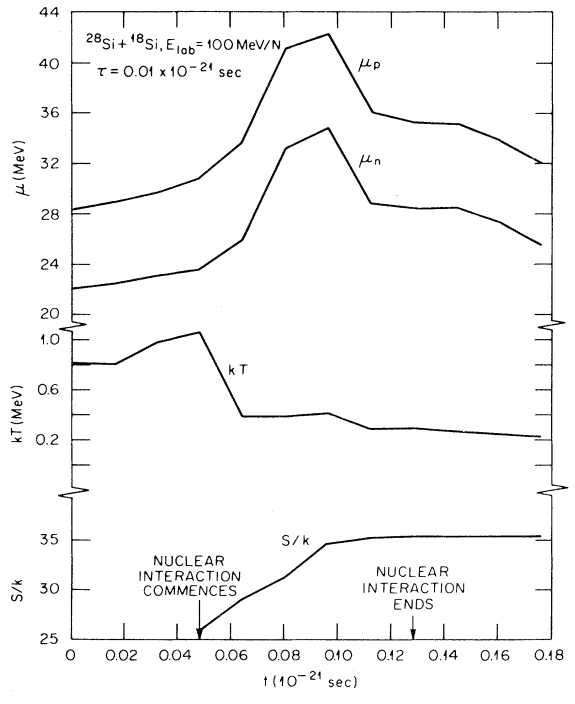

FIG. 4. The parameters μ_p, μ_n, and kT, and the entropy S/k, as functions of time, for the head-on collision of ^{28}Si on ^{28}Si at a laboratory bombarding energy of 100 MeV per nucleon. The parameter τ is 0.01×10^{-21} sec. The arrows indicate the times at which the residual nuclear interactions are turned on or off.

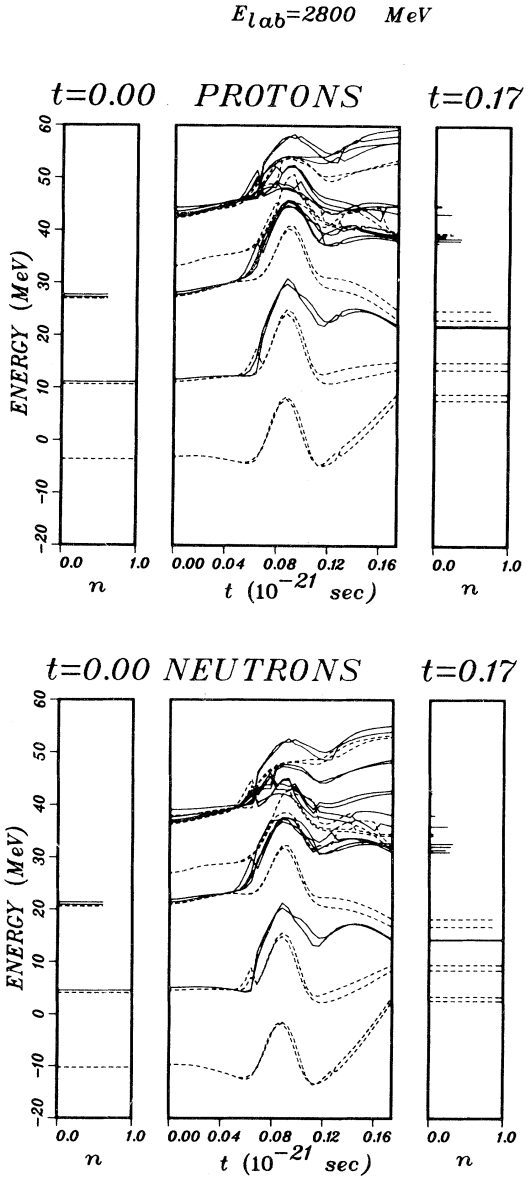

FIG. 5. Same as in Fig. 2 but for the collision of ^{28}Si on ^{28}Si at 100 MeV per nucleon with $\tau=0.01\times10^{-21}$ sec. The right panels in each picture give the occupation numbers at $t=0.17\times10^{-21}$sec.

TDHF calculations.[25] How do we understand this peculiar result? Clearly, it is not due to the presence of a shell gap between occupied and unoccupied states since the closed-shell $^{16}O + ^{40}Ca$ system and the non–closed-shell $^{28}Si + ^{28}Si$ system both exhibit this behavior. In fact, in the $^{28}Si + ^{28}Si$ reaction there is a substantial rearrangement of the occupation numbers $\{n_\lambda\}$, but the final relative kinetic energy is not much affected.

The results obtained here are unphysical and indicate that some important degrees of freedom are likely missing in the implementation of the model. We now attempt to find these degrees of freedom. We first note that the con-

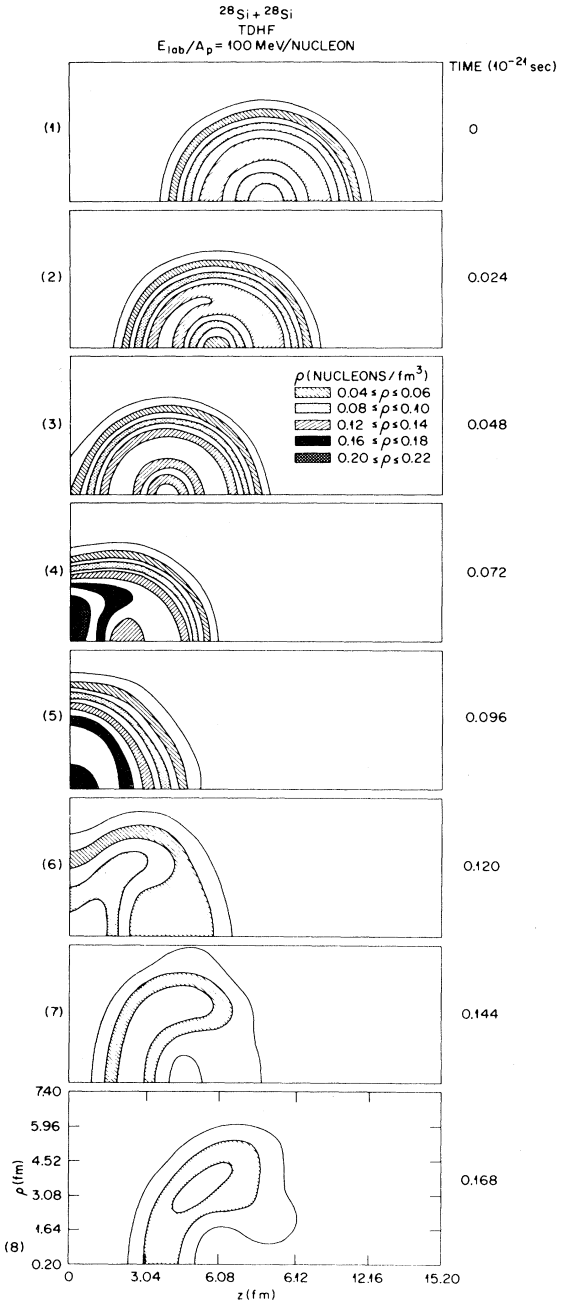

FIG. 6. Density contours for the head-on collision of ^{28}Si on ^{28}Si at a laboratory bombarding energy of 100 MeV per nucleon. These results are for a TDHF calculation with no particle collisions.

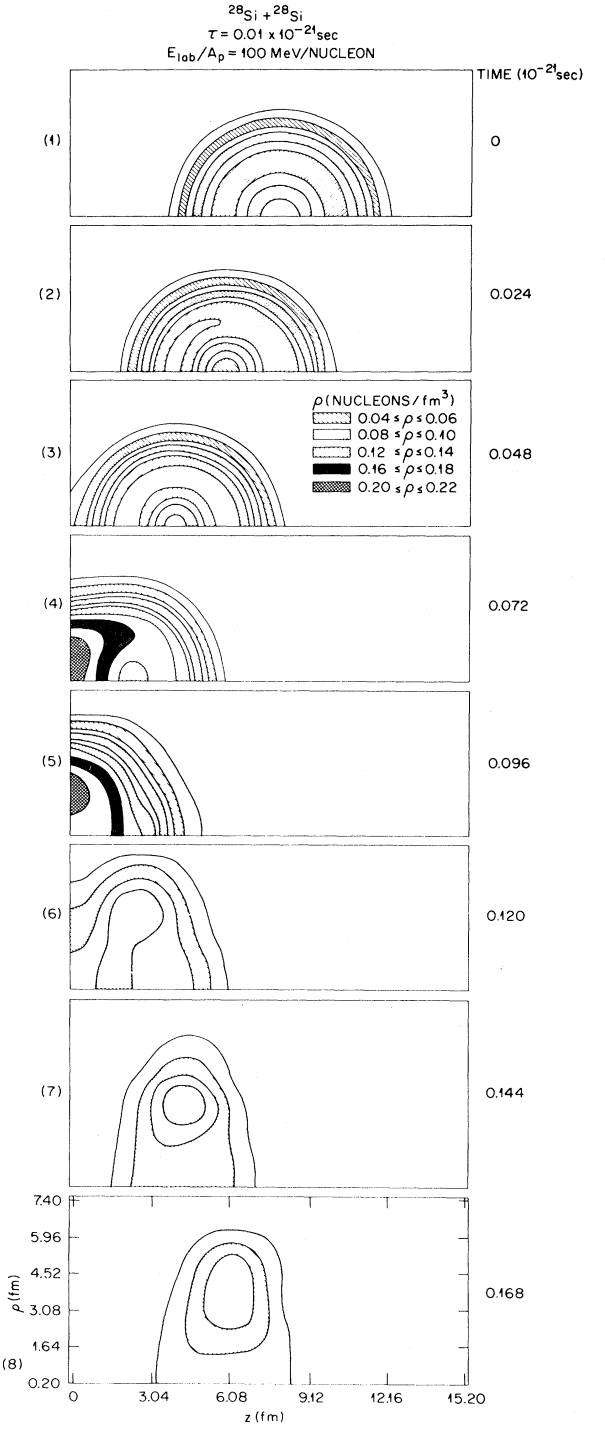

FIG. 7. Density contours for the head-on collision of ^{28}Si on ^{28}Si at a laboratory bombarding energy of 100 MeV per nucleon. They are obtained with the collision model and $\tau = 0.01 \times 10^{-21}$ sec.

ventional basis states we use give wave packets which maintain a large longitudinal momentum in the direction of motion. This is a well-known feature of TDHF theory.[1,2] Both the occupied and the unoccupied states have roughly the same expectation values of linear momentum, and even substantial shifts in the occupation probabilities do not affect the momenta of the colliding nuclei after the collision. Thus, the damping of the relative collective motion is largely insensitive to changes in the occupation numbers.

Since we now understand the origin of the damping behavior, we may well ask whether the present conventional single-particle basis is capable of describing properly the effects of particle collisions. This set of states, in effect, restricts the products of nucleon-nucleon collisions to be strongly forward and backward peaked. On the other hand, for collisional energy up to a few hundred MeV per nucleon, the angular distribution for nucleon-nucleon collisions is almost isotropic. In a realistic time-dependent description, the collision of two nucleons represented by two initial wave packets should result in wave packets moving radially outward in the center-of-mass system. This type of spherical wave packet is obviously not included in the present choice of basis states.

In future work, we plan to include the transverse degree of freedom by choosing a better description of the final states after particle collisions take place. The model calculation may then proceed in the following way. As before, the occupied HF states are first evolved, without changing their occupation numbers. When the two nuclei begin to interact, we will include additional unoccupied states which contain spherical waves propagating outward. The proper choice of this additional set of states needs to be investigated. One possible choice for this additional set consists of modifying the phase of each single-particle wave function $\psi_\lambda(r,t)$ of the standard set such that

$$\bar{\psi}_\lambda(\vec{r},t) - e^{i\vec{\kappa}_\lambda\cdot\vec{r}} e^{+i\vec{\kappa}_\lambda r}\psi_\lambda(\vec{r},t) ,$$

where $\vec{\kappa}_\lambda = \vec{p}_\lambda - m\vec{v}_0$, $\vec{v}_0$ is the velocity of the equal-velocity frame, and $\kappa_\lambda = |\vec{\kappa}_\lambda|$. The first factor $e^{-\vec{\kappa}_\lambda\cdot\vec{r}}$ is to ensure that this state has zero linear momentum in the equal velocity frame and the second factor $e^{i\kappa r}$ is to boost the wave function isotropically in that frame. This set of unoccupied states satisfies Gallilean invariance since the phase factor depends on the difference of momenta $\vec{p}_\lambda - m\vec{v}_0$. The additional set of unoccupied single-particle states needs to be initially orthonormalized with the standard set of basis states, after which the TDHF equation (2.1) automatically guarantees orthonormality as a function of time.[1,2] As time proceeds, the additional unoccupied states begin to be occupied, as governed by the occupation number equation (2.17). For these states, since the kinetic energy in the equal-velocity frame is minimal, $\epsilon_\lambda(\text{eff})$ is expected to be relatively small. Thus, these unoccupied states embed themselves among the occupied states in the $\epsilon_\lambda(\text{eff})$ spectrum. There can be substantial changes of occupancy and of relative kinetic energy when nucleons switch from occupied states to previously unoccupied states propagating in the transverse direction. Future investigations using the collision model with the new basis states will be of great interest. We also mention that other authors[2,27,28] have carefully examined various problems associated with the asymptotic, final-state TDHF wave functions.

Finally, we emphasize that the neglect of the appropriate transverse degrees of freedom is *not* solely confined to the intermediate-energy, heavy-ion reactions discussed here. This problem is a general feature found at *all* heavy-ion energies for all TDHF calculations,[1,2] including those[29–33] in which pairing effects[34] are included. Also, results of recent TDHF calculations indicate that, for heavy-ion reactions, pairing has little effect on the low-energy dynamics.[35] However, in such pairing studies the single-particle states are all chosen in the conventional way as discussed above. On the other hand, it seems physically reasonable that a pair of particles interacting via the residual pairing interaction should mostly scatter isotropically. Thus, in order to properly take into account pairing effects in low-energy reactions, it may be useful again to include, in the basis states, those which propagate in the transverse direction.

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APPENDIX: EVALUATION OF $n_\lambda^{(e)}$

We wish to evaluate $n_\lambda^{(e)}$ for each time interval $(t, t+\Delta t)$ within which it is assumed to be a constant. Thus, we need to determine the parameters specifying $n_\lambda^{(e)}$ in Eq. (3.1). For a linear form of $f(\delta n_\lambda)$, the conservation equations (3.9), (3.10), (3.12), and (3.14), at $t+\frac{1}{2}\Delta t$ can be written as

$$D_1 = \sum_{\lambda=1} n_\lambda^{(e)}\delta(\tau_{\lambda z}, \tfrac{1}{2}) - Z = 0 , \tag{A1}$$

$$D_2 = \sum_{\lambda=1} n_\lambda^{(e)}\delta(\tau_{\lambda z}, -\tfrac{1}{2}) - N = 0 , \tag{A2}$$

$$D_3' = \sum_{\lambda=1} \left[n_\lambda^{(e)} - n_\lambda\left(t+\frac{\Delta t}{2}\right)\right]\vec{p}_\lambda\left(t+\frac{\Delta t}{2}\right) = 0 , \tag{A3}$$

and

$$D_4' = \sum_{\lambda=1} \left[n_\lambda^{(e)} - n_\lambda\left(t+\frac{\Delta t}{2}\right)\right]\epsilon_\lambda\left(t+\frac{\Delta t}{2}\right) = 0 . \tag{A4}$$

Since p_λ and ϵ_λ are evaluated at the end points of each time interval,[26] we take

$$\vec{p}_\lambda\left(t+\frac{\Delta t}{2}\right) = \tfrac{1}{2}[\vec{p}_\lambda(t) + \vec{p}_\lambda(t+\Delta t)] \tag{A5}$$

and

$$\epsilon_\lambda\left[t+\frac{\Delta t}{2}\right]=\tfrac{1}{2}[\epsilon_\lambda(t)+\epsilon_\lambda(t+\Delta t)]\ . \tag{A6}$$

From Eq. (4.4) we find that, to lowest order in $\Delta t/2$, Eqs. (A3) and (A4) become

$$D_3=\sum_{\lambda=1}[n_\lambda^{(e)}-n_\lambda(t)]\vec{p}_\lambda\left[t+\frac{\Delta t}{2}\right]=0 \tag{A7}$$

and

$$D_4=\sum_{\lambda=1}[n_\lambda^{(e)}-n_\lambda(t)]\epsilon_\lambda\left[t+\frac{\Delta t}{2}\right]=0\ . \tag{A8}$$

In head-on collisions, $\vec{p}_\lambda$ and $\vec{p}_0$ have only z components. The four unknown parameters in the four equations of (A1), (A2), (A7), and (A8) are μ_p, μ_n, p_o, and $\beta\equiv 1/kT$. Using Newton's method, we obtain

$$\begin{pmatrix}\mu_p\\ \mu_n\\ p_0\\ \beta\end{pmatrix}=\begin{pmatrix}\bar{\mu}_p\\ \bar{\mu}_n\\ \bar{p}_0\\ \bar{\beta}\end{pmatrix}-\begin{pmatrix}\frac{\partial D_1}{\partial\mu_p}&\frac{\partial D_1}{\partial\mu_n}&\frac{\partial D_1}{\partial p_0}&\frac{\partial D_1}{\partial\beta}\\ \frac{\partial D_2}{\partial\mu_p}&\frac{\partial D_2}{\partial\mu_n}&\frac{\partial D_2}{\partial p_0}&\frac{\partial D_2}{\partial\beta}\\ \frac{\partial D_3}{\partial\mu_p}&\frac{\partial D_3}{\partial\mu_n}&\frac{\partial D_3}{\partial p_0}&\frac{\partial D_3}{\partial\beta}\\ \frac{\partial D_4}{\partial\mu_p}&\frac{\partial D_4}{\partial\mu_n}&\frac{\partial D_4}{\partial p_0}&\frac{\partial D_4}{\partial\beta}\end{pmatrix}^{-1}\begin{pmatrix}D_1\\ D_2\\ D_3\\ D_4\end{pmatrix}, \tag{A9}$$

where $\bar{\mu}_p$, $\bar{\mu}_n$, $\bar{p}_0$, and $\bar{\beta}$ are the values from the previous iteration. The derivatives in (A9) can be written out explicitly using Eq. (3.1) and the quantities in the last term are evaluated with $\bar{\mu}_p$, $\bar{\mu}_n$, $\bar{p}_0$, and $\bar{\beta}$. We begin the iteration choosing trial values from the previous half time step. The iterations in Eq. (A9) converge rapidly as long as the trial values for μ_p, μ_n, p_0, and β are not too different from the true values. This condition is usually satisfied for any smooth dynamical process.

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