PHYSICAL REVIEW C VOLUME 35, NUMBER 5 MAY 1987

Physical interpretation of time-dependent Hartree-Fock density matrix for heavy ion scattering

Abraham Klein and A. S. Umar
Department of Physics, University of Pennsylvania, Philadelphia, Pennsylvania 19104

(Received 14 April 1986)

We suggest a quantum mechanical interpretation of the density matrix of the time-dependent Hartree-Fock theory for heavy ion scattering. We show how with this interpretation the time-dependent Hartree-Fock equations can be derived provided we admit (i) a generalized factorization of a suitably defined average of two-body density matrix elements in terms of a sum of products of the corresponding one-particle elements and (ii) additional semiclassical approximations which convert a sum of products into an antisymmetric product of sums. These ideas, previously recognized within the framework of soliton models, are extended here to include inelastic processes with the excitation of collective modes as the mechanism for producing deep inelastic scattering. An essential feature of the approach is that it provides, in principle, a theoretical method of obtaining exclusive amplitudes. We describe how these might be calculated.

I. INTRODUCTION

The usual derivation of the time-dependent Hartree-Fock (TDHF) equations[1,2] from the time-dependent variational principle, as the equations which determine an optimal Slater determinant, has the twin virtues of simplicity and almost unlimited flexibility in the choice of systems to which such a description might apply. On the other hand, this second virtue can easily become a vice, since it is left for us, in any particular instance, to supply both the physical interpretation and the conditions for validity of the approximation. In the case of TDHF theory for heavy ion reactions, it is the problem of physical interpretation which has so far evaded any cogent solution.[3]

Our aim in this paper is to define a fully quantum mechanical amplitude associated with the scattering of two heavy ions and "prove" that in the semiclassical limit it satisfies both the TDHF equations and the supplementary conditions which identify it as the density matrix expression of a Slater determinant. The approach followed in this work is another application of the philosophy that was first espoused by one of us more than two decades ago[4] and that we have recently revived for another go round.[5]

According to this point of view every different application of Hartree-Fock or related ideas should be derived *ab initio* from the Heisenberg equations of motion. This forces us in each separate case both to supply a quantum mechanical definition of the amplitude and to devise the approximations needed to reach the semiclassical limit from the quantum equations, precisely the two elements missing from the usual derivation. (A weakness of our approach, on the other hand, is that it too is quite flexible. We provide a sufficient set of conditions, which we think are sensible, but in the end we must retain an open mind concerning the completeness of the physics input.)

In the body of the paper we utilize three ideas:

(i) The most general quantity which we can hope will satisfy TDHF equations is a Fourier superposition (series or integral depending on the variable) of quantum amplitudes of the form $\langle F|\hat{\rho}|I\rangle$, i.e., of a single particle density operator $\hat{\rho}$ connecting some initial state $|I\rangle$ with some final state $|F\rangle$. The Fourier superposition is always with respect to the *difference* in the value of the quantum numbers specifying initial and final states.

(ii) Going to the semiclassical limit requires the assumption that $\langle F|\hat{\rho}|I\rangle$ is a slowly varying function of the *average* value of the quantum numbers in initial and final states and a peaked function of the differences. Thus the quantity which is to satisfy TDHF equations is in consequence of (i) a slowly varying function of all its arguments.

(iii) It is assumed that a corresponding average two-body density matrix which enters in the standard way in the equation of motion for the one-body density matrix can be approximated by a generalized factorization in terms of the one-body quantities.[5] When, *in addition,* we utilize the properties described under (i) and (ii), this factorization can be turned into the standard Hartree-Fock factorization, thus providing the promised derivation.

What is really new about this paper is not the above technique which we showed quite some time ago[6] could be utilized to understand the quantum significance of the purely elastic classical soliton scattering for the nonlinear Schrödinger equation. It is our current willingness—forced by experiment—to finally admit that similar arguments might indeed be applicable to deeply inelastic processes.

In the body of the paper, we repeat the basic ideas twice, first in Sec. II, assuming that the only inelastic processes involve particle transfer. This is the analog of the derivation given previously[6] for a soliton model, except that in the latter particle transfer occurs only virtually, and in the asymptotic region only elastic scattering is "observed." In Sec. III we add the formal remarks necessary to describe transfer from translational energy to internal energy of rotation and vibration. By this point it becomes evident that we are dealing with a multiparameter family of inclusive amplitudes, but, as described in Sec. IV, we can obtain exclusive amplitudes (in a semiclassical approximation) by inverse Fourier transformation, *provided* we are willing to do TDHF calculations on a sufficiently large grid of initial conditions. After a summary in Sec. V, we include a brief appendix on the generalized factorization which is one of the fundamental tools of this paper.

We conclude this Introduction by commenting briefly on previous research in the area covered by this paper. We are unaware of any previous work other than the paper previously cited[6] which suggests a quantum mechanical definition of the TDHF amplitude for heavy ion (HI) scattering. However, several related programs seem to have grown out of the interest in this problem. These address the question of how to modify TDHF in order to be able to extract exclusive scattering information. One program is based on the application of path integral methods to calculate a mean field approximation to S-matrix elements.[7,8] This work appears to be theoretically sound—but practically extremely difficult to implement. The other, the S-matrix TDHF method,[3,9,10] contains physical ideas which have some kinship with those of the present work, but its mathematical basis contains some intuitive elements which require further study and evaluation. Our own approach to extracting individual reaction channel information will be exposed in a succeeding paper.

II. TDHF FOR HEAVY ION SCATTERING: EXTENDED SOLITON LIMIT

We study a standard nonrelativistic nuclear Hamiltonian ($\hbar = m = 1$)

$$H=\int dx\, \psi^\dagger(x)(-\tfrac{1}{2}\nabla^2)\psi(x)+\tfrac{1}{4}\int dx_1 \cdots dx_4 \psi^\dagger(x_1)\psi^\dagger(x_2)V(x_1x_2\,|\,x_3x_4)\psi(x_4)\psi(x_3)\ . \tag{2.1}$$

Here $\psi(x)$ and $\psi^\dagger(x)$ are single nucleon destruction and creation operators, V is an antisymmetrized matrix element of the interaction, and x refers to all single particle degrees of freedom. We shall suppress any explicit reference to spin and charge in the following.

We consider a very special matrix element of the density operator

$$\rho_{12}^{N_1N_2}(x_1t,x_2t\,|\,\theta)\equiv \sum_\nu e^{i\nu\theta}\int d\mathbf{k}_1 d\mathbf{k}_2 \langle (N_1-\nu)(\mathbf{p}_1-\mathbf{k}_1),(N_2+\nu)(\mathbf{p}_2-\mathbf{k}_2)\,|\,\psi^\dagger(x_2t)\psi(x_1t)\,|\,N_1(\mathbf{p}_1),N_2(\mathbf{p}_2)\rangle\ . \tag{2.2}$$

Here $|N_1(\mathbf{p}_1),N_2(\mathbf{p}_2)\rangle$ describes a collision experiment in which the nucleus "N_1" moving with momentum $\mathbf{p}_1$ is incident on the nucleus "N_2" moving with momentum $\mathbf{p}_2$. As the result of a density fluctuation at time t, there is a transition to a two-nucleus state with some particle and some momentum transfer, but we do not—for the moment—allow any internal excitation of the individual nuclei. Finally we integrate over all momentum transfers and form a Fourier series with respect to particle transfer. As remarked in the Introduction, the form (2.2) was suggested by our study of the nonlinear Schrödinger equation[6] where it was established that the classical two-soliton solution, an exact solution of a time-dependent Hartree equation, could be identified as the classical limit of the average (2.2). Furthermore, the individual Fourier coefficients could be used to extract individual S-matrix elements. [It is implied by (2.2) that we limit the considerations of this work to processes which involve two objects colliding and the same number emerging.]

Our aim here is to show that under well-defined approximations, the amplitude (2.2) satisfies the TDHF equations. Naturally, we shall provide only a sufficient set of assumptions. In the next section we shall then generalize the argument to include internal excitation to collective degrees of freedom.

Starting from the Heisenberg equation of motion

$$\begin{aligned} i\partial_t\psi^\dagger(yt)\psi(xt)= &-\tfrac{1}{2}(\nabla x^2-\nabla y^2)\psi^\dagger(yt)\psi(xt)+\tfrac{1}{2}\int \psi^\dagger(yt)\psi^\dagger(x_2t)V(xx_2\,|\,x_3x_4)\psi(x_4t)\psi(x_3t)\\ &-\tfrac{1}{2}\int \psi^\dagger(x_1t)\psi^\dagger(x_2t)V(x_1x_2\,|\,yx_4)\psi(x_4t)\psi(xt)\ , \end{aligned} \tag{2.3}$$

we can form the average in (2.2) and study the interaction terms. Consider, for instance, the term

$$\begin{aligned} &\rho_{12}^{N_1N_2}(x_3t,x_4t,yt,x_2t\,|\,\theta)\\ &\quad\equiv \sum_\nu e^{i\nu\theta}\int d\mathbf{k}_1 d\mathbf{k}_2 \langle (N_1-\nu)(\mathbf{p}_1-\mathbf{k}_1),(N_2+\nu)(\mathbf{p}_2-\mathbf{k}_2)\,|\,\psi^\dagger(yt)\psi^\dagger(x_2t)\psi(x_4t)\psi(x_3t)\,|\,N_1(\mathbf{p}_1)N_2(\mathbf{p}_2)\rangle\ . \end{aligned} \tag{2.4}$$

To the nuclear matrix element we apply the generalized Hartree-Fock factorization,

$$\begin{aligned} &\langle (N_1-\nu)(\mathbf{p}_1-\mathbf{k}_1),(N_2+\nu)(\mathbf{p}_2-\mathbf{k}_2)\,|\,\psi^\dagger(y)\psi^\dagger(x_2t)\psi(x_4t)\psi(x_3t)\,|\,N_1(\mathbf{p}_1)N_2(\mathbf{p}_2)\rangle\\ &\quad=\tfrac{1}{2}\int d\mathbf{p}'_1 d\mathbf{p}'_2 \sum_{\nu'}[\langle (N_1-\nu)(\mathbf{p}_1-\mathbf{k}_1),(N_2+\nu)(\mathbf{p}_2-\mathbf{k}_2)\,|\,\psi^\dagger(yt)\psi(x_3t)\,|\,(N_1-\nu')(\mathbf{p}_1-\mathbf{p}'_1)(N_2+\nu')(\mathbf{p}_2-\mathbf{p}'_2)\rangle\\ &\qquad\qquad\times\langle (N_1-\nu')(\mathbf{p}_1-\mathbf{p}'_1),(N_2+\nu')(\mathbf{p}_2-\mathbf{p}'_2)\,|\,\psi^\dagger(x_2t)\psi(x_4t)\,|\,N_1(\mathbf{p}_1)N_2(\mathbf{p}_2)\rangle\\ &\qquad\qquad-(y\leftrightarrow x_2)-(x_3\leftrightarrow x_4)+(y\leftrightarrow x_2,x_3\leftrightarrow x_4)]\ . \end{aligned} \tag{2.5}$$

This factorization has been discussed at length in previous work.[5] A brief account is given in the appendix.

In order to transform (2.5) into the form sought, it is necessary to introduce changes of variable followed by several assumptions. First we set

$$k_i \rightarrow p_i' + p_i'' ,\quad dk_i \rightarrow dp_i'' \; . \tag{2.6}$$

Then in the first factor displayed on the right-hand side of (2.5) we write, for instance,

$$\begin{aligned}\langle (N_1-\nu)(\mathbf{p}_1-\mathbf{p}_1'-\mathbf{p}_1''),(N_2+\nu)(\mathbf{p}_2-\mathbf{p}_2'-\mathbf{p}_2'') \mid \psi^\dagger(y)\psi(x_2) \mid (N_1-\nu')(\mathbf{p}_1-\mathbf{p}_1'),(N_2+\nu')(\mathbf{p}_2-\mathbf{p}_2') \rangle \\ \cong \langle (N_1-\nu+\nu')(\mathbf{p}_1-\mathbf{p}_1''),(N_2+\nu-\nu')(\mathbf{p}_2-\mathbf{p}_2'' \mid \psi^\dagger(y)\psi(x_2) \mid N_1(\mathbf{p}_1),N_2(\mathbf{p}_2) \rangle \; .\end{aligned} \tag{2.7}$$

This entails the following approximations:

(i) The dependence on particle transfer is a slowly-varying function of the total number of nucleons for $\nu \ll N_1$ or N_2.

(ii) By suppressing the dependence on $\mathbf{p}_i'$, the momentum transfer in the accompanying factor, we are assuming that this momentum transfer is small compared to the initial momenta,

$$| \mathbf{p}_i' | \ll | \mathbf{p}_i | \; . \tag{2.8}$$

This condition can be satisfied by an appropriate choice of $|\mathbf{p}_i|$ if N_i is large. If we make $|\mathbf{p}_i|$ too large, however, the single particle picture will certainly break down because of increased particle emission. A reasonable upper bound to the applicability of the present picture (as is well known) is

$$| \mathbf{p}_i | \ll N_i p_F \; , \tag{2.9a}$$

where p_F is the Fermi momentum. On the other hand, the form factor (2.2) will not support momentum transfer larger than p_F,

$$| p_i' | \lesssim p_F \; . \tag{2.9b}$$

For heavy ions a reasonable domain of application is thus established.

If the approximation (2.7) is accepted and applied to (2.4) and (2.5) utilizing the definition (2.2), we find that we can put the result into the form

$$\rho_{12}^{N_1N_2}(x_3t,x_4t;yt,x_2t \mid \theta)=\rho_{12}^{N_1N_2}(x_3t,yt \mid \theta)\rho_{12}^{N_1N_2}(x_4t,x_2t \mid \theta)-\rho_{12}^{N_1N_2}(x_3t,x_2t \mid \theta)\rho_{12}^{N_1N_2}(x_4t,yt \mid \theta) \; . \tag{2.10}$$

Thus the approximation (2.7) is exactly what is needed to decouple the sums in (2.5). The abundance of indices should not obscure the fact that this has the standard form for the Hartree-Fock factorization of a two-particle density matrix element even though the object on the left-hand side of (2.10) is a special *sum* of such elements. Indeed, as argued, it is only for such an appropriate sum that we can expect (2.10) to hold.

Finally applying (2.10) to (2.3), the latter may be written

$$i\dot{\rho}_{12}^{N_1N_2}(x_1t,x_2t \mid \theta)=[\mathscr{H}_{12}^{N_1N_2},\rho_{12}^{N_1N_2}](x_1t_1x_2t \mid \theta) \; , \tag{2.11}$$

where

$$\mathscr{H}_{12}^{N_1N_2}(xt,yt \mid \theta)=h(x,y)+V_{12}^{N_1N_2}(xt,yt \mid \theta) \; , \tag{2.12}$$

$$V_{12}^{N_1N_2}(xt,yt \mid \theta)=\int V(xx' \mid yy')\rho_{12}^{N_1N_2}(y't,x't \mid \theta) \; , \tag{2.13}$$

and $h(x,y)$ is the single-particle part of the nuclear Hamiltonian represented as the kinetic energy operator in (2.1). In addition to Eqs. (2.11)–(2.13), it is easy to verify from the definition (2.2) and the definition of the number operator that

$$\int dx\, \rho_{12}^{N_1N_2}(xt,xt \mid \theta)=N_1+N_2 \tag{2.14}$$

and from (2.10) together with (2.14) that

$$\int dy\, \rho_{12}^{N_1N_2}(xt,yt \mid \theta)\rho_{12}^{N_1N_2}(yt,x't \mid \theta) =\rho_{12}^{N_1N_2}(xt,x't \mid \theta) \; . \tag{2.15}$$

Since this is all quite formal, it is natural to ask how we may in fact calculate the dependence of the density matrix on the parameter θ. According to Eq. (2.4) the Fourier coefficients of this periodic function describe exclusive particle-transfer channels and therefore contain information we would very much like to have. We ask the reader's indulgence in postponing the discussion of this basic element of the theory to Sec. IV, since we would like first to generalize the derivation of this section.

Thus we have established a *sufficient* set of conditions for the TDHF equations to describe heavy ion scattering. The problem with these conditions is that they omit a central element of deep inelastic scattering, the transformation of collective translational energy into internal excitation of the outgoing fragments. The best known attempt[11,12] to study this process in a semimicroscopic way does so through the assumption that this transfer takes place through available collective modes. From our point of view there is no other way of understanding TDHF. To include these processes, we push the generalized factorization to the utmost. But it is of the nature of this factorization[4] that if it holds at all, it holds only for collective transitions. This formal extension is described in the next section.

III. TDHF FOR HEAVY ION SCATTERING: INCLUSION OF COLLECTIVE EXCITATION

In the definition (2.2), we have allowed for momentum transfer and particle-number transfer and have subsequently assumed a peaked behavior in both variables. We now assume that each incident ion has a collective spectrum described by a K-dimensional Hilbert space $|\lambda_1 \cdots \lambda_k\rangle$ and that

$$\psi_{\lambda_1 \cdots \lambda_k}(q_1 \cdots q_k) \equiv \langle q_1 \cdots q_k | \lambda_1 \cdots \lambda_k \rangle \qquad (3.1)$$

are the wave functions of a microscopically based collective model, which allow us to go back and forth between bases. Here q_i, $i=1 \cdots K$ are assumed to be Cartesian collective coordinates, including the five (canonical) quadrupole degrees of freedom of the original Bohr-Mottelson model, collective coordinates for various giant resonances, etc. We choose to describe the enlarged space by the collective coordinates q_i, rather than by the associated quantum numbers λ_i. We need to assume in the following that the same collective Hilbert space can be used for neighboring nuclei, i.e., the collective space varies smoothly with particle number. This is a reasonable assumption certainly for the giant resonances.

The definition (2.2) can then be generalized by means of a Wigner transform with respect to the collective coordinates.[13] Introducing average and difference coordinates,

$$Q_i = \tfrac{1}{2}(q_i' + q_i), \quad \eta_i = q_i' - q_i , \qquad (3.2)$$

we can define the generalized density matrix

$$\begin{aligned}\rho_{12}^{N_1 N_2}(x_1 t, x_2 t \,|\, \theta, \mathbf{Q}, \mathbf{P}) &= \sum_{\nu} e^{i\nu\theta} \int d\mathbf{k}_1 d\mathbf{k}_2 \int d\boldsymbol{\eta} \exp(i\mathbf{P}^{(1)}\cdot\boldsymbol{\eta}^{(1)} + i\mathbf{P}^{(2)}\cdot\boldsymbol{\eta}^{(2)}) \\ &\quad \times \langle (N_1-\nu)(\mathbf{p}_1-\mathbf{k}_1)(\mathbf{q}^{(1)\prime});(N_2+\nu)(\mathbf{p}_2-\mathbf{k}_2)(\mathbf{q}^{(2)\prime}) \,|\, \psi^\dagger(x_2 t)\psi(x_1 t) \,|\, N_1(\mathbf{p}_1)(\mathbf{q}^{(1)}), N_2(\mathbf{p}_2)(\mathbf{q}^{(2)}) \rangle ,\end{aligned} \qquad (3.3)$$

where, for instance,

$$\mathbf{q}^{(1)} = (q_1^{(1)} \cdots q_k^{(1)}) . \qquad (3.4)$$

[In (3.3), $\mathbf{Q}$ and $\mathbf{P}$ can be considered classical canonical variables.] With the generalized definition (3.3) we can now repeat, line by line, the steps starting at (2.3). The essential additional observations necessary to ensure that we end up with the analogs of (2.10)—(2.13) are as follows:

(i) The generalized Hartree-Fock factorization includes as intermediate states the same class of states admitted in the initial discussion. Thus, there is now a sum over intermediate collective states.

(ii) The Wigner transform of a product of operators, though in general a complicated object, is equal, in the *classical limit*, to the product of the individual transforms.

(iii) The Wigner transforms which intervene in our problem are slowly varying functions of their arguments. With these assumptions the reasoning and conclusions of Sec. II follow almost without change and only with an augmentation of notation.

We take one final step in the direction of increased realism by changing the representation of the initial and final states to that which corresponds more closely to what is used in TDHF calculations. Thus, instead of the designation of the individual three-momenta of incident and target ions, we choose instead the total momentum $\mathbf{P}$ and the relative momentum $\mathbf{p}$. Next we replace $\mathbf{p}$ by its magnitude $|\mathbf{p}|$ and by a vector impact parameter $\mathbf{b}=(b,\phi)$, where we understand that the relative orbital angular momentum l is given by the equation $b=(l/|\mathbf{p}|)$. A full six-dimensional integration over $\mathbf{P}$, $\mathbf{b}$, and $|\mathbf{p}|$ now takes care of total momentum, relative angular momentum, and energy transfer in the center of mass system.

IV. EXTRACTION OF EXCLUSIVE AMPLITUDES FROM TDHF

The fundamental result of this paper is Eq. (3.3) or some modification of it such as the replacement of the relative momentum analysis by an impact parameter analysis as mentioned at the end of the preceding section. An equation such as (3.3) gives substance to the common understanding that the TDHF approach to HI reactions provides an inclusive description.

Nevertheless it is unsatisfactory to stop at this point. We must go on to ask whether it is possible to obtain exclusive amplitudes from a suitably modified analysis. We shall solve this problem in this section. In a second paper in preparation we shall study the question of what detailed reaction information is actually contained in one of the exclusive amplitudes.

In order to explain the basic concept, let us consider just one of the collective degrees of freedom, which we call q ($q^{(1)}$ for one of the ions, $q^{(2)}$ for the other). We rewrite (3.3) in a condensed form as

$$\begin{aligned}\rho_{12}(x_1 t, x_2 t \,|\, \mathbf{Q},\mathbf{P};\mathbf{R},\mathbf{S}) &= \int (d\boldsymbol{\rho}) \exp(i\boldsymbol{\rho}\cdot\mathbf{S}) \int d\eta_1 d\eta_2 \exp[i(P^{(1)}\eta^{(1)} + P^{(2)}\eta^{(2)})] \\ &\quad \times \langle \mathbf{r}' q^{(1)\prime}, q^{(2)\prime} \,|\, \psi^\dagger(x_2 t)\psi(x_1 t) \,|\, \mathbf{r}, q^{(1)}, q^{(2)} \rangle .\end{aligned} \qquad (4.1)$$

Here $\mathbf{Q}=(Q^{(1)},Q^{(2)})$ and $\eta^{(1)},\eta^{(2)}$ are related to $q^{(i)}$ and $q^{(i)\prime}$ as in Eq. (3.2), $\mathbf{r}$ refers to all other (collective) quantum numbers specifying a state of two ions, $\boldsymbol{\rho}=\mathbf{r}'-\mathbf{r}$, and $\mathbf{R}$ and $\mathbf{S}$ are the canonical coordinates and momenta associated with all these degrees of freedom. In fact, (4.1) does not correspond precisely to a condensed form of (3.3). For example, the dependence on the number (or mass) variables in (3.3) has not been put into this form. This can be done, but we shall prefer, below, to discuss this variable separately.

Once we accept (4.1) as the "canonical" form for the density matrix describing HI scattering in TDHF theory, the extraction of exclusive amplitudes is, *in principle,* trivial. Two steps are necessary. First we calculate the inverse Fourier transform (inverse Wigner transform). This yields the amplitude $\langle \mathbf{r}',q^{(1)\prime},q^{(2)\prime} \,|\, \psi^\dagger(x_2t)\psi(x_1t) \,|\, \mathbf{r},q^{(1)},q^{(2)}\rangle$. As a second step we utilize the collective wave functions $\langle \boldsymbol{\alpha},\lambda^{(1)},\lambda^{(2)} \,|\, \mathbf{r},q^{(1)},q^{(2)}\rangle$ of a suitable microscopic (or phenomenological) collective model to extract the quantity

$$\langle \boldsymbol{\alpha}',\lambda^{(1)\prime},\lambda^{(2)\prime} \,|\, \psi^\dagger(x_2t)\psi(x_1t) \,|\, \boldsymbol{\alpha},\lambda^{(1)}\lambda^{(2)}\rangle = \int d\mathbf{r}'d\mathbf{r}\,dq^{(1)\prime}dq^{(2)\prime}dq^{(1)}dq^{(2)}\langle \boldsymbol{\alpha}',\lambda^{(1)\prime},\lambda^{(2)\prime} \,|\, \mathbf{r}'q^{(1)\prime}q^{(2)\prime}\rangle$$
$$\times\langle \mathbf{r}',q^{(1)\prime},q^{(2)\prime} \,|\, \psi^\dagger(x_2t)\psi(x_1t) \,|\, \mathbf{r},q^{(1)},q^{(2)}\rangle\langle \mathbf{r},q^{(1)},q^{(1)} \,|\, \mathbf{r},\lambda^{(1)}\lambda^{(2)}\rangle\ , \tag{4.2}$$

which may properly be called an exclusive amplitude. It is understood that we have at best a semiclassical approximation to this amplitude; this is implicit in all that has preceded.

In the above we are taking it for granted that time independent S-matrix elements (or equivalent information) can be extracted from the exclusive amplitudes such as those defined in Eq. (4.2), i.e., these amplitudes do not suffer from the difficulty discussed in Ref. 3. The proof of this assertion, in the general case, is rather involved, and will be the subject of a separate publication. However, in Ref. 6, which was the inspiration for the further development, the proof has already been given for the nonlinear Schrödinger equation.

What remains is the problem of computing the left-hand side of (4.1), i.e., in order to achieve our goal, we need not one TDHF calculation per choice of impact parameter, but a multidimensional phase space of such calculations, a formidable task from both the technical and the economic viewpoints. How do we, in principle, generate this space of solutions? Let t_0 be the initial time for calculation ($t_0 \to -\infty$). The initial condition is chosen so that ρ_{12} describes two separated but approaching ions and is thus a sum of terms referring to each of these objects,

$$\rho_{12}(x_1t_0,x_2t_0 \,|\, \mathbf{Q},\mathbf{P};\mathbf{R},\mathbf{S}) = \rho_1(x_1t_0,x_2t_0 \,|\, Q^{(1)},P^{(1)},\mathbf{R}^{(1)},\mathbf{S}^{(1)}) + \rho_2(x_1t_0,x_2t_0 \,|\, Q^{(2)},P^{(2)},\mathbf{R}^{(2)},\mathbf{S}^{(2)})\ , \tag{4.3}$$

where nonvanishing values require both x_1 and x_2 to be in each other's neighborhood and both within one of the colliding ions. The variables which label ρ_1 and ρ_2 describe (classically) orientation, shape, distortion, and composition variables together with their associated momenta. Thus to obtain the space of required density matrices, we need to solve TDHF for an associated space of initial conditions. These initial conditions are contained in density matrices which are themselves the solutions of auxiliary TDHF problems.

These problems are auxiliary only in the sense of their relations to the reaction problem. They are of fundamental importance themselves in that ρ_1 and ρ_2 are the basic elements for constructing a theory of collective motion of the nuclei in question. The calculation of microscopic density matrices for a full panoply of collective variables is certainly beyond present possibilities. It is nevertheless of importance to understand the full dimensions of the problem. It may not be out of the question to study the dependence on selected degrees of freedom in a self-consistent way or to make some compromises with the help of cranking theory,[14] or even to utilize a plausible single-particle theory. We consider it of importance to make some start in this direction.

We must add some remarks concerning particle transfer, a subject which is not properly covered by the discussion leading to (4.3). This discussion is relevant for those collective variables which describe states in one of the ions. Under these conditions the action of the density operator can cause excitation in each of the ions at or near the initial time when they are well separated. In (4.3) the way in which the manifold of solutions of TDHF depends on a manifold of initial conditions should be clear. For the particle transfer variable (or for similar variables such as charge transfer) matters are a little more complex.

In order to see what to do here in relation to the form (2.2), we have to consider the two colliding nuclei to provide a single mean field—a two-center model. We then wish to fill N_1+N_2 orbitals. We shall write for the occupied orbitals when the ions are well separated ($h=1,\ldots,N_1+N_2$)

$$\phi_h = \phi_h^{(1)} + \phi_h^{(2)}\ , \tag{4.4}$$

where the superscripts refer to orbitals centered in one or the other of the wells. For $N_1 \neq N_2$, in general, asymptotically the functions should be concentrated in one or the other wells, and only as the nuclei approach each will there be "leakage" of the single particle functions. We define

$$\phi_h(\theta) = \phi_h^{(1)}e^{i\theta} + \phi_h^{(2)}\ . \tag{4.5}$$

Asymptotically there will be no sign of θ dependence in the density matrix, despite the formal appearance of (4.5) until we develop some leakage, i.e., until both terms of (4.5) are nonvanishing for one or more orbitals. After that the Fourier components necessary to form (2.2) build up rapidly.

In practice, this may be the easiest variable to deal with.

V. SUMMARY AND CONCLUSIONS

To summarize our findings, we have argued that the TDHF equations for heavy ion scattering can be interpreted as the equations for a multidimensional Wigner transform and/or Fourier series of exclusive matrix elements of the one-particle density matrix. Each Wigner transform integral is with respect to the change in some collective degree of freedom: These should include orientation and shape variables among others. The Fourier series are with respect to particle transfer variables. The ultimate goal of a TDHF program may therefore be defined as the calculation of the inverse Wigner transforms or Fourier coefficients, in order to obtain exclusive scattering information. This requires the solution of the TDHF equations for families of initial conditions. We suggest that at least restricted versions of this program may be currently feasible.

Detailed analysis of the reaction information contained in an exclusive density matrix element will be given in a succeeding paper.

This work was supported in part by Department of Energy Grant 40132-5-25351.

APPENDIX

Let $|A\rangle, |A'\rangle, \ldots,$ be preassigned elements of a subspace of the complete many-body Hilbert space for a fixed number N of particles. This subspace may itself be a complete Hilbert space of smaller—usually much smaller—dimensionality. We require an approximation for the two-body density matrix

$$\rho(1234\,|\,AA') \equiv \langle A'\,|\,\psi_4^\dagger\psi_3^\dagger\psi_2\psi_1\,|\,A\rangle \tag{A1}$$

whose validity is tied both to the nature of the forces acting between particles and to a sagacious choice of the set $|A\rangle$. Here the indices $1,\ldots,4$ may be spatial, momentum, or shell model indices, depending on the application. We assume that the required factorization is[5]

$$\rho(1234\,|\,AA') \cong \tfrac{1}{2}\sum_{A''}\left[\langle A'\,|\,\psi_4^\dagger\psi_1\,|\,A''\rangle\langle A''\,|\,\psi_3^\dagger\psi_2\,|\,A\rangle - (1\leftrightarrow 2) - (3\leftrightarrow 4) + (1\leftrightarrow 2, 3\leftrightarrow 4)\right] . \tag{A2}$$

This factorization has the following attractive properties:

(1) The antisymmetry and hermiticity properties of (A1) are preserved.

(2) If $|A\rangle$ is a single state, we regain one-state Hartree-Fock theory.

(3) The random phase approximation can be derived by assuming that diagonal (in A) elements are zero order and certain off-diagonal elements are first order.

(4) Time-dependent Hartree-Fock theory can be derived generally for the Wigner transform of (A2).[5] This is essentially the application used in this paper.

(5) If we ask for the *physical* justification for (A2), this was essentially argued originally[4] to be a combination of coherence of retained matrix elements and random phase cancellation of those omitted.

---

[1] J. W. Negele, Rev. Mod. Phys. **54**, 913 (1982).
[2] K. T. R. Davies, K. R. S. Devi, S. E. Koonin, and M. R. Straayer in *Treatise on Heavy-Ion Science,* edited by D. Allan Bromley (Plenum, New York, 1985), Vol. 3.
[3] J. J. Griffin, in *Proceedings of the Creek Falls Conference on Heavy Ion Collisions,* edited by E. C. Halbert (National Technical Information Service, Springfield, Va., 1977), p. 1.
[4] A. Kerman and A. Klein, Phys. Lett. **1**, 185 (1962); Phys. Rev. **132**, 1326 (1963).
[5] A. Klein, Phys. Rev. C **30**, 1680 (1984); A. Klein and A. S. Umar, University of Pennsylvania Report UPR-0022NT, 1986.
[6] A. Klein and F. Krejs, Phys. Rev. A **18**, 1343 (1978).
[7] Y. Alhassid and S. E. Koonin, Phys. Rev. C **23**, 1590 (1981).
[8] H. Reinhardt, Nucl. Phys. **A390**, 70 (1982); Phys. Lett. **121B**, 9 (1983).
[9] J. J. Griffin, P. C. Lichtner, and M. Dworzecka, Phys. Rev. C **21**, 1351 (1980).
[10] J. J. Griffin, M. Dworzecka, P. C. Lichtner, and K. K. Kan, Phys. Lett. **93B**, 235 (1980).
[11] R. A. Broglia, C. H. Dasso, and A. Winther, Phys. Lett. **61B**, 113 (1976); R. A. Broglia, O. Civitarese, C. H. Dasso, and A. Winther, *ibid.* **73B**, 405 (1978).
[12] P. N. Isaev, Yad. Fiz. 32, 978 (1980) [Sov. J. Nucl. Phys. **32**, 5056 (1980)]; 34, 717 (1981) [**34**, 399 (1981)].
[13] R. E. Johnson, A. Klein, and R. M. Dreizler, Ann. Phys. (N.Y.) **49**, 496 (1968).
[14] J. F. Berger, M. Girod, and D. Gogny, in *Theoretical Approaches to Heavy Ion Reaction Mechanisms,* edited by M. Martinot, C. Ngo, and F. Lepage (North-Holland, Amsterdam, 1984), p. 23c.