GENERALIZED DENSITY DYNAMICS

D. J. Rowe
Department of Physics, University of Toronto
Toronto, Ontario, M5S 1A7, Canada

THE HARTREE-FOCK DENSITY DYNAMICS

The HF approximation, in one form or another underlies most of many-body quantum mechanics. One reason for this is that the only many-body problem that can be solved, generally speaking, is the independent-particle problem. Another is that HF theory is a theory of Slater determinants, which represent particle-hole vacuum states and are therefore particularly simple to work with. In this talk, I shall consider HF as a dynamical theory of the one-body density.

A one-body density ρ contains all the one-body properties of the state ψ to which it corresponds. Thus if we define its components

$$\rho_{\beta\alpha} = \langle\psi|\ a^{+}_{\alpha}a_{\beta}\ |\psi\rangle, \tag{1}$$

then the expectation of any one-body operator X is given by

$$\langle\psi|\ X\ |\psi\rangle = \rho(X) = \sum_{\alpha\beta} X_{\alpha\beta}\ \rho_{\beta\alpha}\ . \tag{2}$$

Since most physical observables of interest (with the exception of the Hamiltonian) are one-body operators, the one-body density is a particularly useful entity.

Given a Slater determinant ψ, with density ρ, HF theory gives the dynamical equation

$$\frac{d}{dt}\langle\psi|X|\psi\rangle = i\langle\psi|[H_0,X]|\psi\rangle\ , \tag{3}$$

where $H_0=H_0(\rho)$ is the HF density dependent Hamiltonian. This equation has two very important features. Firstly, since $[H_0,X]$ is a one-body operator, for all one-body X, it follows that eq. (3) can be written

$$\dot{\rho}(X) = i\rho([H_0,\ X]), \tag{4}$$

which demonstrates that HF theory is a closed one-body density dynamics; i.e. one needs to know only the one-body density ρ to evaluate the r.h.s.

of eq. (4). A closed dynamical equation for the one-body density of the type (3) is sometimes called a kinetic equation.[1] Secondly, the HF Hamiltonian satisfies the equation

$$\langle\psi|[H_o, \hat{X}]|\psi\rangle = \langle\psi|[H, \hat{X}]|\psi\rangle \ , \tag{5}$$

where H is the unconstrained many-body Hamiltonian. As a consequence, it follows that $\hat{\rho}(X)$ takes precisely the same value at each ρ in the constrained HF dynamics as it would in the full unconstrained quantum mechanics.

To put the HF density dynamics into perspective, it is profitable to consider the following three questions: (i) What is special about the set of one-body operators and hence about the one-body densities? (ii) Are there other subsets of observables of interest with corresponding densities? (iii) Can we construct for them a closed density dynamics?

One soon recognizes that what is special about the one-body operators is that they span a closed lie algebra; i.e. the commutator of two one-body operators is again a one-body operator. But the generators of any lie group of transformations of the many-particle Hilbert space span a closed lie-algebra. In particular, the generators of collective motions, e.g. su(3), sp(3,R), ..., are collective observables of considerable interest. We therefore consider how to define the densities and construct a density dynamics for any such Lie algebra of observables. Fuller details can be found in ref. 2, 3.

GENERALIZED DENSITIES

Let G be a lie group of unitary transformations of the many-particle Hilbert space $\mathbb{H}$. We denote the action of a group element $g \in G$ on a state $\psi \in \mathbb{H}$ simply by $g\psi$.

Let $\mathfrak{g}$ denote the lie algebra of G. The structure of $\mathfrak{g}$ is given in terms of a basis $\{E_\alpha\}$ by the commutation relations

$$[E_\alpha, E_\beta] = C_{\alpha\beta}^{\gamma} E_\gamma \ , \tag{6}$$

where $\{C_{\alpha\beta}^{\gamma}\}$ are the structure constants. An arbitrary element $X \in \mathfrak{g}$ is a vector with components (X^α), defined in terms of the basis by the expansion

$$X = X^\alpha E_\alpha \ . \tag{7}$$

To any state $\psi \in \mathbb{H}$ there now corresponds a density ρ defined by

$$\rho(X) = -i \langle\psi| X |\psi\rangle \tag{8}$$

for all $X \in \mathfrak{g}$. Note that the factor $(-i)$, not present in eq. (2), is included to make $\rho(X)$ real and is necessitated by the fact that I am using the mathematicians convention of choosing X to be anti-Hermitian rather than Hermitian. If one prefers, one can replace X by $Y = -iX$ and regard the Hermitian operator Y as the physical observable.

Inserting the expansion (7) into (8) gives

$$\rho(X) = X^{\alpha} \rho_{\alpha} , \tag{9}$$

where $\rho_{\alpha} = \rho(E_{\alpha})$, and reveals that ρ is a covector with components (ρ_{α}). Evidently ρ is a vector in $\mathfrak{g}^*$, the dual space of the lie algebra $\mathfrak{g}$.

Note that the definition (8) can be extended to a mixed (e.g. thermal) state in the standard way by

$$\rho(X) = -i \sum_{\lambda} C_{\lambda} \langle\psi_{\lambda}| X |\psi_{\lambda}\rangle , \tag{10}$$

where (C_{λ}) are the (positive) weighting factors for the incoherent components of the mixed state.

GROUP ORBITS AND COADJOINT ORBITS

The set of Slater determinants is an orbit of the group of one-body unitary transformations. An orbit of a group G is a set of states

$$M = \{\psi(g) = g\psi \, ; \, g \in G\}, \tag{11}$$

where ψ is any given fixed state in $\mathbb{H}$. Clearly G has many possible distinct orbits in $\mathbb{H}$ depending on the choice of representative state ψ. To each such orbit there corresponds a coadjoint orbit of densities.

$$N = \{\rho_g \, ; \, g \in G\}, \tag{12}$$

where ρ_g is the density corresponding to $\psi(g)$. It follows from the definition (8) that

$$\rho_g(X) = \rho(g^{-1} X g). \tag{13}$$

For densities of mixed states, one observes that eq. (13) still applies.

DENSITY DYNAMICS

We seek a dynamical equation that can be integrated to give paths $\rho(t)$ in $\mathfrak{g}^*$. Ideally, we would like paths that correspond precisely to solutions $\psi(t)$ of the full time-dependent Schrodinger equation.

The Schrodinger equation gives

$$\frac{d}{dt} \langle\psi| X |\psi\rangle = i\langle\psi|[H, X]|\psi\rangle, \tag{14}$$

where H is the Hamiltonian. Now if iH were an element of the Lie algebra, we could immediately set

$$\dot{\rho}(X) = \rho([iH, X]) \tag{15}$$

to obtain a density dynamics in accord with eq. (14). However, this is a trivial case which parallels the HF equation for a one-body Hamiltonian.

The interesting situation is when neither iH nor [iH, X] are in the lie algebra. The r.h.s. of eq. (15) is then not defined because [iH, X] is outside the domain of the density.

In HF theory the problem is solved by finding a one-body HF Hamiltonian H_0 that satisfies the equation

$$\langle\psi|[H_0, X]|\psi\rangle = \langle\psi|[H, X]|\psi\rangle, \tag{16}$$

for all one-body X, whenever ψ is a Slater determinant. We therefore enquire if there might similarly exist some $iH_0 \in \mathfrak{g}$ at each ψ on a G-orbit M that satisfies eq. (16) for all $X \in \mathfrak{g}$. For, if so, we can set

$$\dot{\rho}(X) = \rho([iH_0, X]), \tag{17}$$

in parallel with the HF eq. (4), and again obtain a density dynamics in accord with eq. (14). The answer is that there does exist such a Hamiltonian $H_0(\rho)$ if and only if the energy

$$H = \langle\psi|H|\psi\rangle \tag{18}$$

is a single-valued function $H(\rho)$ of the density for all $\psi \in M$.[3]

Note that the map $M \to N$; $\psi \to \rho$ is, in general, many-to-one in which

case there are many energies to each ρ. In the special case that M and N are isomorphic, one can already construct a dynamics on M as was done in ref. 4. However, if the map $M \to N$ is many-to-one, it can be shown[3] that the dynamics on M is not well-defined (due to the fact that M is not a phase space). A very special situation arises when the energy is nevertheless a single-valued function of the density due to a symmetry leading to an invariance of the Hamiltonian. This is a most interesting situation considered by Dirac[5] in other language. However, it is straightforward and so we shall not focus specifically on it here. Instead we consider the general situation where $H(\rho)$ is not a priori well-defined by eq. (18). Eq. (18) is then replaced by

$$H(\rho) = \langle\langle\psi|H|\psi\rangle\rangle \ , \tag{19}$$

by which we mean an average over all states $\psi \in M$ having the same density ρ.

We can now define $H_0(\rho)$ by

$$\langle\langle\psi|[H_0, X]|\psi\rangle\rangle = \langle\langle\psi|[H, X]|\psi\rangle\rangle \ , \tag{20}$$

which is easily shown to have a solution[3]. Thus we can again use eq. (17) to define a density dynamics.

The implication of this result is that the average dynamics for a set of states of density ρ is well defined whereas it was not defined for the individual members of the set. This is perhaps not surprising since, to distinguish members of the set, we need additional densities beyond those in $\mathfrak{g}^*$. An average dynamics is nevertheless useful because, in many practical situations, one may expect the time-derivatives of densities of states of the same density to differ only slightly. One might also contemplate treating first the average density dynamics with the intention of subsequently developing a theory for the fluctuations about the average.

Finally, we show that the above density dynamics is a Hamiltonian dynamics. Let $(\bar{E}_\nu)$ be a maximal subset of linearly independent vectors in $\mathfrak{g}$ having the property that

$$\rho([X,\bar{E}_\nu]) \neq 0 \quad \text{for some } X \in \mathfrak{g}. \tag{21}$$

Substituting $g=\exp(x^\nu\bar{E}_\nu)$ in the expression (13) for ρ_g and differentiating gives

$$\frac{\partial \rho(\underline{x})}{\partial x^\nu} = \rho([X, \bar{E}_\nu]) \tag{22}$$

revealing that the vectors $(\bar{E}_\nu)$ are a basis of generators of infinitesimal displacement on N. It also follows from eq. (19) that

$$\frac{\partial H}{\partial x^\nu} = \langle\langle\psi | [H, \bar{E}_\nu] | \psi\rangle\rangle \tag{23}$$

Hence, by eq. (20), the equation of motion (17) gives

$$\dot{\rho}_\nu = \frac{\partial H}{\partial x^\nu} \tag{24}$$

or, in coordinate independent language,

$$\dot{\rho} = dH. \tag{25}$$

Now, for any smooth function $F(\rho)$ of the density,

$$\dot{F} = \frac{\partial F}{\partial \rho_\nu} \dot{\rho}_\nu = \frac{\partial F}{\partial \rho_\nu} \frac{\partial H}{\partial x^\nu} . \tag{26}$$

To evaluate $\partial F/\partial \rho_\nu$, observe that

$$\frac{\partial F}{\partial x^\nu} = \frac{\partial F}{\partial \rho_\mu} \sigma_{\mu\nu} , \tag{27}$$

where

$$\sigma_{\mu\nu} = \frac{\partial \rho_\mu}{\partial x^\nu} = \rho([\bar{E}_\mu, \bar{E}_\nu]). \tag{28}$$

It follows that

$$\frac{\partial F}{\partial \rho_\mu} = \frac{\partial F}{\partial x^\nu} \sigma^{\nu\mu} , \tag{29}$$

where $(\sigma^{\mu\nu})$ is the inverse of the matrix $(\sigma_{\mu\nu})$, which by eq. (21) must exist. Thus eq. (26) becomes a Hamilton's equation

$$\dot{F} = \{H, F\} \tag{30}$$

with Poisson bracket

$$\{H,F\} = \sigma^{\nu\mu} \frac{\partial H}{\partial x^{\mu}} \frac{\partial F}{\partial x^{\nu}} \quad . \tag{31}$$

APPLICATION

If one simply wanted the ground state of a one-body Hamiltonian H_o, it would make sense to seek it in the space of independent-particle states (Slater determinants). However, for the time-dependent problem, one may also be interested in the time evolution $\psi(t)$ of an initial state ψ that is not a Slater determinant. Since

$$\psi(t) = e^{-iH_o t} \psi \tag{32}$$

and $\exp(-iH_o t)$ is a one-body unitary transformation, it follows that the path $\psi(t)$ lies on an orbit of the one-body unitary group. This suggests that it might be useful, even when the Hamiltonian H is not one-body, to consider an approximate dynamics constrained to an orbit of the one-body unitary group. For example, it might be appropriate for describing the scattering of two heavy-ions like $^{12}C + {}^{12}C$ with initial state given by the product of two shell-model ground states. This seems like a natural way of lifting the sometimes unrealistic TDHF restriction to Slater determinants.

However, as we have shown elsewhere[4], the dynamics on an orbit of wave functions is only defined when the orbit is a phase space which is an exceptional case. It is in fact the situation when the orbit of wave functions is isomorphic to the corresponding coadjoint orbit of densities[3]. On the other hand, coadjoint orbits are always phase spaces[3] and, as we have shown here, always support a well-defined Hamiltonian density dynamics.

Densities have another advantage over wave functions in that they can represent mixed states as well as pure states. Mixed states might correspond to thermal distributions or simply to one's incomplete knowledge of the system. One possibility is to let a density correspond to a whole shell-model space of states. Consider, for example, a shell model space corresponding to a partition of the single-particle Hilbert space into subspaces of occupied (hole) states, valence states and unoccupied (particle) states. The conventional procedure for partitioning the space is initiated by constructing an energy ordered basis of single-particle eigenstates of some physically reasonable shell-model Hamiltonian. But what is the optimal partition?

To answer this question, consider the one-body densities, corresponding to a particular shell-model partition, as a point on a manifold.

Since any other partition is obtained by some unitary transformation of the single-particle basis, it follows that the manifold in question is an orbit of the one-body unitary group. The optimal shell-model space can therefore be defined as the stationary points on this manifold. This gives the equation

$$\langle\langle\psi|[H, X]|\psi\rangle\rangle = 0 \tag{33}$$

for all one-body X, where the average is over all shell-model states. Eq. (33) obviously has a close resemblance to the HF equation and can likewise be solved by self-consistent field methods. A solution is obtained when the following off-diagonal single-particle matrix elements all vanish:

$$\begin{aligned}
\varepsilon_{hp} &= T_{hp} + \sum_{h'} V_{hh'ph'} + \frac{n}{N} \sum_{v} V_{hvpv} \\
\varepsilon_{hv} &= T_{hv} + \sum_{h'} V_{hh'vh'} + \frac{n}{N-1} \sum_{v'} V_{hv'vv'} \\
\varepsilon_{vp} &= T_{vp} + \sum_{h'} V_{vh'ph'} + \frac{n-1}{N-1} \sum_{v'} V_{vv'pv'}
\end{aligned} \tag{34}$$

where h,h' label hole states, v,v' valence states, and p,p' label particle states. n is the number of particles in the valence space and N is its dimensionality. T is the kinetic energy and V is the two body interaction.

One notes that in a mean field, rather than the above variational, theory the factors in front of the 3rd term would all be n/N. The differences can be interpreted as blocking effects.

REFERENCES

1. E.A. Remler, to be published.
2. G. Rosensteel and D.J. Rowe, Phys. Rev. A24 (1981) 673.
3. D.J. Rowe, M. Vassanji and D.J. Rowe, to be published.
4. D.J. Rowe and R. Basserman, Can. J. Phys. 54 (1976) 1941; A.K. Kerman and S.E. Koonin, Ann. Phys. (N.Y.) 100 (1976) 332; D.J. Rowe, A. Ryman and G. Rosensteel, Phys. Rev. A22 (1980)2362; P. Kramer and M. Saraceno, Lecture Notes in Physics 140 (Springer-Verlag, 1981)
5. P.A.M. Dirac, Can. J. Math. 2 (1950) 129.