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Thermodynamic coefficients of hot nuclei

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We present a general method to evaluate large amplitude time-dependent Hartree Fock dynamics in a single mode and in the presence of a thermal bath. We apply the method in the small oscillation regime to isothermal and isentropic breathing mode oscillations. We employ realistic microscopic effective Hamiltonians with phenomenological extensions to large model spaces and obtain thermodynamic coefficients for ^{16}O and ^{40}Ca. Coefficients for the incompressibilities, specific heats, and thermal expansion are obtained along with breathing mode frequencies as a function of temperature. A significant effect due to the nonlocality of the interaction on the collective mass is obtained. The interaction produces a remarkably low value for the incompressibility while providing an adequate description of the breathing mode energy.

I. INTRODUCTION

The time evolution of hot nuclei has been investigated within a variety of many-body methods. One set of mean-field approaches based upon extending time-dependent Hartree-Fock (TDHF) considers the time evolution with assumed global thermodynamic equilibrium.[1–3] This is closest in spirit to our own work. Other time-dependent approaches begin with TDHF but move closer to a hydrodynamic picture by including effects of two-body scattering[4] and viscosity and thermal conduction[5,6] via classical approximations.

We have several major goals in the present work. First, we will generalize the approach of Ref. 1 to arbitrary pairs of conjugate operators and demonstrate the contact with TDHF. The approach is developed for "mode-selected" large amplitude collective motion. Second, we implement the method with realistic effective Hamiltonians which, in principle, have more predictive power than purely phenomenological Hamiltonians. This is important in view of the demonstration by Có and Speth[7] that dynamical quantities, such as the breathing mode frequency, vary widely with different phenomenological Hamiltonians whose parameters are fixed solely by ground state properties. Third, we will demonstrate that many other thermodynamic coefficients are easily obtained and should serve to broaden the basis for comparisons between theory and experiment and between different theories. Fourth, we will present results for initial applications to ^{16}O and ^{40}Ca. These results are obtained in the domain of small amplitude motion and we reserve the large amplitude applications for future efforts.

Since we anticipate eventual comparisons of the present results with experimental data it is important to keep in mind the chief limitations of our approach: we only include mean-field dynamics, we select a single mode and thereby preclude Landau damping, and we assume global thermal equilibrium. With regards to the last assumption we derive considerable encouragement from the recent work of Nemeth *et al.*[5] where the results of local and global thermodynamic equilibrium assumptions in a semiclassical approach were shown to be comparable even for large amplitude processes in nuclei.

The outline of the paper is as follows: in Sec. II we review TDHF dynamics in a single mode and restricted to zero temperature. In Sec. III we present the extension to finite temperatures. In Sec. IV we consider isothermal and isentropic small oscillations and define the thermodynamic coefficients which we will evaluate. Section V recounts the ingredients of our calculations: the realistic effective Hamiltonian, its phenomenological adjustments, and the choice of conjugate operators for the breathing mode. In Sec. VI we present our results for ^{16}O and ^{40}Ca while Sec. VII summarizes our conclusions.

II. TDHF DYNAMICS IN ONE MODE: A REVIEW OF THE $T=0$ CONSTRAINED HARTREE-FOCK THEORY WITH TWO CONJUGATE PARAMETERS

The time-dependent mean-field theory provides currently the best microscopic description of nuclear dynamics at low energies.[8] Viewed as an initial value problem it has proven reliable in explaining the evolution of one-body observables in a wide range of nuclear phenomena.[9] In its adiabatic version, adiabatic time-dependent Hartree-Fock (ATDHF),[10,11] it provides a self-consistent way of adding kinetic energy terms to potential energy surfaces. Finally, in its small amplitude limit it leads to the random-phase approximation (RPA) which is the standard way of studying the harmonic part of the nuclear spectrum near the ground state. This is a broad subject with many subtleties and ramifications. As our interests focus on the study of collective nuclear motion under different thermal conditions we only consider here the simplest case of TDHF motion in one predetermined mode.

The purpose of this section is mainly pedagogical as the theory is simple and well known.[10] It will allow us to introduce the notation and will set the stage for the extension to finite temperature.

We consider two single-particle operators $\hat{P},\hat{Q}$ interpreted as a collective momentum and a collective coordinate. Their nature depends on the kind of motion that we want to focus upon and the formalism does not depend on their precise form except for some general properties that allow a reasonable physical interpretation. We require the following

$$\left.\begin{array}{r}\hat{P}\rightarrow-\hat{P}\\ \hat{Q}\rightarrow\hat{Q}\end{array}\right\}\text{ under time reversal} \tag{1a}$$

$$[\hat{P},\hat{Q}]\neq 0 \; . \tag{1b}$$

The next step is to set up a constrained Hartree-Fock (CHF) calculation using $\hat{P}$ and $\hat{Q}$ as constraining operators. This is done formally by minimizing the following functional

$$G[\rho]=H[\rho]-\lambda_1 Q[\rho]-\lambda_2 P[\rho] \; , \tag{2}$$

where

$$H[\rho]=\mathrm{tr}t\rho+\tfrac{1}{2}\mathrm{tr}\,\mathrm{tr}\rho v^{A}\rho \; , \tag{3}$$

$$Q[\rho]=\mathrm{tr}q\rho \; , \tag{4}$$

$$P[\rho]=\mathrm{tr}p\rho \; . \tag{5}$$

In Eq. (3) t is the kinetic energy operator, v^A the antisymmetrized two-body interaction, q and p are the single-particle constraining operators, and ρ is the one-body density operator. The usual requirements on ρ

$$\mathrm{tr}\rho=A, \quad \rho^2=\rho \tag{6}$$

force the trial wave function to be a determinant of A particles. In this case the functionals defined above are simply the mean values of the operators in the CHF Slater determinant. Variation of Eq. (2), with due regard to conditions Eq. (6) results in the usual CHF equation

$$[h-\lambda_1 q-\lambda_2 p,\rho]=0 \; , \tag{7}$$

where h is the HF Hamiltonian

$$h=t+\mathrm{tr}v^{A}\rho \; . \tag{8}$$

The standard way to solve Eq. (7) is to solve the eigenvalue problem

$$g\phi_i=\epsilon_i\phi_i \; , \tag{9}$$

where

$$g=h-\lambda_1 q-\lambda_2 p \; . \tag{10}$$

The result of this procedure is a density matrix which is a function of the constraining parameters $\rho=\rho(\lambda_1,\lambda_2)$. The eigenvalue problem represented by Eq. (9) does not have time-reversal invariance because, while h and q have been assumed time-even, p is time-odd. This means that the wave functions will be complex and that the equilibrium density matrix $\rho(\lambda_1,\lambda_2)$ will have a time-odd part representing a net collective current.

We now write down some relationships that follow from the Feynmann-Hellman theorem. Let us call $G(\lambda_1,\lambda_2),H(\lambda_1,\lambda_2),Q(\lambda_1,\lambda_2),P(\lambda_1,\lambda_2)$ the functions obtained by evaluating the functionals in Eqs. (2)–(5) at the self-consistent density $\rho(\lambda_1,\lambda_2)$. Then these quantities are related by

$$\frac{\partial G}{\partial\lambda_1}=-Q, \quad \frac{\partial G}{\partial\lambda_2}=-P \; . \tag{11}$$

A Legendre transformation with respect to the variables P and Q provides the complementary relationships

$$\frac{\partial H}{\partial Q}=\lambda_1, \quad \frac{\partial H}{\partial P}=\lambda_2 \; . \tag{12}$$

For the latter we have assumed that the functions $Q(\lambda_1,\lambda_2)$ and $P(\lambda_1,\lambda_2)$ can be inverted everywhere. This poses some convexity requirements on the functions G and H which are related to the stability of the CHF minimum. We will not, at this stage, elaborate further on these requirements and assume that the Jacobian $[\partial(Q,P)/\partial(\lambda_1,\lambda_2)]$ is nonsingular.

The equations of motion are obtained by requiring that the Heisenberg equations for the operators $\hat{P},\hat{Q}$ be satisfied in mean value, i.e., we require that

$$\begin{aligned}\hbar\frac{d}{dt}\mathrm{tr}\rho q&=\mathrm{tr}\rho i[h,q] \; ,\\ \hbar\frac{d}{dt}\mathrm{tr}\rho p&=\mathrm{tr}\rho i[h,p] \; .\end{aligned} \tag{13}$$

These equations are also easily derived from a time-dependent variational principle where the density matrix is constrained to depend on time only through the parameters λ_1,λ_2.

Although we have chosen to look at Eq. (13) as averaged Heisenberg equations for $\hat{P}$ and $\hat{Q}$ they can also, of course, be considered as equations for the density matrix. If we rewrite them as

$$\begin{aligned} &\mathrm{tr}\,q\,(i\hbar\dot{\rho}-[h,\rho])=0\ ,\\ &\mathrm{tr}\,p\,(i\hbar\dot{\rho}-[h,\rho])=0\ , \end{aligned} \tag{13a}$$

we can also interpret them as an attempt to satisfy the full time-dependent Hartree-Fock equations $i\hbar\dot{\rho}=[h,\rho]$ in the special "directions" specified by p and q. Viewed in this light, we have simply selected a particular mode of the more general TDHF dynamics and have forced the system in this mode. Of course, whether the procedure is at all justified depends on the residual couplings that our selected mode has with the rest.

It is worthwhile at this point to comment on the physical meaning of this procedure. The operators $\hat{P},\hat{Q}$ are independent of the Hamiltonian and are used to define a "collective path"[12] in the many-dimensional phase space of density matrices. There is a large amount of literature on attempts to relate this collective path back to the dynamics of the Hamiltonian. At small amplitudes this leads to the identification of $\hat{P}$ and $\hat{Q}$ to a low frequency collective RPA mode.[13] In the adiabatic approximation it leads to linking the $\hat{P}$ operator to $\partial/\partial Q$ and to the extraction of a collective mass of the Thouless-Valatin form. In the truly large amplitude regime one has to face squarely the fact that extracting a low-dimensional invariant collective manifold decoupled from the noncollective degrees of freedom is a very difficult and, many times, impossible task. Results on how to follow the RPA modes to large amplitudes in an optimal way have been discussed by Marumori[14] and collaborators. In our present effort we will be concerned with the small amplitude response of nuclei.

We can combine Eqs. (13a) and (7) and use again the cyclic invariance of the trace to obtain

$$\begin{aligned} \dot{Q}&=\frac{d}{dt}\mathrm{tr}\rho q=\lambda_2\mathrm{tr}\rho i[p,q]/\hbar\ ,\\ \dot{P}&=\frac{d}{dt}\mathrm{tr}\rho p=\lambda_1\mathrm{tr}\rho i[q,p]/\hbar\ . \end{aligned} \tag{14}$$

Using Eq. (12) to replace λ_1 and λ_2 we finally obtain the equations of motion

$$\begin{aligned} \dot{Q}&=\frac{\partial H}{\partial P}\xi(P,Q)\ ,\\ \dot{P}&=-\frac{\partial H}{\partial Q}\xi(P,Q)\ , \end{aligned} \tag{15}$$

where

$$\xi(P,Q)=\mathrm{tr}\rho i[p,q]/\hbar\ . \tag{16}$$

Except for the common factor ξ these are canonical equations for the conjugate pair P,Q. The motion is governed by the Hamiltonian function H, which is just the mean value of the Hamiltonian expressed as a function of the mean values of the constraining operators.

The factor $\xi(P,Q)$ is not very important in what follows. Notice that it would just disappear if the operators $\hat{P},\hat{Q}$ were canonically conjugate. It can be scaled away by a renormalization of the p,q operators or more practically by a rescaling of the time variable, as is obvious from Eq. (15). In what follows, we just carry this factor along and compute it when necessary.

One important consequence of Eq. (15) is that, as in ordinary TDHF, the energy is conserved. Similarly these equations are not restricted to small amplitudes.

III. FINITE TEMPERATURE FORMALISM

The extension to finite temperature of the results in the preceding section follows in a standard and straightforward manner.

The method that we develop here extends the approach of Sagawa and Bertsch[1] which was applied to study the vaporization of hot nuclei. We show that the method is applicable to the study of any collective mode and emphasize the need to specify the thermodynamic conditions under which it happens. This is important because the readily calculated isothermal coefficients are not necessarily those applicable to realistic situations. This point has been stressed by Goodman[15] in connection with calculations of moments of inertia and collective rotational bands in nuclei at $T\neq 0$. We explore below the isothermal and isentropic regimes with a fixed number of particles but the methods can be readily adapted to other situations such as the case of a fixed chemical potential.

Instead of the energy we minimize the grand potential with the temperature and the chemical potential constraining the values of the entropy and the particle number. Thus we consider variations of the functional

$$\Omega[\rho]=G[\rho]-TS[\rho]-\mu N[\rho]\ , \tag{17}$$

where $G[\rho]$ is defined in Eq. (2) and

$$S[\rho]=-\mathrm{tr}\{\rho\ln\rho+(1-\rho)\ln(1-\rho)\}\ , \tag{18}$$

$$N[\rho]=\mathrm{tr}\rho\ . \tag{19}$$

Variation of Ω yields immediately the constrained finite-temperature Hartree-Fock (FTHF) equation

$$\rho=\left\{1+\exp\left[\frac{h-\mu-\lambda_1 q-\lambda_2 p}{T}\right]\right\}^{-1}\ . \tag{20}$$

This is solved as usual by requiring the simultaneous diagonalization of ρ and $g=h-\lambda_1 q-\lambda_2 p$. Notice that again, when self-consistency is achieved

$$[h-\lambda_1 q-\lambda_2 p,\rho]=0\ . \tag{21}$$

Now the self-consistent density will be a function of $\lambda_1,\lambda_2,T,\mu$ and the value of the corresponding functional will yield the following functions

$$H(\lambda_1,\lambda_2,T,\mu)=\mathrm{tr}t\rho+\tfrac{1}{2}\mathrm{tr}\,\mathrm{tr}\rho v^{A}\rho\ , \tag{22a}$$

$$N(\lambda_1,\lambda_2,T,\mu)=\mathrm{tr}\rho\ , \tag{22b}$$

$$S(\lambda_1,\lambda_2,T,\mu)=-\mathrm{tr}\{\rho\ln\rho+(1-\rho)\ln(1-\rho)\}\ , \tag{22c}$$

$$Q(\lambda_1,\lambda_2,T,\mu)=\mathrm{tr}q\rho\ , \tag{22d}$$

$$P(\lambda_1,\lambda_2,T,\mu)=\mathrm{tr}p\rho\ , \tag{22e}$$

$$\Omega=H-\mu N-TS-\lambda_1 Q-\lambda_2 P\ . \tag{22f}$$

These quantities are related by the analogs of Eq. (11)

$$\frac{\partial\Omega}{\partial\mu}=-N,\quad \frac{\partial\Omega}{\partial T}=-S,\quad \frac{\partial\Omega}{\partial\lambda_1}=-Q,\quad \frac{\partial\Omega}{\partial\lambda_2}=-P\ . \tag{23}$$

A Legendre transformation with respect to all variables yields the equivalent of Eq. (12)

$$\frac{\partial H}{\partial Q}=\lambda_1,\quad \frac{\partial H}{\partial P}=\lambda_2,\quad \frac{\partial H}{\partial S}=T,\quad \frac{\partial H}{\partial N}=\mu\ . \tag{24}$$

These relations assume that H has been rewritten as a function of Q,P,S,N by inversion of Eqs. (22b)–(22e).

Other partial Legendre transforms are, of course, possible and will be relevant in different situations. For example, at constant T and N we want to consider the free energy

$$F=H-TS=\Omega+\lambda_1 Q+\lambda_2 P+\mu N \tag{25}$$

which gives

$$\frac{\partial F}{\partial Q}=\lambda_1,\quad \frac{\partial F}{\partial P}=\lambda_2,\quad \frac{\partial F}{\partial T}=-S,\quad \frac{\partial F}{\partial N}=\mu\ . \tag{26}$$

For the dynamical equations to be derived below the important part of Eqs. (24) and (26) is that λ_1 and λ_2 are derivatives of the energy (or free energy).

Again we will not analyze the conditions for the existence of the various Legendre transforms although it should be realized that important phenomena related to phase transitions may cause these transforms to become singular.

The establishment of the dynamical equations proceeds exactly as before. All the manipulations leading up to Eq. (14) carry through unaltered except, of course, that now ρ is the solution of the FTHF Eq. (20).

However, the step that leads from Eq. (14) to (15) depends on what thermal conditions we want to explore. If the oscillation occurs at constant entropy, i.e., without exchange of heat energy with the thermal bath, then it is appropriate to use Eq. (24) for λ_1 and λ_2. In that case we obtain equations formally similar to Eq. (15).

$$\dot{Q}=\left.\frac{\partial H}{\partial P}\right|_{S,N}\xi\ ,\qquad \dot{P}=-\left.\frac{\partial H}{\partial Q}\right|_{S,N}\xi\ . \tag{27}$$

In Eq. (27) we have indicated explicitly which variables are held constant in the partial derivative. The consequence of Eq. (27) is that the motion occurs at constant energy and without heat exchange with the environment. Of course, the internal energy is shifted between kinetic and potential during the motion. The temperature is not constant and can be computed using Eq. (24) as

$$T=\left.\frac{\partial H}{\partial S}\right|_{P,Q,N}\ . \tag{28}$$

In this case, then, the energy H computed at constant entropy provides the Hamiltonian function for the collective motion.

It is also possible to explore the isothermal regime which may be relevant to astrophysical applications. In that case we use Eq. (26) instead of Eq. (24) in computing λ_1 and λ_2. Then the isothermal motion is given by the equations

$$\dot{Q}=\left.\frac{\partial F}{\partial P}\right|_{T,N}\xi\ ,\qquad \dot{P}=-\left.\frac{\partial F}{\partial Q}\right|_{T,N}\xi\ . \tag{29}$$

In this case it is the free energy that plays the role of a Hamiltonian for the collective motion. To keep the temperature constant energy has to be exchanged with the thermal bath and this will be done following the lines of constant free energy. The energy at any point on the trajectory can be computed as

$$E=F-T\frac{\partial F}{\partial T}\ . \tag{30}$$

The fluctuating term $T(\partial F/\partial T)$ is the thermal energy exchanged with the heat bath.

In both cases above we have considered that the number of particles is held fixed (while the chemical potential changes). A straightforward extension can be done to consider the motion at constant chemical potential.

IV. ISOTHERMAL AND ISENTROPIC SMALL OSCILLATIONS

The study of large amplitude collective motion at finite temperature is now reduced to the study of an energy surface obtained from a constrained Hartree-Fock (HF) calculation with at least four Lagrange parameters. Two of them (λ_1,λ_2) are of dynamical nature and represent the force and velocity fields needed to describe collective motion in a given mode. The other two (T,μ) embody the thermal constraints on the motion. The numerical determination of these surfaces is quite feasible with realistic Hamiltonians. It is a rather large undertaking involving thousands of standard HF calculations. The output of such a computation is, for example, the function $H(P,Q,S,N)$ which for constant S,N yields the trajectory of isentropic motion as the line of constant H in the phase space of P and Q. In a similar way the free energy $F(P,Q,T,N)$ for constant T,N yields the trajectory of isothermal motion as the line of constant F.

In what follows we study the small amplitude limit of these surfaces near an equilibrium point. If such a point exists with values

$$P=0,\quad Q=q_0 \tag{31}$$

for a certain value of T,μ then the relevant surface (H or F) can be expanded in its neighborhood up to quadratic terms as

$$H(P,Q,S,N)=\tfrac{1}{2}k_S(S,N)(Q-q_0)^2+\tfrac{1}{2}B_S(S,N)P^2\ , \tag{32a}$$

$$F(P,Q,T,N)=\tfrac{1}{2}k_T(T,N)(Q-q_0)^2+\tfrac{1}{2}B_T(T,N)P^2\ , \tag{32b}$$

where

$$\begin{aligned}
k_S&=\left.\frac{\partial^2 H}{\partial Q^2}\right|_{S,N}=\left.\frac{\partial\lambda_1}{\partial Q}\right|_{S,N},\\
B_S&=\left.\frac{\partial^2 H}{\partial P^2}\right|_{S,N}=\left.\frac{\partial\lambda_2}{\partial P}\right|_{S,N},\\
k_T&=\left.\frac{\partial^2 F}{\partial Q^2}\right|_{T,N}=\left.\frac{\partial\lambda_1}{\partial Q}\right|_{T,N},\\
B_T&=\left.\frac{\partial^2 F}{\partial P^2}\right|_{T,N}=\left.\frac{\partial\lambda_2}{\partial P}\right|_{T,N}.
\end{aligned}\tag{33}$$

No cross terms are present because $\hat{P}$ is time odd. The equations of motion following from Eq. (27) or Eq. (29) become

$$\begin{aligned}
&\frac{d}{dt}(Q-q_0)=-BP\xi\ ,\\
&\frac{dP}{dt}=k\xi(Q-q_0)\ ,
\end{aligned}\tag{34}$$

where B and k have the subscript appropriate to isentropic or isothermal conditions and ξ is calculated at the equilibrium point.

From Eq. (34) we obtain immediately harmonic motion with frequency

$$\begin{aligned}
&\omega_S=\xi\sqrt{k_S B_S}\ ,\\
&\omega_T=\xi\sqrt{k_T B_T}\ .
\end{aligned}\tag{35}$$

The calculation above is a simple example of how thermodynamic coefficients can be obtained from constrained FTHF calculations. These coefficients are defined in general as second derivatives of energy (or free energy) at an equilibrium point. Here k and B have the meaning of a generalized spring constant and mass parameter. The precise physical significance of these coefficients will depend on the nature of the operators $\hat{P}$ and $\hat{Q}$. Symmetry and positivity requirements will restrict them.

Isothermal and isentropic coefficients are connected by Maxwell type relations as in ordinary thermodynamics. As an example of practical importance below we now show how to compute isentropic coefficients in terms of isothermal ones. The constrained FTHF calculation is performed at specified values of λ_1, λ_2, and T. The values of μ for the protons and neutrons are adjusted at each iteration to satisfy particle number constraints. After convergence, values of H,Q,P,S,F among others, are calculated. The functions

$$\begin{aligned}
&Q=Q(\lambda_1,\lambda_2,T)\ ,\\
&P=P(\lambda_1,\lambda_2,T)\ ,\\
&S=S(\lambda_1,\lambda_2,T)
\end{aligned}\tag{36}$$

are therefore obtained and their partial derivatives can be calculated numerically. We omit the μ (or N) dependence as we will always consider motion at constant N.

Thermodynamic coefficients are obtained from the differentials

$$\begin{aligned}
dQ&=\frac{\partial Q}{\partial\lambda_1}d\lambda_1+\frac{\partial Q}{\partial\lambda_2}d\lambda_2+\frac{\partial Q}{\partial T}dT\ ,\\
dP&=\frac{\partial P}{\partial\lambda_1}d\lambda_1+\frac{\partial P}{\partial\lambda_2}d\lambda_2+\frac{\partial P}{\partial T}dT\ ,\\
dS&=\frac{\partial S}{\partial\lambda_1}d\lambda_1+\frac{\partial S}{\partial\lambda_2}d\lambda_2+\frac{\partial S}{\partial T}dT\ .
\end{aligned}\tag{37}$$

The matrix of partial derivatives is symmetric because of Eq. (23). Thus, in Eq. (37) we have

$$\frac{\partial P}{\partial\lambda_1}=\frac{\partial Q}{\partial\lambda_2},\quad \frac{\partial S}{\partial\lambda_1}=\frac{\partial Q}{\partial T},\quad \frac{\partial S}{\partial\lambda_2}=\frac{\partial P}{\partial T}\ .\tag{38}$$

If we specialize the calculation at $\lambda_2=0$, the time-reversal properties assumed for $\hat{P}$ and $\hat{Q}$ imply

$$\frac{\partial S}{\partial\lambda_2}=\frac{\partial Q}{\partial\lambda_2}=0\quad\text{at } \lambda_2=0\ .\tag{39}$$

The matrix in Eq. (37) therefore simplifies to

$$Y=\begin{bmatrix} k_T^{-1} & 0 & a\\ 0 & B_T^{-1} & 0\\ a & 0 & C\end{bmatrix}\tag{40}$$

where k_T and B_T are defined in Eq. (33) and where

$$\begin{aligned}
a&=\left.\frac{\partial Q}{\partial T}\right|_{\lambda_1,\lambda_2},\\
C&=\left.\frac{\partial S}{\partial T}\right|_{\lambda_1,\lambda_2}.
\end{aligned}\tag{41}$$

It is now easy to invert Eq. (37) using Eq. (40)

$$\begin{aligned}
d\lambda_1&=\frac{k_T}{1-\alpha}dQ+\frac{a^{-1}}{1-\alpha^{-1}}dS\ ,\\
d\lambda_2&=B_T dP\ ,\\
dT&=\frac{a^{-1}}{1-\alpha^{-1}}dQ+\frac{C^{-1}}{1-\alpha}dS\ .
\end{aligned}\tag{42}$$

α is a dimensionless number which characterizes the passage from isothermal to isentropic conditions

$$\alpha=k_T\frac{a^2}{C}\ .\tag{43}$$

The thermodynamic coefficients at constant entropy can now be read off from Eq. (42)

$$\begin{aligned}
k_S&=\left.\frac{\partial\lambda_1}{\partial Q}\right|_S=\frac{k_T}{1-\alpha}\ ,\\
B_S&=\left.\frac{\partial\lambda_2}{\partial P}\right|_S=B_T\ .
\end{aligned}\tag{44}$$

Using Eq. (35) we find the ratio of the isothermal to isentropic frequencies

$$\omega_S/\omega_T=(1-\alpha)^{-1/2}\ ,\tag{45}$$

We can give a physical interpretation to α if we use the last relation in Eq. (42) to write

$$\left.\frac{\partial S}{\partial T}\right|_{Q} = C(1-\alpha) = \left.\frac{\partial S}{\partial T}\right|_{\lambda_1}(1-\alpha) . \tag{46}$$

Considering now that $\partial S/\partial T$ is proportional to a specific heat we find

$$\left.\frac{\partial S}{\partial T}\right|_{Q} \Big/ \left.\frac{\partial S}{\partial T}\right|_{\lambda_1} = 1-\alpha . \tag{47}$$

Thus α is related to a ratio of specific heats quite analogous to the ratio C_p/C_v of elementary thermodynamics. In Sec. V B 2 we make this analogy precise.

V. INGREDIENTS OF THE CALCULATIONS

A. Realistic effective Hamiltonian

The full Hamiltonian acting on all A nucleons is defined by

$$H = \sum_{i<j} h_{ij} = T_{\mathrm{rel}} + V + V_c , \tag{48}$$

where we use a relative kinetic energy operator

$$T_{\mathrm{rel}} = \sum_{i<j} \frac{(\mathbf{p}_i - \mathbf{p}_j)^2}{2Am} , \tag{49}$$

the realistic nucleon-nucleon potential V, and the Coulomb potential V_c. The quantities p and m signify the single-nucleon momentum and mass, respectively. From Eq. (48) we develop an effective Hamiltonian based on the major assumption that the many-body method we invoke is suitable to approximate the results of a shell-model diagonalization in a very large but finite basis. In particular, we choose a no-core basis space in order to avoid the calculation of core-polarization effects with realistic effective interactions. We approximate the temperature-independent effective no-core Hamiltonian with

$$H_{\mathrm{eff}} = T_{\mathrm{rel}} + V_{\mathrm{eff}} + V_c . \tag{50}$$

In the approximation we neglect renormalization effects on T_{rel} and on V_c and we calculate only leading order contributions to V_{eff}. We anticipate that these approximations become less severe as we increase the size of the no-core model space and increase the dependence on the adequacy of the many-body method. We do, however, introduce certain phenomenological adjustments below which are aimed at compensating for these approximations and for deficiencies in the Hartree-Fock approximation. The method of calculating the leading term of V_{eff},[16] which is the Brueckner G matrix[17] based on the Reid soft core potential,[18] has been presented elsewhere.[19–21] We also include the lowest order folded diagram in V_{eff} which we find substantially reduces the dependence of V_{eff} on the energy gap between the model space states and the remaining (excluded) states.

Since we employ a large no-core model space, the Pauli operator in the G matrix excludes scattering to intermediate two-particle states where each particle is in a set of major shells spanning the Fermi surface. Our basic assumption of reliance upon the many-body dynamical framework in a large but fixed basis space is equivalent to assuming the important temperature dependent effects are incorporated by that framework. That is, in contrast with thermal Brueckner Hartree-Fock theory, we assume H_{eff} is temperature independent, as would be appropriate, for example, in a microcanonical treatment. It is possible to generate theoretical alternatives to our approach which incorporate temperature dependent corrections to H_{eff}. However, due to our choice of partitioning of the model space and our restricted application to temperatures below 6 MeV we expect such corrections will not alter our results in a significant way.

These effective Hamiltonians (in some cases prior to including the folded diagram) have been employed in a number of many-body studies with no-core methods. In particular, we have used moment methods to obtain spectral distributions[21] and we have introduced[22] and applied[23] a coherent correlated pair method as well as a dynamical basis generation scheme.[24] Most relevant to the current effort is a detailed study of the thermal properties of ^{16}O and ^{40}Ca in the spherical FTHF approximation.[25,26] For more details on the effective Hamiltonian one should consult Ref. 26.

We have also extended the FTHF calculations with these effective Hamiltonians to include deformation.[27] In ^{24}Mg we obtained results indicating that first order deformed to deformed and that second order deformed to spherical phase transitions occur at temperatures less than 3 MeV.

For the sake of completeness we briefly summarize the strategy and rationale of introducing model space dependent phenomenological adjustments to the realistic effective Hamiltonians. The matrix elements of each of the operators in Eq. (50) are obtained in a harmonic oscillator basis with energy spacing $\hbar\omega$ for a particular nucleus consisting of A nucleons. We have found that, in a given model space, the matrix elements of H_{eff} (signified by $\langle\ \rangle$) are approximately dependent on $\hbar\omega$ and on A in the following way

$$\langle H_{\mathrm{eff}} \rangle \simeq \frac{\hbar\omega}{A}\langle t_{\mathrm{rel}} \rangle + \hbar\omega \langle v_{\mathrm{eff}} \rangle + \sqrt{\hbar\omega}\langle v_c \rangle . \tag{51}$$

Here we signify the A- and $\hbar\omega$-independent parts of the matrix elements by lower case letters. The dependence specified for the kinetic and Coulomb terms is exact while that of V_{eff} is approximate and is most accurate for the largest matrix elements.[26]

We have calculated H_{eff} in a sequence of model spaces abbreviated as the two-space (0*s*, 0*p*, and 1*s*-0*d* shells), the three-space (two-space plus 1*p*-0*f* shell), the four-space (three-space plus 2*s*-1*d*-0*g* shell), and the five-space (four-space plus 2*p*-1*f*-0*h* shell). With these model spaces we have evaluated the convergence rates of properties of ^{16}O and ^{40}Ca as a function of temperature.[25,26] We estimated that for both these systems, the thermostatic properties were converged in the FTHF approximation for temperatures $T \lesssim 7$ MeV when evaluated in the five-space.[26] For the current effort we are evaluating thermodynamic coefficients for these systems near their equilibrium configurations and for $T \lesssim 6$ MeV. However, based on systematics of the breathing mode in ^{16}O presented below we estimated that ^{40}Ca calculations required one more major shell to be converged to the level of less than a 10% error. We therefore adopted a phenomenological extension of our effective Hamiltonian to larger model spaces which we now describe.

In order to approximately include the effects of higher oscillator states we add a phenomenological single-particle Hamiltonian which acts between all shells and those above the first six shells. Thus, it does not act between two oscillator single-particle states both of which are within the first six shells. This phenomenological Hamiltonian consists of the single-particle kinetic energy operator, a Woods-Saxon potential (strength $=-60$ MeV, diffuseness $=0.6$ fm, and radius $=1.1A^{1/3}$ fm) and a Coulomb potential of a uniform charge sphere of radius $1.1A^{1/3}$ fm. In addition, to achieve a smooth matching of the added self-consistent states with the HF spectrum at $T=0$, an additional overall positive shift of 20 MeV was added to the oscillator diagonal terms of the phenomenological Hamiltonian. The need for this shift can be traced to the use of a two-body relative kinetic energy operator for the lowest six shells. Since the overall effects of this additional single-particle Hamiltonian are not large for these light nuclei we felt these approximations were adequate.

We also continue with the philosophy of making phenomenological adjustments to H_{eff} in order to cure the well-known problem that it does not reproduce simultaneously the ground state binding and rms radii of nuclei within the Brueckner-Hartree-Fock approximation. In our previous efforts[25,26] we varied $\hbar\omega$ in Eq. (51) and introduced overall strength parameters for T_{rel} and V_{eff} which we will call λ_t and λ_v for purposes of the present work. We adjusted $\hbar\omega$, λ_t, and λ_v within the spherical Hartree-Fock (SHF) approximation to obtain reasonable ground state properties. A detailed study of these parameters, the underlying rationale, the model space dependence, the nuclear dependence, and the resulting values have already been presented.[26] Since we are extending the Hamiltonian to larger spaces we have conducted a new study to determine optimum values for these parameters. Note that λ_t and λ_v only multiply the two-body terms associated with the realistic H_{eff} of the first six shells. We present in Table I a listing of the parameters and resulting ground state properties of ^{16}O and ^{40}Ca in the SHF approximation. The values of the parameters for four and five shell calculations have been chosen to give reasonable ground state properties in those spaces. However, for larger spaces a parameter set which gives good results in the largest space is selected for study. Then Table I shows the slow trend for increased binding and smaller rms radius that results. Unless otherwise specified we now adopt the 10-shell oscillator space for ^{16}O and the 11-shell oscillator space for ^{40}Ca.

B. Choice of $\hat{P}$ and $\hat{Q}$ for the breathing mode

To describe isoscalar monopole motion we use for $\hat{P}$ and $\hat{Q}$ the operators

$$\hat{Q}=\frac{1}{A}\sum_{i=1}^{A} r_i^2 \ , \tag{52}$$

$$\hat{P}=\frac{1}{2\hbar}\sum_{i=1}^{A} (\mathbf{p}_i\cdot\mathbf{r}_i+\mathbf{r}_i\cdot\mathbf{p}_i) \ . \tag{53}$$

$\hat{Q}$ measures the mean square radius and is used as collec-

TABLE I. Parameters of the effective Hamiltonian and resulting SHF properties of ^{16}O and ^{40}Ca as a function of the number of oscillator shells in which the calculation is performed. The rms radii quoted here are the point mass radii without corrections for spurious center of mass effects. For comparison the experimental binding of ^{16}O (^{40}Ca) is 127.6 (342.1) MeV and the charge rms of ^{16}O (^{40}Ca) is 2.75 (3.45) fm.

Nucleus	Model space	No. shells	$\hbar\omega$ (MeV)	λ_t	λ_v	E_{HF} (MeV)	rms (fm)
^{16}O	3	4	8.520	0.889	1.189	−127.8	2.74
	4	5	8.628	0.902	1.253	−127.6	2.70
	5	6	8.650	0.977	1.350	−124.9	2.62
		7	8.650	0.991	1.350	−125.1	2.62
		8	8.650	0.991	1.350	−127.3	2.59
		9	8.650	0.991	1.350	−127.3	2.58
		10	8.650	0.991	1.350	−127.7	2.56
^{40}Ca	4	5	7.950	0.980	1.220	−342.6	3.41
	5	6	7.610	1.000	1.290	−320.7	3.48
		7	7.610	1.000	1.290	−338.5	3.39
		8	7.610	1.000	1.290	−338.8	3.38
		9	7.610	1.000	1.290	−342.5	3.30
		10	7.610	1.000	1.290	−342.6	3.30
		11	7.610	1.000	1.290	−343.2	3.28

tive coordinate, while $\hat{P}$ is proportional to the radial flow and is used as collective momentum. The commutator is

$$\hat{\xi}=[i\hat{P},\hat{Q}]/\hbar=\frac{2\hat{Q}}{\hbar} \; . \tag{54}$$

Having made a choice for $\hat{Q}$ and $\hat{P}$ we can now assign a physical meaning to the thermodynamic coefficients defined in Eqs. (33) and (41). The fact that the operator $\hat{Q}$ is the mean square radius of the nucleus and therefore determines its volume allows the interpretation of λ_1 as an external pressure parameter which forces the system to have a given size. The term $\lambda_1 Q$ is therefore analogous to pV in ordinary thermodynamics. Quantities calculated at constant λ_1 can thus be loosely said to be at constant pressure, while constant Q means that volume is held fixed. With this in mind we now proceed to relate the partial derivatives studied in Sec. IV to quantities with a more physical interpretation.

1. *Incompressibility*

It is customary[28] to define the finite nucleus incompressibility as

$$K_A=r_0^2\frac{d^2}{dr^2}(E/A)\,|_{r=r_0} \tag{55}$$

where r_0 is the rms radius of the nucleus. In our case

$$r_0=\left[\frac{1}{A}\mathrm{tr}\rho r^2\right]^{1/2}=Q^{1/2} \; . \tag{56}$$

K_A is related to k defined in Eq. (33) by

$$K_A=\frac{4\langle r^2\rangle^2}{A}\frac{\partial\lambda_1}{\partial Q}=\frac{4Q^2}{A}k \; .$$

At temperature T we can then define the isothermal (or isentropic) incompressibility as

$$K_A\,|_{T \text{ or } S}=4\frac{\langle r^2\rangle^2}{A}\frac{\partial\lambda_1}{\partial Q}\bigg|_{T \text{ or } S} \; . \tag{57}$$

Both quantities are equal at $T=0$ and they are related by Eq. (44)

$$\frac{K_A\,|_T}{K_A\,|_S}=1-\alpha \; , \tag{58}$$

where α will be computed below.

2. *Specific heat*

In terms of the entropy, the specific heat is defined as

$$C_{p \text{ or } V}=T\frac{\partial S}{\partial T}\bigg|_{p \text{ or } V} \; , \tag{59}$$

where the entropy is written as a function of p, V or V, T. For our problem we use the correspondence of λ_1, Q with p, V to define

$$C_{\lambda_1}=T\frac{\partial S}{\partial T}\bigg|_{\lambda_1} \; , \quad C_Q=T\frac{\partial S}{\partial T}\bigg|_Q \; . \tag{60}$$

In our units these are pure numbers and their ratio is given by Eq. (47)

$$\frac{C_Q}{C_{\lambda_1}}=1-\alpha \; . \tag{61}$$

3. *Thermal expansion coefficient*

It is customary to define the volumetric thermal expansion coefficient as

$$\beta=\frac{1}{V}\frac{\partial V}{\partial T}\bigg|_p \tag{62}$$

where V is the volume as a function of T,p. In analogy, we define

$$\beta=\frac{3}{2}\frac{1}{\langle r^2\rangle}\frac{\partial\langle r^2\rangle}{\partial T}\bigg|_{\lambda_1} \; . \tag{63}$$

Then, using Eq. (41)

$$\beta=\frac{3}{2}\frac{1}{Q}\frac{\partial Q}{\partial T}\bigg|_{\lambda_1}=\frac{3}{2}\frac{a}{Q} \; . \tag{64}$$

If the expansion occurs isentropically the coefficient is

$$\beta_S=\frac{3}{2}\frac{1}{Q}\frac{\partial Q}{\partial T}\bigg|_S \; . \tag{65}$$

The ratio obtained from Eq. (42)

$$\frac{\beta_S}{\beta}=1-\alpha^{-1} \; . \tag{66}$$

4. *The quantity α*

According to Eq. (43), α is the dimensionless parameter that characterizes passage from isothermal to isentropic conditions. It can be related to the quantities defined above using Eq. (43)

$$\alpha=\frac{k_T a^2}{C}=\frac{A}{9}K_A\,|_T\frac{\beta^2 T}{C_{\lambda_1}} \; . \tag{67}$$

In terms of specific heats α is given by

$$\alpha=\frac{C_{\lambda_1}-C_Q}{C_{\lambda_1}} \; . \tag{68}$$

Using this form and the general inequalities satisfied by specific heats[29]

$$C_{\lambda_1}>C_Q>0 \tag{69}$$

we conclude that

$$0<\alpha<1 \; . \tag{70}$$

This in turn implies the following inequalities between the coefficients

$$\begin{gathered} K_A\,|_T<K_A\,|_S \; , \\ \omega_T>\omega_S \; . \end{gathered} \tag{71}$$

5. *The collective mass*

If the Hamiltonian contains only local two-body interactions the doubly constrained HF monopole problem for $\hat{H}-\lambda_1\hat{Q}-\lambda_2\hat{P}$ can be easily related to the singly constrained one for $\hat{H}-\lambda\hat{Q}$. In fact using the commutation relations of $\hat{P},\hat{Q}$ and the kinetic energy it is possible to show that if $|\psi(\lambda)\rangle$ is the Slater determinant which is a solution of the variational problem

$$\langle\delta\psi\,|\,\hat{H}-\lambda\hat{Q}\,|\,\psi\rangle=0\ . \tag{72}$$

Then the Slater determinant

$$|\,\psi(\lambda_1,\lambda_2)\rangle=e^{i\lambda_2(mA/2\hbar^2)\hat{Q}}\left|\psi\left[\lambda_1+\lambda_2^2\frac{mA}{2\hbar^2}\right]\right\rangle \tag{73}$$

solves the doubly constrained problem

$$\langle\delta\psi\,|\,\hat{H}-\lambda_1\hat{Q}-\lambda_2\hat{P}\,|\,\psi\rangle=0\ . \tag{74}$$

This result is not changed when we add the thermal constraints. This means that for local interactions the dependence of all quantities on λ_2 comes from the geometry of the monopole operators and need not be computed. For example, using Eq. (73) we find

$$Q(\lambda_1,\lambda_2)=Q\left[\lambda_1+\lambda_2^2\frac{mA}{2\hbar^2}\right]\ , \tag{75}$$

$$P(\lambda_1,\lambda_2)=\lambda_2\frac{mA}{\hbar^2}Q\left[\lambda_1+\lambda_2^2\frac{mA}{2\hbar^2}\right]\ , \tag{76}$$

where Q with a single argument is the solution of Eq. (72).

The consequence of Eq. (76) is that the collective mass parameter is

$$B^{-1}=\left.\frac{\partial P}{\partial\lambda_2}\right|_{\lambda_2=0}=\frac{mA}{\hbar^2}Q\ . \tag{77}$$

This result is only valid for local interactions, but it has been shown to be true also for interactions of Skyrme type by Bohigas.[30]

In our case, the interaction described in detail in Sec. V A is nonlocal and therefore Eq. (77) will not hold. However we can define a ratio

$$\eta=\frac{\hbar^2}{mAQ}\frac{\partial P}{\partial\lambda_2}\ . \tag{78}$$

This ratio will be different from unity for nonlocal forces. In terms of η we can write the collective mass [Eq. (77)] for nonlocal forces as

$$B^{-1}=M^*\frac{A}{\hbar^2}Q\ , \tag{79}$$

where

$$M^*=\eta m\ , \tag{80}$$

and therefore assign the nonlocality effects of the interaction to an effective mass. We do not expect this mass to be related to the effective nucleon mass calculated for infinite nuclear matter. Besides the nonlocality, it incorporates in an essential way the finite nucleus effects and the dynamics of the radial flow. Until a more detailed study of this quantity is done we may just think of η as a convenient way of displaying the results for $\partial P/\partial\lambda_2$.

VI. RESULTS AND DISCUSSION

We first present a compilation of the $T=0$ breathing mode frequency and incompressibility for ^{16}O and ^{49}Ca. We feel it is appropriate to present in some detail these $T=0$ properties and compare them with various other methods and forces since this is the first major calculation of these quantities with a realistic effective Hamiltonian. The various methods with which our results are compared include HF, symplectic shell model (SSM),[34] CHF, and RPA. Our results and those from phenomenological potentials are presented in Tables II and III along with the available experimental information for comparison. Note that most phenomenological Hamiltonians as well as our own Hamiltonian have been adjusted to reproduce certain bulk properties of either finite nuclei or nuclear matter. Thus the agreement between experiment and calculations for binding energies and rms radii is not surprising.[39]

In spite of the similarity of values for E/A and rms radii it is well known that a wide range of results for the breathing mode frequency, finite nucleus incompressibility and infinite matter incompressibility can nevertheless result. This is clearly evident in Tables II and III. It has also been demonstrated[7] that it is possible to generate phenomenological Hamiltonians which yield approximately the same binding, rms radius, *and* breathing mode frequency but dramatically different values for K_∞.

Our results for the breathing mode frequency fall within the lower range of results from phenomenological forces. Experimental information is sparse for these light systems but, for ^{40}Ca, where it is available, there is good agreement with our results.

For the finite nucleus incompressibility K_A a somewhat different picture emerges. In ^{16}O our results for K_A follow a general correlation pattern between K_A and $\hbar\omega$ found for these particular Hamiltonians.[31,34] That is, our K_A is also in the lower range of results from phenomenological forces. However, in ^{40}Ca our K_A is substantially lower than the results for *all* phenomenological forces. The reason we can have such a low value for K_A while maintaining good agreement for $\hbar\omega$ is due to the role of an effective mass arising from the nonlocal features of our Hamiltonian. We return to this major point later.

The results for K_A from SSM[34] are based on the third moment of the monopole strength function. The values of K_A we compute and the others we quote are based on the first negative moment of the monopole strength function. The size of the difference for the same Hamiltonian is an indicator of the breathing mode width. As pointed out by Bohigas *et al.*[30] and by Blaizot[31] the method for obtaining K_A from the first negative moment of the monopole strength function gives the lower value.

TABLE II. A compilation of $T=0$ results for ^{16}O.

	BE/A (MeV)		$\langle r^2\rangle^{1/2}$ (fm)[a]		$\hbar\omega$ (MeV)		K_A (MeV)		K_∞ (MeV)	
exp	7.98		2.71–2.73						≤ 105[b] 210 ± 30[c] ~ 350[d]	
This work	7.98		2.56[e]		24.7		98.2			
Force	HF	SSM[f]	HF	SSM[f]	RPA[g]	SSM[f]	RPA[g]	SSM[f]	HF[g]	SSM[i]
B1		5.82		2.74		22.0		92		
MDI	7.99[h]	7.84	2.76[h]	2.72						200
SkM		7.81		2.73					220	216
D1	8.19[j]	7.80	2.76[j]	2.70	24.6		101		228	
Ska	7.97[j]	7.56	2.78[j]	2.72	26.3		117		263	
SV	8.00[k]	7.54	2.67[k]	2.70						306
SIV	8.03[k]	7.56	2.68[k]	2.71	29.0		138		325	
SII	7.89[l]	7.62	2.75[l]	2.69						342
SIII	8.01[k]	7.60	2.69[k]	2.69	29.8		147		356	
SVI	7.99[k]	7.58	2.70[k]	2.71						364
Wong *et al.*[m] (CHF)	6.01				22.2[m]				246	

[a] Measured or calculated charge rms radius unless otherwise specified.
[b] Reference 38.
[c] References 31 and 32.
[d] Reference 7.
[e] Point mass radius including spurious c.m. motion.
[f] Reference 34; scaling incompressibility based on the third moment of the monopole strength function.
[g] Reference 31; based on Hartree-Fock and RPA calculations unless otherwise referenced.
[h] Reference 35.
[i] Reference 34; based on the extrapolation method of Ref. 32.
[j] Reference 28.
[k] Reference 36.
[l] Reference 37.
[m] Reference 33; based on constrained Hartree-Fock (CHF).

There is great interest in obtaining K_∞ to characterize the nuclear matter equation of state. As seen in Tables II and III, various methods to extract the experimental value of K_∞ from properties of finite nuclei yield quite different estimates. Due to the limited model space for the realistic H_{eff} it is unreasonable to attempt calculations of K_A for heavy nuclei. Thus we cannot estimate a value for K_∞. However, the trend of our K_A from ^{16}O and ^{40}Ca gives reason to believe that the K_∞ from our Hamiltonian will be quite low compared to the results for K_∞ obtained from most phenomenological Hamiltonians.

We return to the intriguing issue of how such a low value for K_A, especially in ^{40}Ca, can be compatible with the experimental breathing mode energy. In terms of the effective mass defined in Eq. (79) the monopole energy is given by

$$\hbar\omega=\left[\frac{K_A\hbar^2}{M^*Q}\right]^{1/2}. \tag{81}$$

We have shown that $M^*=m$ for local and Skyrme-type forces. For our nonlocal Hamiltonian at $T=0$ we obtain $M^*=1.01m$ for ^{16}O and $M^*=0.75m$ for ^{40}Ca. It is this feature of our interaction that allows a good agreement of the monopole energy in ^{40}Ca with a substantially reduced incompressibility. This points to the fact that nonlocality of the two-body interaction plays an important role in softening the equation of state while retaining agreement with breathing mode energies. While we show below (see Table V) that M^* is rather insensitive to changes in temperature we have not obtained its dependence on density since we have studied only small variations about equilibrium density. Later efforts will concentrate on the large amplitude behavior in order to have greater contact will heavy ion experiments.

We now concentrate on the main results of the present effort—the T-dependent properties of ^{16}O and ^{40}Ca. First, consider the T dependence of the breathing mode itself. As noted in Sec. IV the monopole energy $\hbar\omega$ depends on the thermodynamic conditions. Note that this distinction is generally absent in the literature. We present in Table IV our results for the isothermal and isentropic values of $\hbar\omega$ as a function of T up to 6 MeV. We see immediately how important is the distinction between the thermodynamic conditions since the $\hbar\omega_T$ falls

TABLE III. A compilation of $T=0$ results for ^{40}Ca.

	BE/A (MeV)		$\langle r^2\rangle^{1/2}$ (fm)[a]		$\hbar\omega$ (MeV)		K_A (MeV)		K_∞ (MeV)	
exp	8.55		3.47–3.49 3.42[b]		20.5[b]				≤105[c] 210±30[d] ~350[e]	
This work	8.56		3.42[f]		21.6		91.1			
Force	HF	SSM[g]	HF	SSM[g]	RPA[h]	SSM[g]	RPA[h]	SSM[i]	HF[h]	SSM[j]
B1					19.1	19	99	104	190	
MDI	8.61[k]	8.44	3.48[k]	3.46		21.8		135		200
SkM		8.37		3.47		21.7		136	220	216
D1	8.67[l]	8.34	3.47[l]	3.45	22.2	22.4	132	142	228	
Ska	8.54[l]	8.20	3.50[l]	3.48	23.0	23.5	144 (165)[i]	160	263	
SV	8.57[m]	8.10	3.44[m]	3.47		25.3		184		306
SIV	8.54[m]	8.09	3.46[m]	3.49	25.3	26.0	171 (203)[i]	195	325	
SII	8.40[n]	8.13	3.49[n]	3.48		26.5		206		342
SIII	8.54[m]	8.08	3.48[m]	3.49	26.3	27.0	186 (227)[i]	215	356	
SVI	8.52[m]	8.03	3.48[m]	3.51		27.3		220		364
Wong *et al.*[o] (CHF)	7.04				23.9[o]				246	

[a] Measured or calculated charge rms radius unless otherwise noted.

[b] From a compilation of experimental results in Ref. 34.

[c] Reference 38.

[d] References 31 and 32.

[e] Reference 7.

[f] Point mass radius including spurious c.m. motion.

[g] Reference 34, based on a symplectic shell model (SSM).

[h] Reference 31, based on Hartree-Fock and RPA calculations unless otherwise noted.

[i] Reference 34; scaling incompressibility based on the third moment of the monopole strength function.

[j] Reference 34, based on the extrapolation method of Ref. 32.

[k] Reference 35.

[l] Reference 28.

[m] Reference 36.

[n] Reference 37.

[o] Reference 33, based on constrained Hartree-Fock (CHF).

TABLE IV. Breathing mode energies ($\hbar\omega$ in MeV) for ^{40}Ca. A variety of methods are employed including constrained time-dependent Hartree-Fock (Ref. 1) (CTDHF) and modified random phase approximation (Ref. 40) (MRPA).

$T=$	0	1	2	3	4	5	6
ISOTHERMAL							
This work	21.6	21.5	20.4	17.5	14.0	11.7	10.6
SGII interaction							
CTDHF[1]			22		9		6
SkM interaction							
MRPA[40]	22.6	22.9	23.2	22.7	21.5	19.9	18.0
ISENTROPIC							
This work	21.6	21.5	20.8	19.0	16.9	15.5	14.7
JMZ interaction[41]							
TDHF[2]	~20.0						23.7
Dissipative Linear Response[42]			23.9[a]				

[a] The actual temperature is 2.3 MeV for this result in Ref. 42.

much faster than $\hbar\omega_S$ with T. At 6 MeV $\hbar\omega_S$ is 40% larger than $\hbar\omega_T$ for ^{40}Ca.

Where available we have presented results in Table IV obtained with other Hamiltonians and other methods. Considerable variation in the admittedly sparse set of results is observed. At $T=6$ MeV the $\hbar\omega_T$ for two similar (Skyrme-type phenomenological forces) has very different values: 6 and 18 MeV. Our result of 10.6 MeV falls between these cases. Note that the method used to obtain the $\hbar\omega_T=6$ MeV result[1] is essentially the same as ours so that the difference from our value is due to the choice of Hamiltonian.

The isentropic results for $\hbar\omega$ are of greater physical interest in relation to heavy ion experiments. However, there is little theoretical information available for this quantity from the previous literature. The very high value of 23.7 MeV at $T=6$ MeV for the Jaquaman-Mekjian-Zamick (JMZ) interaction may not be realistic in view of the fact that this interaction overbinds ^{40}Ca by 3 MeV/nucleon and yields an rms radius of 3.08 fm compared to the experimental rms radius of 3.48 fm.

In Table V we present a complete summary of our results for ^{16}O and ^{40}Ca as a function of T. As a general feature we note that all properties change rather slowly with the initial increase from $T=0$ to $T=1$ MeV. More rapid changes are observed thereafter reflecting the decrease in the importance of the shell effects and the increase in the importance of the vapor phase.

The first three columns contain properties previously reported for 6-shell calculations.[25,26] The minor differences of these large space results from the 6-shell results have been discussed in Ref. 43. We do not extend our calculations beyond 6 MeV where ^{16}O is unbound since we do not include a dynamical treatment of the gas phase. Methods for incorporating the gas phase have been used in Refs. 1 and 2.

We now comment on the incompressibilities in Table V. Again, it is important to specify the thermodynamic condition under which the incompressibility is evaluated. Since the ratio of the K_A's follows the square of the ratios of the $\hbar\omega$'s as seen through Eqs. (44) and (45), $K_A|_T$ falls much faster than $K_A|_S$ with T.

The thermal expansion coefficients in Table V are seen to increase by orders of magnitude from $T=1$ to $T=5$ MeV which reflects the approaching transition to a gas phase. In an infinite system these quantities would actually diverge at the liquid-gas phase transition. The fact that the values for the thermal expansion coefficients of ^{40}Ca are generally lower than those of ^{16}O at a given temperature is explained by the fact that a greater percentage of the particles in ^{16}O are in the last filled shell at zero temperature. This point was previously discussed in the context of the rms radius vs T.[25,26]

The specific heat at constant volume C_Q is an important thermodynamic coefficient especially at low T. Up to this point it has not appeared in discussions of theoretical or experimental results with finite nuclei. On the other hand specific heat defined as the simple derivative of the excitation energy with respect to temperature (no quantities held fixed)[44] and as the derivative at constant angular momentum have been evaluated.[45] Attempts to fully understand the nuclear equation of state from laboratory experiments must determine all these specific heats. We present our results for C_λ/A and C_Q/A in Table V along with their ratio.

VII. CONCLUSIONS

We have described a general method for evaluating large amplitude temperature-dependent TDHF dynamics in a single mode and have presented illustrative results in the small-amplitude regime. We have utilized a realis-

TABLE V. Thermodynamic coefficients for ^{16}O and ^{40}Ca.

					Monopole energy		Incompressibility		Thermal expansion		Specific heats			
	T (MeV)	BE/A (MeV)	S/A	$\langle r^2\rangle^{1/2}$ (fm)	$\hbar\omega_T$ (MeV)	$\hbar\omega_S$ (MeV)	$K_A\|_T$ (MeV)	$K_A\|_S$ (MeV)	β (MeV)$^{-1}$	β_s (MeV)$^{-1}$	C_{λ_1}/A	C_Q/A	C_{λ_1}/C_Q	η
^{16}O	0	7.981	0.0	2.558	24.73	24.73	98.2	98.2	0.0	0.0	0.0	0.0	1	1.016
	1	7.97	0.013	2.558	24.64	24.69	97.6	97.9	0.5×10^{-2}	-0.2×10^{-4}	0.069	0.069	1	1.016
	2	7.739	0.157	2.576	22.30	23.21	81.0	87.7	0.4×10^{-1}	-0.33×10^{-2}	0.38	0.35	1.08	1.016
	3	7.148	0.390	2.645	15.86	18.68	43.0	61.0	0.133	-0.056	0.86	0.61	1.42	1.014
	4	5.879	0.755	2.841	10.61	15.14	21.8	44.5	0.308	-0.319	1.80	0.88	2.03	0.995
	5	3.481	1.303	3.258	7.87	13.47	14.9	43.5	0.509	-0.982	3.24	1.11	2.93	0.936
	5.8[a]	0.575	1.871	3.787	6.80	13.32	13.8	52.9	0.593	-1.68	4.22	1.10	3.84	0.860
^{40}Ca	0	8.579	0.0	3.283	21.56	21.56	91.1	91.1	0.0	0.0	0.0	0.0	1.0	0.752
	1	8.550	0.0368	3.285	21.46	21.51	90.5	90.8	0.73×10^{-2}	-0.31×10^{-4}	0.126	0.125	1.0	0.753
	2	8.318	0.194	3.303	20.37	20.82	83.0	86.7	0.28×10^{-1}	-0.13×10^{-2}	0.35	0.33	1.04	0.759
	3	7.835	0.392	3.357	17.46	19.05	63.6	75.7	0.71×10^{-1}	-0.14×10^{-1}	0.67	0.57	1.19	0.767
	4	7.010	0.642	3.472	14.02	16.92	44.2	64.3	0.132	-0.6×10^{-1}	1.09	0.75	1.46	0.772
	5	5.824	0.933	3.662	11.75	15.46	34.2	59.2	0.184	-0.135	1.53	0.88	1.73	0.765
	6	4.326	1.250	3.915	10.63	14.72	31.3	60.0	0.212	-0.194	1.95	1.02	1.92	0.748

[a] At $T=5.9$ MeV, ^{16}O becomes unbound.

tic microscopic effective Hamiltonian and have compared with results from phenomenological Hamiltonians where available. The nonlocality present in our Hamiltonian due to the Brueckner G matrix and higher-order graphs gives rise to significant effects in the thermodynamic coefficients in ^{40}Ca.

It has been one of the major goals of this effort to indicate the relative ease with which these coefficients can be calculated in finite nuclei via thermal CHF calculations. Another goal has been to call attention to the dependence of these coefficients on the thermodynamic conditions. These coefficients probe the energy surface in independent directions and therefore serve as a physical basis for defining the nuclear equation of state. Furthermore, where results from other Hamiltonians are available, we have shown they are sensitive to details of the interaction. We strongly encourage attention to the issue of the experimental determination of these thermodynamic coefficients.

We close with the remark that the tendency we have found for a low incompressibility relative to previous results may provide a basis for understanding supernova explosions in certain models.[46]

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