Relativistic temperature-dependent Hartree-Fock calculation of spherical nuclei

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The temperature-dependent Hartree-Fock approach is extended to the relativistic quantum-field-theory framework; exchange of σ, ω, ρ, and π mesons and photons are included. Application is made to two spherical nuclei, ^{16}O and ^{40}Ca. Temperature dependences of excitation energies, single-particle spectra, charge densities, and entropies are evaluated and compared to corresponding nonrelativistic calculations. We find a considerably larger thermal response for these nuclei when compared to the nonrelativistic results.

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In recent years, stimulated by the heavy-ion physics and astrophysics, there has been a growing interest in the properties of highly excited nucleus [1–3]. At the laboratory level, these nuclei can be produced efficiently through the compound-nucleus reactions in heavy-ion collisions. Early attempts [4] of studying highly excited nuclei were carried out by statistical mechanical methods, level densities were calculated on the basis of single-particle levels obtained by schematic models, or more realistic models such as Woods-Saxon. Such a calculation is not self-consistent in that the result of level densities does not feed back to the single-particle energies, and also only the zero-temperature energy levels are used in the calculation. Later a temperature-dependent Hartree-Fock (TDHF) theory was developed for the Schrödinger equation for nonrelativistic nucleons interacting through static, two-body potentials. In most of these calculations [5,6] phenomenological effective zero-range forces were used. As the energies of experiments have been increasing, especially at energies attainable in the Relativistic Heavy-Ion Collider (RHIC), it is necessary to extend these studies to the relativistic realm. A recent covariant mean-field calculation [7] of nuclear matter at finite temperature is such an effort. In this work, however, we are concerned with a temperature-dependent relativistic approach for the finite nucleus.

Quantum relativistic field theories of nucleons, coupled to explicit mesonic degrees of freedom, have been successfully applied to a wide range of nuclear phenomena such as nuclear matter, neutron stars, finite nuclei and hypernuclei, as well as dynamic processes like nucleon-nucleus and electron-nucleus scattering [8]. In the nuclear structure problem, self-consistent Hartree (H) and Hartree-Fock (HF) calculations in relativistic mean-field theory have been shown to reproduce many ground-state and low-excited-state properties of the spherical nucleus. Recently these calculations [9–12] were successfully extended to the nonspherical nuclei. Examples range from light deformed nuclei in the *sd* shell to heavy deformed nuclei in the rare-earth region and include both even-even and odd-A nuclei.

In this work, using the framework of relativistic quantum theory, we extend the relativistic mean-field theory to a relativistic temperature-dependent Hartree-Fock (RTDHF) calculation to study the highly excited nuclei. We calculate results for two representative nuclei ^{16}O and ^{40}Ca, with special attention paid to the thermal response of these two nuclei.

It has usually been assumed that in the heavy-ion collision process these highly excited nuclei can reach thermal equilibrium, thus the method of quantum statistical mechanics can effectively be employed to study properties of hot nuclei. There are arguments about the validity of standard methods of quantum statistics mechanics when applied to a system which has a small number of particles, such as a nucleus. However, recent model studies of quantum spin chains have demonstrated that a quantum system with few degrees of freedom displays quantum-statistic behavior and can be described properly by the canonical ensemble in spite of the fact that only 2^7 states are presented in Hilbert space. So the validity of the quantum statistics mechanics in the present study is assumed.

In the mean-field approach, usually the grand canonical ensemble is employed. The use of grand canonical equilibrium for the description of excited nuclei is meaningful only when the nuclear temperature T is small compared to the chemical potential, so the occupation probabilities for unbound states are not so large as to lead to the nonequilibrium processes of particle emission; under this condition T is usually constrained below 5–6 MeV. This is also the limit we adopt for our study in this paper.

We start with the following Lagrangian which couples nucleons to four mesons (σ, ω, π, and ρ) and the photon (A^μ):

$$\begin{aligned}\mathcal{L}&=\mathcal{L}_F+\mathcal{L}_I\ ,\\ \mathcal{L}_I&=g_\sigma\bar{\Psi}\sigma\Psi-g_\omega\bar{\Psi}\omega^\mu\gamma_\mu\Psi-\frac{f_\pi}{m_\pi}\bar{\Psi}\gamma_5\gamma^\mu\tau\Psi\partial_\mu\pi\\ &\quad-g_\rho\bar{\Psi}\rho^\mu\tau\gamma_\mu\Psi-e\bar{\Psi}\gamma_\mu\tfrac{1}{2}(1+\tau_3)A^\mu\Psi\ .\end{aligned}\tag{1}$$

Note that we adopt the pseudovector (PV) coupling for the pion, since the relativistic nuclear matter HF calculation and other considerations favor this coupling scheme [13]. From this Lagrangian the Hamiltonian can be ob-

tained by the usual procedure; then by using Green's functions to express the meson fields in terms of the nuclear sources, the Hamiltonian can be expressed in terms of the nucleon fields only [10]. Then quantizing the nucleon field we get the following Hamiltonian:

$$H=\sum_{\alpha\beta}\langle\alpha|T|\beta\rangle C_\alpha^\dagger C_\beta+\tfrac{1}{2}\sum_{\alpha\beta\gamma\delta}\langle\alpha\beta|V|\delta\gamma\rangle C_\alpha^\dagger C_\beta^\dagger C_\gamma C_\delta\ , \tag{2}$$

$$T=-i\gamma_0\boldsymbol{\gamma}\cdot\boldsymbol{\nabla}+\gamma_0 M\ ,$$

$$V=V_v+V_s+V_e\ ,$$

$$V_s=-g_\sigma^2\gamma_0(1)\gamma_0(2)\frac{e^{-m_\sigma r}}{4\pi r}+g_\omega^2\gamma_0(1)\gamma_0(2)\gamma_\mu(1)\gamma^\mu(2)\frac{e^{-m_\omega r}}{4\pi r}\ , \tag{3}$$

$$V_v=\tau(1)\cdot\tau(2)\left[g_\rho^2\gamma_0(1)\gamma_0(2)\gamma_\mu(1)\gamma^\mu(2)\frac{e^{-m_\rho r}}{4\pi r}+\left[\frac{f_\pi}{n_\pi}\right]^2\gamma_0(1)\gamma_5(1)\gamma^\mu(1)\gamma_0(2)\times\gamma_5(2)\gamma_\nu(2)\partial_\mu(1)\partial^\nu(2)\frac{e^{-m_\pi r}}{4\pi r}\right]\ ,$$

$$V_e=\tfrac{1}{4}[1+\tau_3(1)][1+\tau_3(2)]e^2\gamma_0(1)\gamma_0(2)\gamma_\mu(1)\gamma^\mu(2)\frac{1}{4\pi r}\ .$$

The retardation effect in the exchange terms of Eq. (3) is neglected for simplicity; however, according to our calculation [14] this effect is small for the light nuclei, and for the purpose of this investigation its effect should be negligible.

The greek letters in Eq. (2) denote the set of quantum numbers characterizing the single-particle states. Since we consider spherical nuclei, j (angular momentum), and its third component m are good quantum numbers, along with t_3 (third component of isospin) and π (parity), i.e., $\alpha=\alpha\,(t_3,\pi,j,m)$. Single-particle states are expanded in a spherical basis $|i\rangle$ as

$$|\alpha\rangle=\sum_i c_i^\alpha|i\rangle\equiv\sum_n c_n^\alpha\begin{bmatrix} i\dfrac{G_{n\kappa}(r)}{r}\phi_{\kappa m}(\hat{r}) \\ -\dfrac{F_{n\kappa}(r)}{r}\phi_{-\kappa m}(\hat{r})\ . \end{bmatrix} \tag{4}$$

In principle, we can choose any complete orthogonal set for the basis functions, for example, spherical harmonic oscillator wave functions. However, in this work we choose a basis which is the set of solutions of a Dirac equation with a potential as close as possible to that of the nucleus in question, since our earlier study [10] showed that a good basis can reduce the number of terms required in the expansion when the convergence test is performed. Another merit of our basis is that it has a realistic asymptotic behavior. We employ the same basis states as we used in Ref. [10], namely, the set of Hartree solutions for the same nucleus. For the highly excited states, it is crucial that the continuum should be properly included. The basis states in the continuum have been discretized by confining all wave functions within a large sphere ($R=10$ fm), then imposing the linear boundary condition of the MIT bag model. Our results showed for the nuclear ground state ($T=0$) that the artificial boundary condition had a very small effect for states near the Fermi surface when compared with states satisfying the true boundary condition; for those deep inside there are almost no effects at all. By extension we believe that the effect of the boundary will be similarly small for the self-consistent states resulting from our calculation, and this gives us a convenient way to deal with the continuum.

We consider the ground state of an A particle system is in the form

$$|\phi_g\rangle=\prod_{\alpha=1}^{A}C_\alpha^\dagger|0\rangle\ . \tag{5}$$

In the finite temperature we have the following contractions [15]:

$$C_\alpha^\dagger C_\beta=n_\alpha\delta_{\alpha\beta}\ ,$$
$$C_\beta C_\alpha^\dagger=(1-n_\alpha)\delta_{\alpha\beta}\ . \tag{6}$$

Here n_α is the mean occupation number for the single-particle state α.

The grand potential can be written as

$$\Omega=\langle\langle H\rangle\rangle-\mu\langle\langle N\rangle\rangle-TS\ . \tag{7}$$

Here $\langle\langle H\rangle\rangle$ and $\langle\langle H\rangle\rangle$ are the ensemble average of the Hamiltonian and the number operator, μ is the chemical potential, S is the entropy, and T is the temperature. As is conventional, temperature T is given in energy units in this work.

TABLE I. Parameters of Lagrangian. The meson masses are in MeV, the coupling constants are dimensionless.

m_σ	m_ω	m_ρ	m_π	g_σ^2	g_ω^2	g_ρ^2	f_π^2
520	783	770	138	100.0	141.6	5.89	0.9771

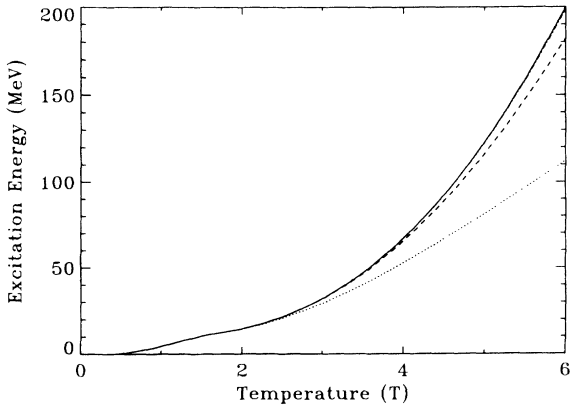

FIG. 1. Excitation energies of ^{40}Ca. Dotted line is four, dashed line is six, dot-dashed line is eight, and solid line is ten major shell basis.

In the HF calculation, the entropy S is given by the form for a system of noninteracting fermions:

$$S=-\sum_{\alpha}\{n_{\alpha}\ln n_{\alpha}+(1-n_{\alpha})\ln(1-n_{\alpha})\} . \tag{8}$$

By minimizing the grand potential Ω with respect to the mean occupation number we are able to obtain the distribution function (9); and by minimizing the grand potential with respect to the single-particle wave functions (in our case the expansion coefficients), with the constraint that the wave function be normalized, we can get the finite temperature Hartree-Fock equation (10):

$$n_{\alpha}=\frac{1}{1+\exp[(\epsilon_{\alpha}-\mu)/kT]} , \tag{9}$$

$$\sum_{i_1'}\Bigg[\langle i|T|i_1'\rangle+\sum_{\alpha}n_{\alpha}\Bigg\{\sum_{i_2i_2'}c_{i_2}^{\alpha*}\langle ii_2|V_s|i_1'i_2'\rangle c_{i_2'}^{\alpha}+(-1)^{t_3(\gamma)-1/2}\sum_{i_2i_2'}c_{i_2}^{\alpha*}(-1)^{t_3(\alpha)-1/2}\langle ii_2|V_v|i_1'i_2'\rangle c_{i_2'}^{\alpha}$$
$$+[t_3(\gamma)+\tfrac{1}{2}]\sum_{i_2i_2'}c_{i_2}^{\alpha*}[t_3(\alpha)+\tfrac{1}{2}]\langle ii_2|V_e|i_1'i_2'\rangle c_{i_2'}^{\alpha}$$
$$-\delta_{t_3(\alpha),t_3(\gamma)}\sum_{i_2i_2'}c_{i_2}^{\alpha*}\langle ii_2|V_s|i_2'i_1'\rangle c_{i_2'}^{\alpha}-\delta_{t_3(\alpha),t_3(\gamma)}\sum_{i_2i_2'}c_{i_2}^{\alpha*}\langle ii_2|V_v|i_2'i_1'\rangle c_{i_2'}^{\alpha}$$
$$-[t_3(\gamma)+\tfrac{1}{2}]\sum_{i_2i_2'}c_{i_2}^{\alpha*}[t_3(\alpha)+\tfrac{1}{2}]\langle ii_2|V_e|i_2'i_1'\rangle c_{i_2'}^{\alpha}$$
$$-2\delta_{t_3(\gamma),-t_3(\alpha)}\sum_{i_2i_2'}c_{i_2}^{\alpha*}\langle ii_2|V_v|i_2'i_1'\rangle c_{i_2'}^{\alpha}\Bigg\}\Bigg]c_{i_1'}^{\gamma}=\epsilon^{\gamma}c_{i}^{\gamma} . \tag{10}$$

Now at a certain temperature T, for a given set of single-particle states, and restricting the average particle number to be the number of nucleons in the nucleus,

$$\langle N\rangle=\sum n_{\alpha}=A , \tag{11}$$

we can determine the chemical potential μ. Therefore Eqs. (9)–(11) form a set of equations which can be solved self-consistently by the method of iterations. A stable solution can usually be reached within 30 iterations; the criterion for a stable solution we used is that the difference of all single-particle energies during several successive iterations should be less than 5 keV. In actual calculations, we determine the proton and neutron chemical potentials separately from proton and neutron number Z and N.

Before we solve the HF equation (10), we must determine the parameters in the Lagrangian (1). In this work we use parameters fitted to nuclear matter data [16]; they are also successfully used to calculate both spherical and nonspherical nuclei at zero temperature [11,14]. These parameters are shown in Table I.

In a practical calculation, the expansion basis (4) must be truncated after a fixed number of N basis states. Any reliable results should be independent of N, so the number N must be large enough to ensure that satisfactory convergent solution is reached. One should notice, however, that as the temperature increases more highly excited single-particle states will contribute in the distribution function (9); thus it is conceivable that a larger basis is required for a higher temperature. Therefore to test convergence we first calculate the ^{40}Ca excitation energy $E^*(T)=E(T)-E(0)$ from $T=0$ to 6 MeV by using bases of four, six, eight, and ten major shell wavé functions, respectively. The result is shown in Fig. 1. As one can see by using the eight major shell basis the results converge nicely within the temperature range considered in this work. We remark that at $T=0$ a four major shell basis is good enough for ^{40}Ca, which is about one-fifth of the number of states in an eight major shell basis. In the following all the results are obtained by using eight major shells.

We display the neutron single-particle spectra of ^{16}O and ^{40}Ca as a function of temperature in Figs. 2 and 3. One can easily notice that the thermal response of ^{16}O is greater than ^{40}Ca. This can be understood if one realizes that most contributions of thermal response come from

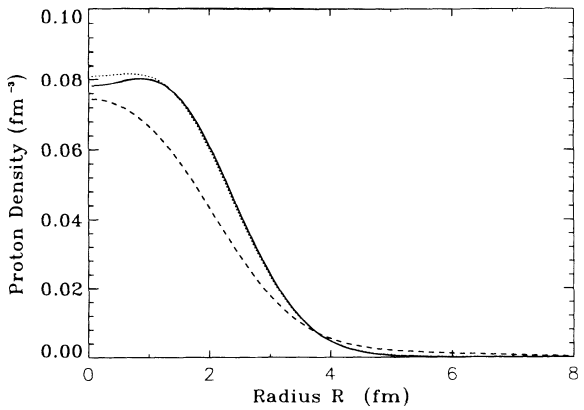

FIG. 2. Neutron single-particle spectrum of ^{16}O.

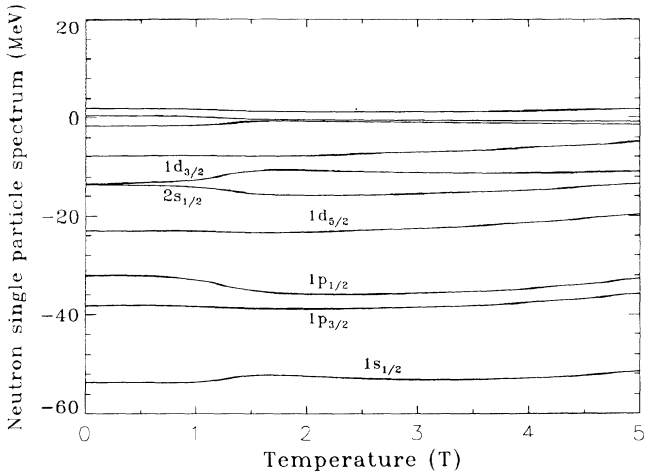

FIG. 3. Neutron single-particle spectrum of ^{40}Ca.

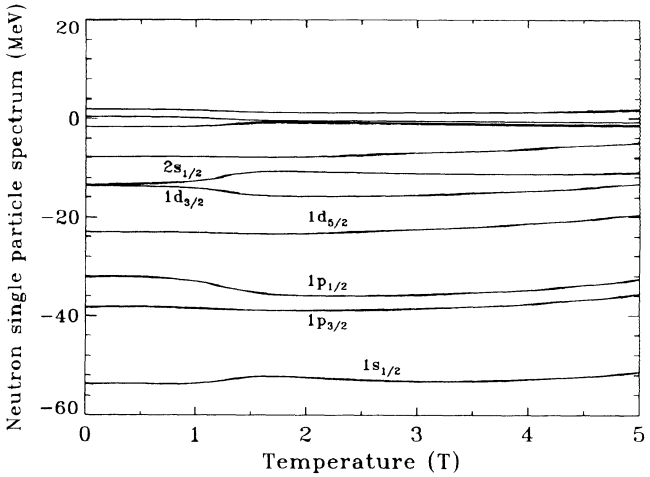

FIG. 5. Charge densities of ^{40}Ca. Solid line is zero, dotted line is 2.5, and dashed line is 5 MeV temperature.

the last filled shell near the Fermi surface at zero temperature, since the particles of last filled shell of ^{16}O compose a large proportion of the total number of particles, this nucleus is prone to get excited. When compared to the nonrelativistic self-consistent calculations [1,5], our results show a greater thermal response for the same nuclei.

In Figs. 4 and 5 the proton charge densities of ^{16}O and ^{40}Ca are shown with $T=0$, 2.5, and 5 MeV. One interesting feature of ^{40}Ca is that as temperature increases from 0 to 2.5 MeV, the charge density in the central region is significantly depressed; however, as T goes from 2.5 to 5 MeV it picks up again. This can be explained in the following way: When ^{40}Ca is moderately heated ($T=2.5$ MeV) the $2s_{1/2}$ state, which has a large contribution to the density at the center and is very close to the Fermi surface at $T=0$, becomes greatly depopulated, thus leaving a "cavity" in the center of the nucleus; as T reaches higher values ($T=5$ MeV) there are higher $ns_{1/2}$ states participating in the excitation; thus the "cavity" is somewhat filled in. We also observe that as higher single-particle states join in when T increases, the nuclear surface is pushed out, which indicates a possible dissolution of the nuclear surface. Our results contrast sharply with the nonrelativistic calculation using a zero-range nuclear force [5], where nuclear surface does not change at all, even at $T=5$ MeV, as compared to $T=0$, and the proton density is unchanged beyond $R=3$ fm. Our results are, however, qualitatively in agreement with the nonrelativistic calculation using realistic effective nuclear forces [1], although we find a greater thermal response. For example, the excitation energy found at $T=5$ MeV is 83, 100, and 123 MeV in Ref. [5], in Ref. [1], and in this work, respectively. This seems to confirm the conclusion that the phenomenological zero-range nuclear force shows a smaller thermal response.

The last point we have investigated is the importance of self-consistency in the temperature-dependent calculation. To do this, we calculate the entropy S in two ways; one is in a completely self-consistent manner (S1), the other (S2) is calculated using the set of occupation numbers n_α obtained from Eq. (9) but with a fixed single-particle spectrum, which is chosen to be the zero-temperature spectrum. The results are shown in Fig. 6

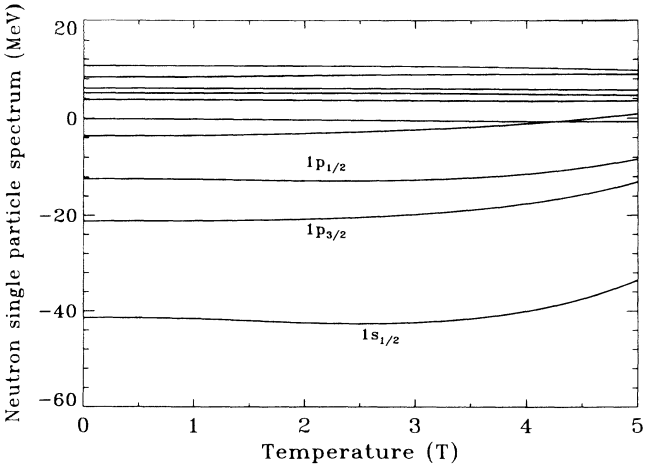

FIG. 4. Charge densities of ^{16}O. Solid line is zero, dotted line is 2.5, and dashed line is 5 MeV temperature.

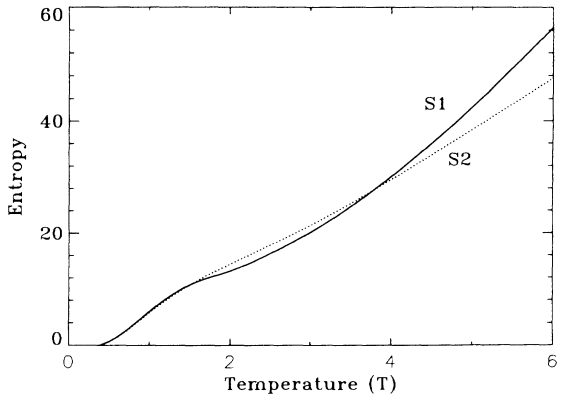

FIG. 6. Entropy of ^{40}Ca as a function of temperature.

for ^{40}Ca. We find S1 and S2 are almost identical at low temperature ($T < 1.5$ MeV); however, at higher temperature there is substantial deviation, especially when T is greater then 5 MeV. We stress that self-consistency is important in the temperature-dependent HF calculations. Entropy is particularly interesting due to its relation with the nuclear energy level density. According to this calculation, we conclude that at low temperatures, $T < 1.5$ MeV, one could use the zero-temperature spectrum to calculate the level density, as in some earlier works [4].

To summarize, we have extended the TDHF to the relativistic framework. We have performed a thorough convergence test to validate our calculation in the temperature range 0–5 MeV. Our results predict substantially greater thermal response for light nuclei as compared to the previous, nonrelativistic TDHF calculations.

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[1] G. Bozzolo and J. P. Vary, Phys. Rev. Lett. **53**, 903 (1984); Phys. Rev. C **31**, 1909 (1985).

[2] H. G. Miller, B. J. Cole, and R. M. Quick, Phys. Rev. Lett. **63**, 1922 (1989); H. G. Miller, R. M. Quick, and B. J. Cole, Phys. Rev. C **39**, 1599 (1989).

[3] P. F. Bortignon, A. Bracco, D. Brink, and R. A. Broglia, Phys. Rev. Lett. **67**, 3360 (1991); B. Lauritzen and J. W. Negele, Phys. Rev. C **44**, 729 (1991); S. Shlomo and J. B. Natowitz, Phys. Lett. B **252**, 187 (1990).

[4] P. B. Kahn and N. Rosenzweig, Phys. Rev. **187**, 1193 (1969); L. G. Moretto, Nucl. Phys. **A182**, 641 (1972). R. Vandenbosch and U. Mosel, Phys. Rev. Lett. **28**, 1726 (1972); V. S. Ramamurthy and S. S. Kapoor, Phys. Lett. **42B**, 399 (1972).

[5] U. Mosel, P.-G. Zint, and K. H. Passler, Nucl. Phys. **A236**, 252 (1974).

[6] M. Brack and P. Quentin, Phys. Lett. **52B**, 159 (1974).

[7] R. J. Furnstahl and B. D. Serot, Phys. Rev. C **41**, 262 (1990).

[8] B. D. Serot and J. D. Walecka, Adv. Nucl. Phys. **16**, 1 (1986).

[9] Suk-Joon Lee, J. Fink, A. B. Balantekin, M. R. Strayer, A. S. Umar, P.-G. Reinhard, J. A. Maruhn, and W. Greiner, Phys. Rev. Lett. **23**, 2916 (1987); W. Pannert, P. Ring, and J. Boguta, *ibid.* **59**, 2420 (1987); Y. K. Gambhir and P. Ring, Phys. Lett. B **202**, 5 (1988); W. Koeph and P. Ring, *ibid.* **212**, 397 (1988); C. E. Price and G. E. Walker, Phys. Rev. C **36**, 354 (1987); R. J. Furnstahl, C. E. Price, and G. E. Walker, *ibid.* **36**, 2590 (1987); Jian-Kang Zhang and D. S. Onley, Phys. Lett. B **209**, 145 (1988).

[10] Jian-Kang Zhang and D. S. Onley, Nucl. Phys. **A526**, 245 (1991).

[11] Jian-Kang Zhang and D. S. Onley, Phys. Rev. C **43**, R942 (1991).

[12] R. V. Jensen and R. Shankar, Phys. Rev. Lett. **54**, 1879 (1985).

[13] C. J. Horowitz and B. D. Serot, Nucl. Phys. **A399**, 529 (1983); A. Bouyssy, J.-F. Mathiod, Nauyen Van Giai, and S. Marcos, Phys. Rev. C **36**, 380 (1987).

[14] Jian-Kang Zhang and D. S. Onley, Phys. Rev. C **44**, 1915 (1991).

[15] A. L. Fetter and J. D. Walecka, *Quantum Theory of Many-Particle Systems* (McGraw-Hill, New York, 1980).

[16] P. G. Blunden and M. J. Iqbal, Phys. Lett. B **196**, 295 (1987).