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The Nuclear Matter Saturation Problem

Zagadnienie wysycania materii jądrowej

Проблема насыщения ядерной материи

INTRODUCTION

The general systematics of nuclear binding energies are well parameterised by the semi empirical mass formula. The volume term in this formula predicts that, in absence of coulomb interactions, an infinite, homogeneous fluid of equal numbers of neutrons and protons will be self bound with a binding energy per nucleon of $E_o \simeq 16 \pm 0.5$ MeV. The symmetry term in the semi empirical mass formula predicts an energy cost of 32 MeV/nucleon in moving away from neutron-proton symmetry. Measurements of the central densities of heavy nuclei suggest that the infinite nuclear matter fluid will saturate at a density $\rho_o \simeq 0.17 \pm 0.01$ nucleons per fm^3 corresponding to a Fermi wave number $k_F \simeq 1.37 \pm 0.03$ fm^{-1}. While it is difficult to unambiguously separate bulk and surface effects, the observation of 'breathing mode' excitations at 12-15 MeV excitation energy in nuclei suggests a bulk compressibility modulus for the nuclear matter fluid

$$K = 9\rho^2 \left.\frac{\partial^2 E}{\partial \rho^2}\right|_{\rho} \simeq 250 \pm 50 \text{ MeV} \qquad (1)$$

Attempts by nuclear many-body theorists to explain this data have a long and frustrating history which we shall review in this short communication.

BRUECKNER AND THE COESTER LINE

The simplest model for nuclear matter is a fluid of non relativistic neutrons and protons interacting through a two-body potential. The hamiltonian is then

$$H = \sum_i -\frac{\hbar^2}{2m}\nabla_i^2 + \sum_{i>j} V_{ij} \qquad (2)$$

The two-body potential must fit the nucleon-nucleon scattering phase shifts and the bound state deuteron properties. There are a number of such 'phase equivalent' potentials on the market. They are either completely phenomenological in nature or guided to a greater or lesser extent by meson exchange models. In general these potentials have a long range one-pion-exchange tail, an intermediate range at which they are attractive, and which is frequently attributed to an enhanced two-pion-exchange, and a short range repulsive core, which may be attributed to vector ρ- and ω-meson exchange. There is clear evidence for the non central nature of the interaction and the observed quadrupole moment of the deuteron would appear to require a tensor force, although there is continuing debate as to the strength of the tensor term.

Whatever the details of the interaction, the strength of the repulsive core alone precludes a direct application of the Hartree-Fock prescription for handling many fermion systems. In the Hartree-Fock prescription a trial wave function in the form of a Slater determinant

$$\Phi = (A!)^{-\frac{1}{2}} \det \phi_i(\underline{x}_j) \qquad (3)$$

is chosen and the expectation value of the hamiltonian (2) is optimised with respect to the single-particle basis ϕ_i. This leads to the equations

$$-\frac{\hbar^2}{2m}\nabla_1^2\phi_i(\underline{x}_1) - \sum_j \int \phi_j^*(\underline{x}_2)\, V(\underline{x}_1,\underline{x}_2)\,[\phi_i(\underline{x}_1)\phi_j(\underline{x}_2) - \phi_i(\underline{x}_2)\phi_j(\underline{x}_1)]d\underline{x}_2 = \epsilon_i\,\phi_i(\underline{x}_1) \qquad (4)$$

for the single-particle basis, and for the ground-state energy expectation value

$$E_o = \frac{1}{2}\sum_i \int \phi_i^*(\underline{x})\left[-\frac{\hbar^2}{2m}\nabla^2 + \epsilon_i\right]\phi_i(\underline{x})\,d\underline{x} \qquad (5)$$

The trial wave function (3) describes a system of particles whose motion is correlated with that of its neighbours only through a mean field. In the nuclear matter problem the strong short-range forces induce two-body correlations which cannot be ignored.

Keith Brueckner attempted to account for those correlations by allowing pairs of particles to undergo multiple scatterings and summing the so called 'ladder diagrams', thus generating a reaction matrix.

$$\langle ij|G|ij\rangle = \langle ij|V|ij\rangle + \sum_{ab}{}' \frac{|\langle ij|V|ab\rangle|^2}{E_{abij}} \qquad (6)$$

The prime on the summation in eqtn (6) denotes that the intermediate states ϕ_a, ϕ_b must honour the Pauli principle and be unoccupied in the uncorrelated ground state Φ of eqtn (3). The energy denominators of eqtn (6) can be written

$$E_{abij} = \epsilon_a + \epsilon_b - \epsilon_i - \epsilon_j \qquad (7)$$

The basis of single-particle states occupied in Φ is now given by

$$-\frac{\hbar^2}{2m}\nabla_1^2\phi_i(\underline{x}_1) + \sum_j \int \phi_j^*(\underline{x}_2)\, G(\underline{x}_1\underline{x}_2)\,[\phi_i(\underline{x}_1)\phi_j(\underline{x}_2) - \phi_i(\underline{x}_2)\phi_j(\underline{x}_1)]d\underline{x}_2 = \epsilon_i\,\phi_i(\underline{x}_1) \qquad (8)$$

and the lowest order expression for the ground-state energy expectation value is

$$E_o^{(1)} = \tfrac{1}{2}\sum_i \int \phi_i^*(\underline{x})\left[-\frac{\hbar^2}{2m}\nabla^2 + \epsilon_i\right]\phi_i(\underline{x})d\underline{x} \qquad (9)$$

Because of the structural similarity of eqtns (8) and (9) to eqtns (4) and (5), this approach is called the Brueckner-Hartree-Fock prescription (BHF). It must be remembered however, that the true Hartree-Fock prescription is based upon the variational principle while the BHF prescription simply represents the lowest order term in a partially summed perturbation theory expansion. The discerning reader will have noted that I have not fully defined the BHF approach because I have not defined the basis of single-particle states unpopulated in Φ which are required in the summation of eqtn (6). The only safe choice is to use a system of plane waves orthogonalised to the states occupied in Φ and to calculate the single particle energies ϵ_a and ϵ_b as expectation values of the kinetic energy operator. A justification of this approach may be that the interaction V is so strong that it scatters particles so far out of the Fermi sea that their potential energy is negligible compared with their kinetic energy.

Going beyond lowest order perturbation theory it is conventional to rearrange the series so that it is no longer in order of ascending powers of the reaction matrix but rather in ascending order of the number of vacancies in the Fermi sea - the so called 'hole-line' expansion. For a central, repulsive hard-core potential of radius r_c the hole-line expansion can be shown to converge with powers of the small parameter

$$\kappa = (r_c/r_o)^3 \qquad (10)$$

where the density of the nuclear fluid is

$$\rho = [4/3\ \pi r_o^3]^{-1} \qquad (11)$$

At the nuclear saturation density ρ_o we have $r_c/r_o \simeq 1/3$ and converge of the hole-line expansion would seem assured.

The results of BHF calculations for a wide range of phase equivalent potentials are summarised in Figure 1.

The results for a wide range of phase equivalent potentials scatter about the line AB, known as the Coester line, and most certainly do not account for the semi empirical mass formula data represented by the black triangle. It is possible to choose a nucleon-nucleon potential which will saturate at the correct density but this fails to give sufficient binding energy. It

is possible to choose a potential which will provide sufficient binding energy, but then it will saturate at too high a density.

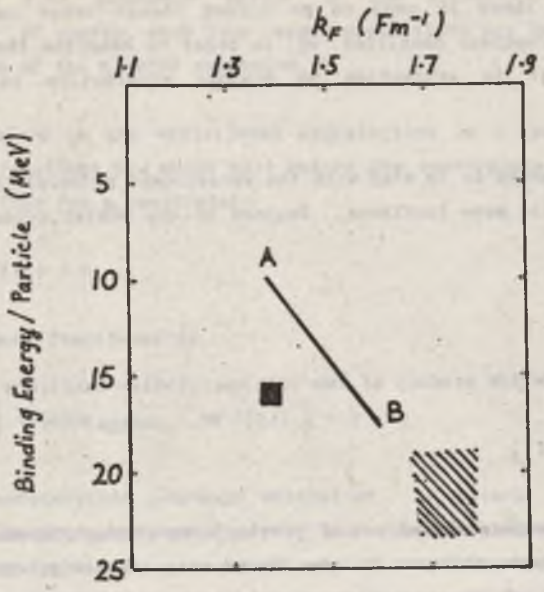

Fig 1 The saturation of nuclear matter. The black rectangle represents the predictions of the semi empirical mass formula. The line AB is known as the Coester line. The results of BHF calculations for nuclear matter with a wide range of phase equivalent potentials scatter about this line.

A closer examination of the results of BHF calculations shows that it is the tensor force which plays an important role in producing saturation. Thus it is no surprise to learn that those bare nucleon-nucleon interactions which have a strong tensor force saturate first and yield results at the upper end A of the Coester line while the results with interactions containing weak tensor forces cluster towards the lower end B.

JASTROW CORRELATIONS: BRUECKNER JUSTIFIED?

Given the complexity of a fully self-consistent BHF calculation, particularly if there is need to go beyond lowest order as might be required at supernuclear densities, eg. in order to describe the core of a neutron star, it is attractive to explore alternative calculational procedures.

One possibility would be to stay with the variational principle and improve the choice of trial wave functions. Instead of the Slater determinant (3) consider

$$\Psi = F\Phi \tag{12}$$

where F is a symmetric product of two-body correlation functions

$$F = \prod_{i>j} f_{ij} \tag{13}$$

designed to accommodate the effect of particularly strong components of our nucleon-nucleon interaction. In the Jastrow approximation the f_{ij} are central functions of the separation between the pair of particles which reduce the two-body wave function at short distances, where the repulsive core forces the particles apart, and which heal to unity at large distances where the interactions are extremely weak.

The full wave function (12) is extremely difficult to work with and it is usual to make some form of cluster expansion of F based upon the relatively low density of the nuclear matter problem as measured by the small parameter κ (10). The problem then is that, if the cluster expansion is terminated at any finite order and the correlation functions f_{ij} freely varied, the energy functional

$$E([F]) = \langle\Psi|H|\Psi\rangle_{Approx} \tag{14}$$

will not saturate, the so called Fmery problem. The notation $\langle\ \rangle_{Approx}$ means that the expectation value in some limited cluster expansion approximation. This problem can be traced to the fact that, in searching for a lower bound to the energy in the variational calculation, one can increase the radius of the wound in the correlated two-body wave function

to completely eliminate the repulsive core and at the same time reduce the rate of healing of the correlation function so that the kinetic energy is negligible. Then we can adjust the long range part of the correlation function to give unbounded weight to the attractive tail of the interaction. Of course, such long range correlations are inconsistent with a termination of the cluster expansion.

What is required in the variational calculations is a constraint on the correlation functions f_{ij} which will ensure the convergence of the cluster expansion. Then for a constraint

$$g([f]) = 0 \tag{15}$$

the variational functional is

$$\delta \int \left\{ \langle \Psi | H | \Psi \rangle_{Approx} - \lambda g([g]) \right\} = 0 \tag{16}$$

with λ an undetermined Lagrange multiplier. A natural choice for the constraint is that it should retain the convergence properties of the hole-line expansion. This can be achieved by requiring that on average the wound volume around any given nucleon contain at most one further nucleon, thus making the restriction to two-body clusters very plausible. Such calculations are generally called lowest order constrained variational calculations (LOCV).

When LOCV calculations are performed for a wide range of phase equivalent nucleon-nucleon interactions the results agree to an impressive extent with BHF calculations using the same potentials. The Coester line is reproduced and once more the saturation predictions disagree with the semi-empirical mass formula.

We note that both LOCV and BHF calculations not only fail to reproduce nuclear matter saturation but that they predict very high compressibilities, typically $K \approx 400$ MeV which is inconsistent with the observation of breathing mode excitations at 12-15 MeV in nuclei.

TENSOR CORRELATIONS: THE MYSTERY, AND THE BINDING-ENERGY, DEEPENS

The full variational principle states that the results of some restricted variational calculation will be an upper bound to the true ground state energy and that the calculated ground state should approach the hamiltonian eigenstate as the restrictions on the scope of the variational calculation are removed. Within the class of LOCV calculations the simplest relaxation would be to free the form of the two-body correlation functions f_{ij}.

The form of our two-body potentials is

$$V_{ij} = \sum_{\lambda} V^{\lambda}{}_{ij} \tag{17}$$

where in different reaction channels λ we have the freedom to include central, tensor, spin-orbit and quadratic spin-orbit forms as appropriate. It seems natural to accord the correlation functions the same degrees of freedom and write

$$f_{ij} = \sum_{\lambda} f_{ij}{}^{\lambda} \tag{18}$$

with

$$f_{ij}{}^{\lambda} = f_C{}^{\lambda}(r_{ij}) + f_T{}^{\lambda}(r_{ij})\, S_{ij} + f_{LS}{}^{\lambda}(r_{ij})\, \underline{L}.\underline{S} + f_Q{}^{\lambda}(r_{ij})(\underline{L}.\underline{S})^2 \tag{19}$$

For all singlet states there are no tensor or spin-orbit terms and thus λ is simply the partial wave $L = \underline{l}_i - \underline{l}_j$, for the triplet states with J=L again λ is simply the partial wave but triplet state with $J = L+1$ are coupled to the partial wave $L' = L+2$ states by the tensor force, eg, $^3S_1$-$^3D_1$, $^3P_2$-$^3F_2$ etc, and in these cases λ refers to the two orthogonal reaction channels associated with the pairs of partial waves.

Since the new correlation functions are designed not simply to take into account the wound in the two-body wave functions produced by the repulsive core of the two-body interaction but also any other possible strong correlations induced by other elements of the force, the constraint used in the Jastrow cluster expansion no longer seems appropriate.

The single-particle energies ϵ_i in the original Hatree-Fock approach (4) are themselves Lagrange multipliers chosen to assure the orthonormality of the single particle functions ϕ_i and hence the normalisations of the trial many-body function Φ (3). In this we shall use as our constraint (15) the normalisation of our two-body correlated wave functions.

$$\Psi_{ij} = f_{ij}\,(2!)^{-\frac{1}{2}} \det \phi_i\,(\underline{x}_j). \tag{20}$$

Later we shall check the convergence of our cluster expansion and show that our termination in lowest order is valid. One consequence of our change in constraint is that because Ψ_{ij} contains a wound at short distances, then, in order to be normalised, f_{ij} must overshoot unity in a region where the interaction is attractive and hence we shall get a slightly increased binding energy.

It has been known for many years that in perturbation theory the tensor force converges relatively slowly. This was recognised by Kuo and Brown in their analysis of the effective central $^3S_1$ interaction in nuclei where they wrote

$$\langle {}^3S_1|V^{eff}|{}^3S_1\rangle = \langle {}^3S_1|V_C|{}^3S_1\rangle + \sum_n \frac{|\langle {}^3S_1|V_T S_{12}|n^3D_1\rangle|^2}{\Delta E n} \,. \tag{21}$$

Using an approximate closure argument $\langle {}^3S_1|S_{12}^2|{}^3S_1\rangle = 8$ they obtained the result

$$V^{eff}_{{}^3S_1} \simeq V_C^{{}^3S_1} + 8V_T^2/E_{eff} \tag{22}$$

Kuo and Brown reasoned that E_{eff} was 200-300 MeV and that this second order tensor contribution yielded a considerable increase in the attractiveness of the $^3S_1$ effective interaction. By putting tensor components directly into our trial wavefunction we include these effects and many more. It transpires that it is the tensor components in the correlation functions (19) which are the really significant new feature and we shall not refer further to the spin-orbit components.

When the new LOCV calculations are carried out for the same range of phase equivalent potentials the results cluster in the cross hatched box in figure 1. Now the results for various phase equivalent potentials are very

similar, instead of being spread along the Coester line they are all grouped together. This is not surprising, we would expect the effect of tensor correlations to be largest for those interactions with strong tensor forces, ie those which were at the end A of the Coester line, and least for those with the weakest tensor forces.

Recently perturbation calculations based on the hole-line expansion have been extended to fourth and fifth order confirming the results of these generalised LOCV calculations. The bad news is that the results of the cross hatched area do not overlap the empirical black rectangle. In addition the compression modulus remains uncomfortably high with $K \geq 350$ MeV for most of the phase equivalent potentials.

Perhaps the most alarming aspect of the results is that the variational calculations predict binding which is greater than the empirical value. This phenomena has happened at least once before in the history of physics. As variational calculations for atomic structure calculations were refined there came a time when the Schrodinger equation for the helium atom yielded a ground state energy below that which was experimentally observed. This violates the upper bound condition of the variational principle. The solution to this apparent paradox is that the model being used must incompletely describe the physics being investigated. In the case of the helium atom the breakdown was traced to the inadequacy of the non relativistic Schrödinger equation. In the next section we shall explore the missing element in the nuclear matter problem.

ISOBARS TO THE RESCUE

Let us review our model which consists of a fluid of non relativistic nucleons interacting through pair potentials. The potentials necessarily contain tensor forces and these we know can be generated by the exchange of pions. So at root our model is a soup of nucleons and pions. The π-nucleon scattering cross section is dominated by a broad resonance at $\sim$ 300 MeV. This is variously referred to as the 3-3 resonance, the Δ particle or the $N^*(1232)$ isobar. Thus it would seem natural to generalise our trial wave function to allow for the possibility that our nucleons may become excited into N^* isobar states. This economically achieved by extending our correlation function (19)

$$f_{ij}^{\lambda} \rightarrow f_{ij}^{\lambda} + f_C^{\lambda}(r_{ij}) + f_T^{\lambda}(r_{ij}) S_{ij} + f^{\lambda}(r_{ij})\, S_{ij}^{II} \qquad (23)$$

where S_{ij}^{II} is the generalised tensor operator connecting the two-component nucleon spinner to the four component spin $^3/_2$ isobar. Such a term arises first in the coupling of the $^1S_0(NN)$ channel to the $^5D_0(NN^*)$ channel. The analogy with the tensor correlations is now complete and is exhibited graphically in figure 2.

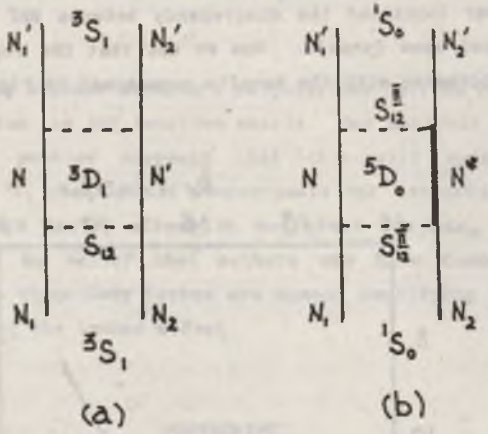

Fig 2 a) The intermediate D-state admixture in the two nucleon $^3S_1$ channel induced by a tensor force, eg, one-pion-exchange.

b) The intermediate D-state N-N* (represented by the heavy line) induced by a one-pion-exchange interaction in the $^1S_0$ nucleon-nucleon channel.

Naturally our hamiltonian must now be extended to include the isobar channels and this is done using the N-N* potentials of Green, Sanio and Niskanen based on the π-N production of N* as analysed by Arenhovel.

The contribution of figure 2b to the N-N $^1S_0$ scattering amplitude is subsumed into the phenomenological potential fits and is responsible for a significant part of the attraction in this channel. Note that one-boson-exchange models of the N-N interaction which try to mimic the

two-pion-exchange with a single fictitious σ-meson exchange miss the richness of this phenomena and thus dangerously hide real physics. When two nucleons interact in the nucleus the amplitude in figure 2b must be modified, the range of momenta allowed to the intermediate nucleon being restricted by the Pauli principle to lie outside the Fermi sea. Thus we must subtract the contribution of this amplitude for all intermediate nucleon momenta $k<k_F$. This subtraction turns this attractive amplitude into a repulsion. Such an effect had been investigated many years earlier by Green and co workers who found it to be a small effect or order 1-2 MeV at the empirical saturation density. Starting from point A on the Coester line this further increased the discrepancy between BHF calculations and the semi empirical mass formula. Now we see that the repulsion increases rapidly as k_F increases with the results summarised in figure 3.

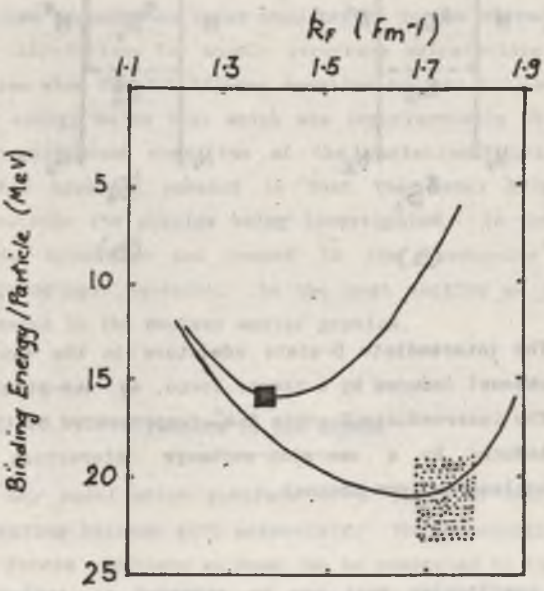

Fig 3. The lower curve represents the reults of a typical LOCV calculation including tensor correlations but excluding isobar effects. The upper curve results when isobars are included.

At last we have a curve that saturates at the empirical binding energy and density. An added bonus is that the curvature of the saturation curve is now reduced and yields a compressibility modulus K ≈ 200-300 MeV. Further studies of asymmetric fluids predict a symmetry term for the semi empirical mass formula of 32 MeV.

We have calculated the three-body cluster contributions to the saturation curve and have found them to be negligible (≲1 MeV) at densities up to $\rho=3\rho_0$ after which they grow rapidly. Thus at higher densities LOCV calcualtions are expected to fail and higher terms in the cluster expansion must be included.

There are still many nuclear structure calculations carried out using as an effective interaction the BHF reaction matrix. Our analysis of the nuclear matter saturation problem suggests that this will underestimate the attraction in the $^3S_1$ channel and overestimate the attraction in the $^1S_0$ channel. While this latter effect is not great for $\rho\lesssim\rho_0$ it is density dependent. It is my belief that authors who have found a need for effective repulsive three-body forces are simply rectifying their omission of the dependence of the isobar effect.

POSTSCRIPT

I would claim that all the essential features of the nuclear matter saturation problem have now been solved. The critical elements missing from the earlier BHF calculations were an adequate treatment of tensor correlations and isobar excitations of the nucleon.

There remains, of course, a much greater mystery. With the discovery of the quark-gluon substructure of nucleons, isobars and mesons, why does such a simple potential model work at all?

I was introduced to this problem by Hans Bethe and educated by Ben Day and Baird Brandow in the mysteries of the BHF approach. The LOCV calculations stemmed from collaborations with Ray Bishop, John Owen and Majid Modarres with useful tuition on the isobar problem from Tony Green.

Details of calculations and further reference are given in ref. [1].

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STRESZCZENIE

Semi-empiryczna formuła masowa dobrze opisuje energię wiązania jąder atomowych w szerokim zakresie mas. Człon objętościowy w tym wzorze pozwala oszacować, przy zaniedbaniu oddziaływania Coulomba, że w jednorodnym, nieskończonym płynie składającym się z neutronów i protonów, tworzy się układ związany przy energii wiązania 16 ± 5 MeV/nukleon. Ze względu na trudności z jednoznacznym rozdzieleniem członu objętościowego i powierzchniowego, eksperymentalnie szacuje się wartość parametru charakteryzującego ściśliwość płynu materii jądrowej: K ≈ 250± 50 MeV. Przegląd prób wyjaśnienia tej wartości jest przedmiotem artykułu.

Р Е З Ю М Е

Полуэмпирическая массовая формула хорошо описывает энергию связи атомных ядер в широком диапазоне масс. Объемный член в этой формуле позваляет оценить, в случае пренебрежения кулоновским взаимодействием, что в однородной, бесконечной жидкости составленной из нейтронов и протонов, образуется связанная система при энергии связи 16±5 МэВ/нуклон. По поводу трудностей с однозначным разделением объемного и поверхностного членов - на основе экспериментов оценивается значение параметра характеризующего сжимаемость жидкости ядерной материи: K = 250±50 МэВ. Обзор работ, пытающихся выяснить это значение является предметом этой статьи.