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LETTER TO THE EDITOR

A constrained variational calculation of the symmetry coefficient

C Howes, R F Bishop and J M Irvine
Department of Theoretical Physics, University of Manchester, Manchester M13 9PL, UK and Daresbury Laboratory, Science Research Council, Daresbury, Warrington WA4 4AD, UK

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Abstract. A lowest-order constrained variational technique previously used by us to describe the bulk properties of neutron and nuclear matter is extended to the case of a nucleon fluid with arbitrary proton to neutron ratio. Calculations with the Reid soft-core potential are performed and a value of the symmetry coefficient in the semi-empirical mass formula is obtained. Inclusion of the saturating effect of the $\Delta(1236)$ described by Green and collaborators is shown to improve this value.

In a previous series of papers (Owen *et al* 1976a, b, c, 1977) we have developed and applied a lowest-order constrained variational method for calculating the energy–density curve for homogeneous quantum fluids. We have used this technique, with the constraint that the correlated wavefunction should be properly normalised, to calculate the nuclear matter saturation curve with realistic NN potentials (Owen *et al* 1977). For the Reid soft-core potential (Reid 1968) we obtained a binding energy per nucleon of 23 MeV at a saturation density corresponding to a Fermi momentum $k_{\mathrm{F}} = 1{\cdot}64\ \mathrm{fm}^{-1}$, which may be compared with the volume coefficient, $a_{\mathrm{V}} \approx 16{\cdot}5$ MeV, in the semi-empirical mass formulae, and the central density of heavy nuclei which corresponds to $k_{\mathrm{F}} \approx 1{\cdot}36\ \mathrm{fm}^{-1}$.

In this work we now consider a general infinite fluid of nucleons at a density $\rho = \rho_N + \rho_Z$, where the proton to neutron ratio $r = \rho_Z/\rho_N$ is allowed to vary. In this case we have two distinct Fermi momenta, for neutrons and protons:

$$\rho_i = k_i^3/3\pi^2 \qquad i = N, Z. \tag{1}$$

We now follow exactly the procedure described by Owen *et al* (1977) except for two changes, namely (i) we sum separately over the distinct neutron and proton Fermi seas and (ii) our two-body correlation functions, which previously carried the labels α ($\equiv (J, S, T)$, respectively the total angular momentum, spin and isospin of the pair) and i (equal to 1 for the channels not coupled by the tensor force and equal to 2,3 for the two channels $L = J \pm 1$ coupled by the tensor force, in the notation of Owen *et al* (1977)) only, now acquire the additional label M_T, the third component of the isospin, to allow for a difference in the n–n, p–p and n–p correlation functions. In our earlier nuclear matter work (Owen *et al* 1977) each of the correlation functions was required to heal to the Pauli function $h(k_{\mathrm{F}}r)$:

$$h(x) \equiv [1 - \tfrac{9}{4}(j_1(x)/x)^2]^{-1/2}. \tag{2}$$

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In the present calculations we continue to require that each of the correlation functions heals to the same Pauli function $H(r)$, which in the case of unequal numbers of neutrons and protons is readily seen by the methods of Owen *et al* (1977), modified by the above changes, to be given by

$$H(r) = \left[1 - \tfrac{9}{2} \sum_{i=N,Z} \left(\frac{\rho_i}{\rho} \frac{j_1(k_i r)}{k_i r}\right)^2\right]^{-1/2}. \tag{3}$$

In another work we shall examine the sensitivity of our results to this restriction that each of the correlation functions heals to the same 'averaged' Pauli function, and in particular we shall examine the effect of allowing the n–n, p–p and n–p correlation functions to heal separately. We do not, however, believe this to be an important effect.

In figure 1 we present the results of our calculations for nucleon matter with the Reid (1968) soft-core potential at various values of the proton to neutron ratio r. From the semi-empirical mass formulae we expect the energy of infinite nucleonic matter at a fixed density ρ to be given by

$$E(\rho,r)/A = -a_V + a_S\alpha^2 \tag{4}$$

where α is the asymmetry parameter, $\alpha = (1 - r)/(1 + r)$. From figure 1 we obtain the value of the volume coefficient $a_V = 22{\cdot}8$ MeV at a saturation density

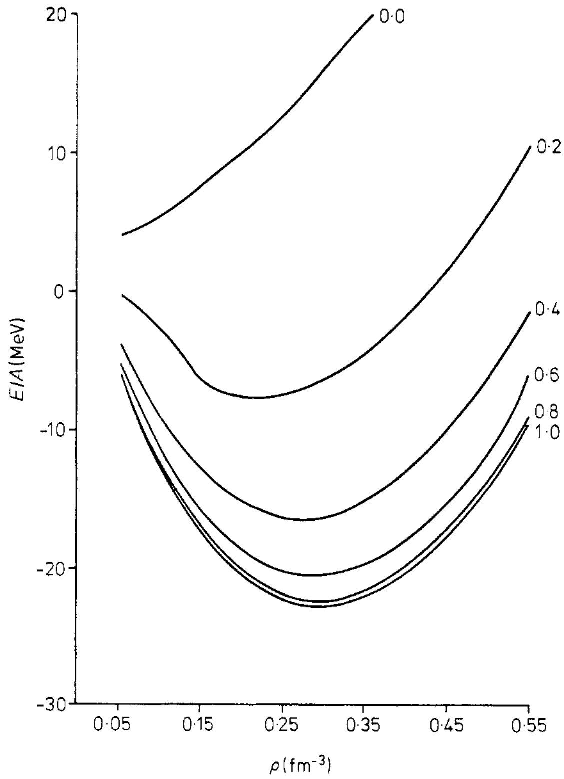

Figure 1. Lowest-order variational calculations with a normalisation constraint of the energy per particle as a function of density for a nucleon fluid with a proton to neutron ratio $r = 0{\cdot}0(0{\cdot}2)1{\cdot}0$.

Table 1. Values of a_S deduced from pairs of curves with different proton to neutron ratio r in figure 1. The asymmetry parameter $\alpha = (1 - r)/(1 + r)$. Values above the major diagonal are at the calculated saturation density of $\rho = 0{\cdot}297\ \mathrm{fm}^{-3}$; values below the major diagonal are at the empirical saturation density of $\rho = 0{\cdot}17\ \mathrm{fm}^{-3}$.

α	α^2 / r / r	0·0 / 1·0	0·01235 / 0·8	0·0625 / 0·6	0·1837 / 0·4	0·4444 / 0·2	1·0 / 0·0
0·0	1·0	...	35·64	35·52	35·88	36·52	38·25
0·1111	0·8	25·11	...	35·49	35·84	36·54	38·28
0·25	0·6	25·92	26·12	...	35·90	36·68	38·43
0·4286	0·4	26·13	26·21	26·24	...	37·01	38·78
0·6667	0·2	26·69	26·73	26·81	27·07	...	39·64
1·0	0·0	27·48	27·51	27·58	27·78	28·12	...

$\rho = 0{\cdot}296\ \mathrm{fm}^{-3}$ for nuclear matter. At a fixed density ρ, any pair of energy curves in figure 1 will also give us a value of the symmetry coefficient a_S. In table 1 we present the matrices of values of a_S so determined for both the calculated saturation density of $0{\cdot}296\ \mathrm{fm}^{-3}$ and the empirical saturation density of $0{\cdot}17\ \mathrm{fm}^{-3}$ for nuclear matter. The spread in the values of a_S may be taken as an indication of how good the assumption of equation (4) is. We see that for $\rho = 0{\cdot}296\ \mathrm{fm}^{-3}$ there is a range of values of a_S from 35–40 MeV with an average of 37·0 MeV. The low values are all clustered in the top left-hand corner of the matrix, which correspond to small values of α. For $\rho = 0{\cdot}17\ \mathrm{fm}^{-3}$ the range of values is from 25 to 28 MeV with an average of 26·8 MeV, and again the lower values tend to be concentrated in the upper left corner. Since the symmetry term was designed to describe the realm of finite nuclei, all of which have $\alpha \leqslant 0{\cdot}2$, we would like to use the values in the top left-hand corner of the matrix in table 1 to define a_S. However, these elements are the most uncertain since they are obtained by taking small differences in large energies and dividing by small values of α^2. Thus an error of $\sim 1\%$ in the binding energy of the $r = 1$ or $r = 0{\cdot}8$ curve can change the estimate of a_S in this regime by $\sim 20\%$.

Brueckner-calculation estimates of the symmetry coefficient have been made by Brueckner *et al* (1968), who give a value of 28 MeV, by Ellis and Sprung (1972) who reanalysed Siemens' (1970) calculations to obtain 29·3 MeV, and again by Ellis and Sprung who obtain 30 MeV, and by Haensel and Haensel (1976) who obtain 23·1 MeV, all of which may be compared with the semi-empirical mass formulae fits of ~ 32 MeV. The proton to neutron ratios used by these workers are given by values of $\alpha = 0{\cdot}0$, $0{\cdot}2$ and $0{\cdot}4$, corresponding to $r = 1{\cdot}0$, $0{\cdot}67$ and $0{\cdot}43$ respectively, and hence they avoid the sensitive upper left-hand corner of the matrix in table 1. If we were to restrict ourselves to these values of r we would obtain a spread of less than 1% in our estimated values of a_S, and would obtain $a_S = 35{\cdot}7$ MeV at the calculated nuclear matter saturation density of $0{\cdot}296\ \mathrm{fm}^{-3}$ and $a_S = 26{\cdot}1$ MeV at the empirical density of $0{\cdot}17\ \mathrm{fm}^{-3}$.

A number of authors (and see Ellis and Sprung (1972)) have also estimated the deviations of the symmetry coefficient from a constant value, assuming, instead of equation (4), the form

$$E(\rho,r)/A = -a_V + a_S\alpha^2(1 + \lambda\alpha^2). \tag{5}$$

Using the whole of table 1 we find that $0{\cdot}0 < \lambda < 0{\cdot}62$ at $\rho = 0{\cdot}17\ \mathrm{fm}^{-3}$ and $-0{\cdot}09 < \lambda < 0{\cdot}12$ for $\rho = 0{\cdot}296\ \mathrm{fm}^{-3}$, which may be compared with the various estimates from Brueckner calculations which yield $-0{\cdot}67 < \lambda < 0{\cdot}24$. The only safe conclusion that may be drawn is that our calculations are compatible with $\lambda = 0$ but seem to favour a small positive value, in agreement with the most recent estimates. It appears to us unlikely that calculations will ever be sufficiently precise to determine λ accurately with any high degree of confidence.

Giving the scatter of results in table 1, it is slightly difficult to make precise statements about the value of the symmetry parameter a_S, but it is clear that at the calculated saturation density of $0{\cdot}296\ \mathrm{fm}^{-3}$ it is too large, while at the empirical saturation density of $0{\cdot}17\ \mathrm{fm}^{-3}$ it is too small, compared with the empirical best-fit value of 32 MeV. The most obvious and far worse failure, however, is in the prediction of the saturation density at $0{\cdot}296\ \mathrm{fm}^{-3}$ with a volume coefficient of 22·8 MeV compared respectively with the empirical values of $0{\cdot}17\ \mathrm{fm}^{-3}$ and 16·5 MeV.

However, Green and Haapakoski (1974), Green and Niskanen (1975) and Day and Coester (1976) have argued that phenomenological interactions, like the Reid interaction we have used, which fit the two-nucleon data will inevitably overestimate the binding of nucleon matter because of the two-meson exchange process depicted in figure 2(*a*), wherein one of the intermediate nucleons has been excited to a $\Delta(1236)$ resonance. Such amplitudes are presumably included in the phenomenological potentials, which are, of course, employed unchanged in nuclear matter calculations, but where in reality in nucleon matter the intermediate nucleon must be excluded from the nucleon Fermi sea (Pauli effect) and the intermediate N and Δ move in the mean field generated by the nucleon background (dispersion effect). Since the process depicted in figure 2(*a*) contributes essentially to the attractive region of the internucleon potential, such a process treated properly will lead to a loss of binding energy for nucleon matter compared with a pure potential calculation. It turns out, however, that this loss of binding energy is to some extent compensated for by the three-nucleon force also mediated by two-meson exchange, whose amplitude is depicted in figure 2(*b*). In our previous work (Owen *et al* 1977) we added the estimates of Green and Niskanen, and Day and Coester, for the effect of the amplitude of figure 2(*a*) to our constrained variational nuclear matter curve, and this had the effect of reducing the binding energy in both cases to 14·7 MeV per particle at saturation densities corresponding to $k_F = 1{\cdot}41\ \mathrm{fm}^{-1}$ and $1{\cdot}45\ \mathrm{fm}^{-1}$ respectively. The amplitude of figure 2(*b*) was originally estimated by Green *et al* (1973) to yield an additional 1–2 MeV binding energy per particle without significantly altering the saturation

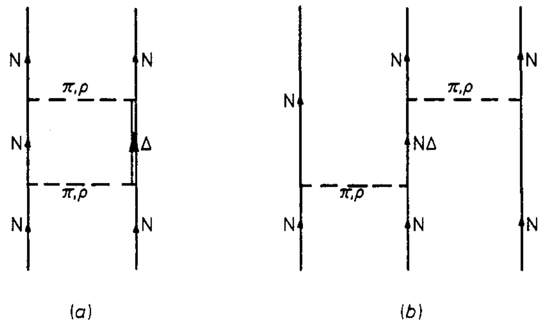

Figure 2. (*a*) A Δ contribution to the N–N interaction. (*b*) The three-nucleon force mediated by two-meson exchange.

density. This is supported by the most recent work of McKellar (1978) in which the 'best' result is given as $1{\cdot}8 \pm 0{\cdot}3$ MeV.

For nuclear matter, Green and co-workers (Green and Niskanen 1975, Green *et al* 1973) quote for the saturation effect of the Δ resonances an additional energy per particle of

$$\delta E(\Delta)/A = (-8{\cdot}5\ \rho^{5/6} + 138\ \rho^{1{\cdot}957})\mathrm{MeV}, \tag{6}$$

with ρ measured in units of fm^{-3}, and where the two terms come from the amplitudes of figures 2(*b*) and 2(*a*) respectively. For neutron matter Green and Haapakoski (1974) suggest that the effect of the amplitude of figure 2(*a*) can be taken into account by multiplying the contribution to the total energy from the $^1S_0$ channel by a factor of $(1 - 4{\cdot}0\ \rho^{1{\cdot}4})$ with ρ in units of fm^{-3}. The effect of the three-body amplitude of figure 2(*b*) in neutron matter is expected to be much smaller than in nuclear matter because of the 'absence of the strong triplet-even tensor potential which plays an important role in nuclear matter' (Green and Niskanen 1975), and with the lack of detailed calculations in this case we consequently feel justified in ignoring it. Adding these effects to our nuclear matter ($r = 1$) and neutron matter ($r = 0$) curves in figure 1, we obtain the modified curves of figure 3. We see that for nuclear matter our calculated volume coefficient is now $16{\cdot}9$ MeV and the predicted saturation density of $0{\cdot}20\ \mathrm{fm}^{-3}$($k_F = 1{\cdot}44\ \mathrm{fm}^{-1}$) is also greatly improved. From the two curves in figure 3 we obtain values of the symmetry coefficient of $a_S = 35{\cdot}1$ MeV at the calculated saturation density of $\rho = 0{\cdot}20\ \mathrm{fm}^{-3}$ and $a_S = 31{\cdot}3$ MeV at the empirical value of $\rho = 0{\cdot}17\ \mathrm{fm}^{-3}$, which are in satisfactory agreement with the best-fit value of 32 MeV. From our calculations it therefore appears that while the Reid interaction is by itself unable to give a good description of nuclear matter, the inclusion of the saturating effects of the $\Delta(1236)$ resonance simultaneously brings each of the three parameters a_V, a_S and the equilibrium density into much closer agreement with their empirical values.

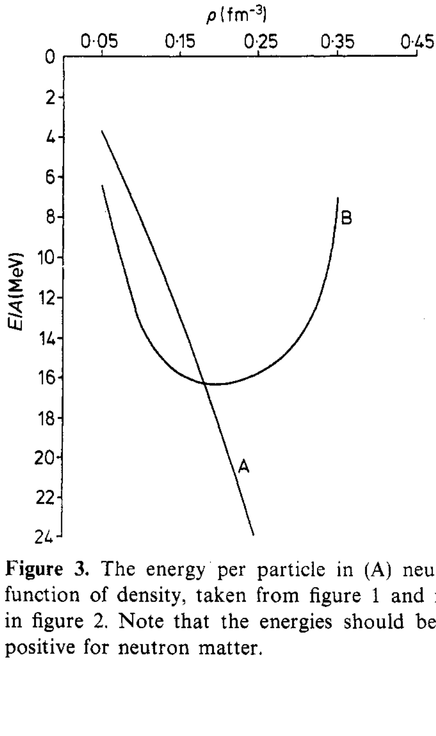

Figure 3. The energy per particle in (A) neutron matter and (B) nuclear matter as a function of density, taken from figure 1 and modified for the effects of the amplitudes in figure 2. Note that the energies should be read as negative for nuclear matter and positive for neutron matter.

A detailed study of the role of the $\Delta(1236)$ resonance in nucleon matter at arbitrary proton to neutron ratio is in progress.

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