

## Nuclear-Matter Calculations Using a Realistic Nucleon-Nucleon Potential

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A realistic nucleon-nucleon potential is used to formulate a simple Thomas-Fermi method for nuclear-structure calculations. The potential-energy density has only one free parameter, which is found by fitting with Bhargava and Sprung's calculation. The short-range repulsion is absorbed in the term containing the free parameter. The compressibility comes out to be good. We illustrate our method in nuclear matter only with  $^1S$  and  $^3S$  states, although the method is applicable in the general case.

Since Bethe<sup>1</sup> developed his Thomas-Fermi theory, several papers<sup>2</sup> have been published on the Thomas-Fermi approximation (TFA). But while Bethe and his collaborators started with realistic nucleon-nucleon interactions, most other authors<sup>2</sup> have used different types of effective interactions for their calculations, probably because the use of realistic two-body potentials is cumbersome even in a TFA calculation. To simplify matters, some<sup>2</sup> of them have assumed, following Bethe, that the interaction can be split up into an attractive long-range part and a repulsive short-range  $\delta$ -function part (both density-dependent and -independent). The parameters of these interactions are determined by the nuclear-matter properties and/or binding energy and r.m.s. radius of, for example, an  $\alpha$  particle, though these interactions may not fit the two-nucleon scattering data.

In this note we give a TFA for use in nuclear-structure calculations in which we start with Reid's<sup>3</sup> hard-core potential. Our aim is to use a realistic two-nucleon potential and obtain a TFA which is simple for the purpose of actual calculations. To illustrate the method we shall consider the  $^1S$  and  $^3S$  states of Reid's potential and use them in the nuclear-matter case. We shall consider the contributions due to all the states for calculations in finite nuclei in future papers.

We start with the standard energy expression

$$(E_{\text{pot}})_{\text{total}} = \sum \int \phi_i^*(\vec{r}_1) \phi_j^*(\vec{r}_2) G(\vec{r}_1, \vec{r}_2; \vec{r}'_1, \vec{r}'_2) \times \phi_i(\vec{r}'_1) \phi_j(\vec{r}'_2) d\vec{r}_1 d\vec{r}_2 d\vec{r}'_1 d\vec{r}'_2, \quad (1)$$

where  $G$  is the Bethe-Brueckner reaction matrix. We write Eq. (1) in terms of center of mass and

relative coordinates

$$\vec{R} = \frac{1}{2}(\vec{r}_1 + \vec{r}_2) \quad \text{and} \quad (2)$$

$$\vec{r} = \vec{r}_1 - \vec{r}_2$$

and expand around  $\vec{R}$  as was done by Kumar, Le Couteur, and Roy.<sup>4</sup>

Now, keeping terms up to the fourth order instead of terms up to the second<sup>4</sup> order in powers of  $r$  for the potential-energy density, we obtain an expression in terms of density and its derivatives:

$$E = -a_1 \rho^2 + a_2 \rho^{8/3} - a_3 \rho^{10/3} + \text{derivative terms}. \quad (3)$$

For simplicity we have put  $\rho_n = \rho_p = \frac{1}{2}\rho$  in Eq. (3). The extension to the case  $\rho_n \neq \rho_p$  is quite easy.

Here,

$$a_1 = -\frac{3}{16} \int G d\vec{r} d\vec{r}', \quad (4a)$$

$$a_2 = -\frac{3}{128} \times 4.8 \times 0.6 \int Gr^2 d\vec{r} d\vec{r}', \quad (4b)$$

$$a_3 = -\frac{27}{700} \int Gr^4 d\vec{r} d\vec{r}', \quad (4c)$$

and coefficients of the derivative terms are given through  $a_2$  and  $a_3$  in a somewhat complicated manner.

As mentioned above, in this note we consider the case of nuclear matter with equal numbers of neutrons and protons with the Coulomb interaction switched off. Also, only contributions from  $^1S$  and  $^3S$  states are considered which contribute most to the binding energy. Then the potential-energy density may be written as

$$E_{\text{nm}} = -a_1 \rho^2 + a_2 \rho^{8/3} - a_3 \rho^{10/3} \\ = -(a_1^1 + a_1^3) \rho^2 + (a_2^1 + a_2^3) \rho^{8/3} + (a_3^1 + a_3^3) \rho^{10/3}, \quad (5)$$

TABLE I. Different values of  $A$ ,  $B$  and  $A'$ ,  $B'$ , as suggested by Sprung and Bhargava and Dahlblom, are listed in this table, where  $R = v(^3S)/v(^1S) = A - Bk_F$ , or  $R = v(^3S)/v(^1S) = A' - B'k_F^2$ .

	$A$	$B$	$A'$	$B'$	
(a)	1.85	0.67			Dahlblom
(b)	2.56	0.96			Sprung and Bhargava
(c)			1.46	0.28	Dahlblom

where  $a_1^1, a_2^1, a_3^1$  may be obtained from  $^1S$  and  $a_1^3, a_2^3$ , and  $a_3^3$  from  $^3S$  states.

To find the values of the quantities  $a_1^1, a_2^1, a_3^1$  the Moszkowski-Scott<sup>5</sup> (MS) separation method is used in which the two-nucleon interaction  $v$  is divided into a short-range and a long-range part  $v = v_s + v_l$  at a separation distance  $d$ .  $a_1^1, a_2^1$ , and  $a_3^1$  are now found from the integrals (4a), (4b), and (4c), where the limits of integration are from  $d$  to  $\infty$ . We follow MS and Bethe in taking  $d = 1$  fm. We can now write the  $^1S$  part of Eq. (5) as

$$(E_{nm})_{1S} = -a_1^1 \rho^2 + a_2^1 \rho^{8/3} (1 - \alpha \rho^{2/3}); \quad (6)$$

using the Reid potential we have  $a_1^1 = 178.3$  MeV fm<sup>3</sup> and  $a_2^1 = 444.7$  MeV fm.<sup>5</sup>

We take  $\alpha$  as a free parameter and fix it by means of Bhargava and Sprung's<sup>6</sup> calculated values. Since in expanding Eq. (1) we had kept up to the fourth-order terms,  $\alpha$  will naturally have a value somewhat different than it would have if we had taken the full series. Also, the short-range repulsive term may be considered to have been absorbed by the term containing  $\alpha$ . In view of the above limitations the reasonable thing to do is to fix the parameter  $\alpha$  by adjusting its value so that one may reproduce the Sprung results.

It is seen that putting  $\alpha = 1.05$ , Eq. (6) gives val-

ues of  $(E_{nm})_{1S}$  which are in fairly good agreement with the Sprung results especially for values of  $k_F$  from 1.2 to 1.5 fm<sup>-1</sup> (Table II). A calculation of compressibility (mentioned below) also gives a reasonable value. We could have increased  $\alpha$  to 1.1, to have still closer agreement of values of  $(E_{nm})_{1S}$  around  $k_F = 1.36$ . But in that case  $(E_{nm})_{1S}$  has a larger value at  $k_F = 1.6$ , which makes the values of  $(E_{nm})_{3S}$  and the total energy unreasonably high. This is due to the fact that the increase in the value of  $(E_{nm})_{1S}$  is much steeper for values of  $k_F$  around 1.6, and this naturally makes the value of compressibility very low. We therefore chose  $\alpha = 1.05$  as a better value.

To calculate the contribution due to the  $^3S$  state we make use of Bethe's suggestion that the ratio of  $^3S$  to  $^1S$  contribution be written as

$$R = v(^3S)/v(^1S) = A - Bk_F, \quad (7a)$$

or

$$R = v(^3S)/v(^1S) = A' - B'k_F^2, \quad (7b)$$

where  $A, B$  or  $A', B'$  are taken from Bhargava and Sprung's<sup>6</sup> and Dahlblom's<sup>1</sup> calculations. It is easy to calculate the  $^3S$ -state contribution using our method. We have considered all three sets of values mentioned by Bethe to see which one is most suitable. These are given in Table I.

Considering the contribution from both  $^1S$  and  $^3S$  states we have for the potential-energy density

$$\begin{aligned} E_{nm} &= (E_{nm})_{1S} + (E_{nm})_{3S} \\ &= [-a_1^1 \rho^2 + a_2^1 \rho^{8/3} (1 - \alpha \rho^{2/3})] (1 + R) \\ &= [-a_1^1 \rho^2 + a_2^1 \rho^{8/3} (1 - \alpha \rho^{2/3})] (1 + A - Bk_F) \\ &= [-a_1 \rho^2 + a_2 \rho^{8/3} (1 - \alpha \rho^{2/3})], \end{aligned} \quad (8a)$$

TABLE II. Values of  $(E_{nm})/\rho$ , the potential energy per particle, for  $^1S$ ,  $^3S$ , and  $^1S + ^3S$  states at different  $k_F$  with different ratios  $R = v(^3S)/v(^1S)$  (viz. Table I) and corresponding compressibility at  $k_F = 1.36$  fm<sup>-1</sup>.

Value of $k_F$ (fm <sup>-1</sup> )	$(E_{nm})_{1S}/\rho$ (MeV)	$R = 2.56 - 0.96k_F$		$R = 1.46 - 0.28k_F^2$		$R = 1.85 - 0.67k_F$		Values given by Sprung and Bhargava	
		$(E_{nm})_{3S}/\rho$ (MeV)	$(E_{nm})/\rho$ (MeV)	$(E_{nm})_{3S}/\rho$ (MeV)	$(E_{nm})/\rho$ (MeV)	$(E_{nm})_{3S}/\rho$ (MeV)	$(E_{nm})/\rho$ (MeV)	$(E_{nm})_{1S}/\rho$ (MeV)	$(E_{nm})_{3S}/\rho$ (MeV)
0.8	-4.63	-8.30	-12.93	-5.93	-10.56	-6.09	-10.72		
1.0	-7.94	-12.70	-20.64	-9.36	-17.30	-9.36	-17.30		
1.2	-11.53	-16.23	-27.76	-12.18	-23.71	-12.06	-23.59	-11.76	-16.27
1.36	-14.58	-18.28	-32.86	-13.73	-28.31	-13.69	-28.27	-14.96	-18.62
1.43	-16.04	-19.04	-35.08	-14.23	-30.27	-14.31	-30.35	-16.28	-19.47
1.5	-17.56	-19.67	-37.23	-14.57	-32.13	-14.84	-32.50	-17.74	-20.34
1.6	-20.38	-20.87	-41.25	-15.15	-35.53	-15.86	-36.24	-19.60	-20.85
Value of compressibility $K$ at $k_F = 1.36$ fm <sup>-1</sup>			55 (Total $K \sim 145$ )		72 (Total $K \sim 160$ )		49		

or

$$E_{nm} = [-a_1^1 \rho^2 + a_2^1 \rho^{8/3}(1 - \alpha \rho^{2/3})](1 + A' - B' k_F^2) \\ = [-a_1 \rho^2 + a_2 \rho^{8/3}(1 - \alpha \rho^{2/3})]. \quad (8b)$$

Taking the usual TF expression for kinetic energy, we write the total energy density as

$$W_{nm} = E_{nm} + K.E. \\ = C \rho^{5/3} - a_1 \rho^2 + a_2 \rho^{8/3}(1 - \alpha \rho^{2/3}), \quad (9)$$

where  $C = 3.6(\hbar^2/2M)$ .

Putting the three sets of values (a), (b), and (c) given in Table I in Eqs. (8a) and (8b) we get the contribution to the potential-energy density from  $^1S$  and  $^3S$  states. We find that for  $R = 2.56 - 0.96k_F$  [(b) in Table I] very good agreement with Sprung's values is obtained; while for (a) and (c) the agreement is not at all good. (See Table II.)

It is worthwhile to mention here that we tried to choose  $A, B$  or  $A', B'$  by fitting with energy values given by Sprung's calculations around  $k_F = 1.36$ . In that case we found  $A = 2.24$ ,  $B = 0.73$  and  $A' = 1.72$ ,  $B' = 0.26$ . But the agreement for  $E_{nm}$  for  $k_F = 1.2$  to  $1.6 \text{ fm}^{-1}$  and compressibility is not at all satisfactory.

We then calculate the nuclear-matter compressibility using the standard expression

$$K = r_0^2 \frac{d^2}{dr_0^2} \frac{W_{nm}}{\rho},$$

where  $r_0$  is equal to  $1.524/k_F$ .

We find that we get reasonably good values of  $K$  for  $R$  given by parameters (b) and (c) (Table I), but not for (a). The values obtained (Table II) are quite good in view of the fact that only  $^1S$  and  $^3S$  states have been considered. A rough check shows that if we include the contributions from the other states,  $K$  comes out to be about 145 for the case (b) and about 160 for (c) at  $k_F = 1.36 \text{ fm}^{-1}$ . This is what we expect from a calculation with a realistic potential.

Table II indicates that an  $R = 2.56 - 0.96k_F$  for the  $^3S$  and  $^1S$  contribution is the best one to use for Reid's hard-core potential.

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