# Hartree-Fock calculations of crystalline structure of nuclear matter with hard-core potentials

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A Hartree-Fock calculation for the binding energy of a crystalline structure of nuclear matter in the presence of a hard-core potential is performed. As expected, a strongly unbound nuclear matter is obtained.

[NUCLEAR STRUCTURE Nuclear matter, Hartree-Fock calculations, hard-core potential.]

It has been sometimes suggested that nuclear matter at normal density may be described by a Slater determinant exhibiting a crystalline structure.[1,2] Recently it has further been argued that such trial functions may be useful in that they may lead to bound nuclei in Hartree-Fock calculations with hard-core potentials.[3] This suggestion appears somewhat surprising in view of what we know about the nuclear interaction. Indeed, in order not to experience the strong short range repulsion with a determinantal wave function, it is necessary to confine each nucleon in a small volume $v$. At normal nuclear matter density the average distance between two nucleons is 1.2 fm. Assuming a hard-core radius $c = 0.4$ fm we find that $v$ should be of the order of $4\pi R^3/3$ with $R \simeq 0.4$ fm. From Heisenberg's uncertainty relation this value implies a kinetic energy per nucleon $T/A \geq (1/2m)(\hbar/R)^2 \simeq 100$ MeV. In contrast the nucleon-nucleon attraction at a distance of 1 fm is of the order of 1 MeV only which makes it difficult to obtain a bound system.

Since the previous qualitative argument does not seem to discourage the kind of speculations mentioned,[1-3] we have performed a Hartree-Fock calculation of nuclear matter in order to provide numbers. We have used the Gammel-Christian-Thaler potential[4]:

$$V = \sum_{S,T} [V_{S,T}(r) + W_{S,T}(r) S_{12}] P_{ST},$$

where $P_{ST}$ is a projector on the subspace with spin $S$ and isospin $T$, and where

$$V_{ST}(r) = \infty \text{ if } r \leq 0.5 \text{ fm},$$
$$= A_{ST} \exp(-\mu_{ST} r)/\mu_{ST} r \text{ if } r > 0.5 \text{ fm}$$
$$W_{ST}(r) = \infty \text{ if } r \leq 0.5 \text{ fm},$$
$$= B_{ST} \exp(-\nu_{ST} r)/\nu_{ST} r \text{ if } r > 0.5 \text{ fm}.$$

We have used the parameter set 5100 of Ref. 5.

Our trial function is a Slater determinant,

$$\Phi(x_1, x_2, \ldots, x_A) = \frac{1}{\sqrt{A}} \det || \varphi_i(x_j) ||,$$

with $x = r, \sigma, \tau$. The single particle functions $\varphi_i$ are of the form

$$\varphi_i(x) = u(|\vec{r} - \vec{R}_i|) \chi_{\sigma_i}(\sigma) \chi_{\tau_i}(\tau),$$

where the values of $\vec{R}_i, \sigma_i, \tau_i$ are assumed to correspond to a bcc lattice, as described in Fig. 1. The nucleon spins have been arranged in order to obtain the largest binding energy from the tensor force.[6] Denoting the lattice constant by $a$ the nucleon density is $\rho = 2/a^3$.

In order to obtain a finite binding energy we have to make sure that the distance between two nucleons is always larger than the hard-core radius $c$. This will be the case if $u(r)$ vanishes outside a sphere of radius $R$ satisfying $2R + c \leq a\sqrt{3}/2$. To determine $u(r)$ we minimize the kinetic energy. This requirement is a plausible approximation to

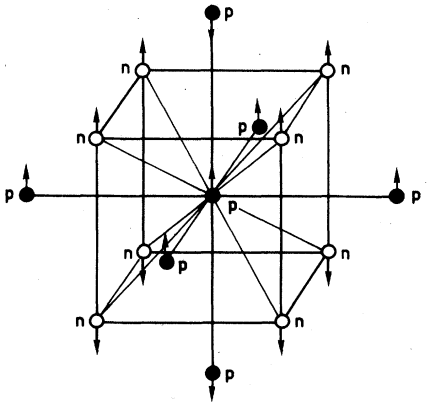


FIG. 1. Body centered cubic crystalline structure for nuclear matter. Small arrows indicate the spin orientation of the nucleons.

 

TABLE I. Binding energy per particle ($E/A$) of nuclear matter as a function of the density $\rho$. The Fermi momentum $k_F$ is also given as well as the lattice constant $a$. The various contributions in the total energy are given in detail, while point Yukawa refers to the classical interaction between two particles (see text). The last column gives the results of a Jastrow calculation performed in Ref. 5 with the same interaction.

| $k_F$ (fm$^{-1}$) | $\rho$ (fm$^{-3}$) | $a$ (fm) | Kinetic $T/A$ (MeV) | Yukawa (MeV) | Point Yukawa (MeV) | Tensor (MeV) | Total energy (MeV) | Ref. 5 MeV |
|---|---|---|---|---|---|---|---|---|
| 1.2 | 0.117 | 2.576 | 273.2 | −11.5 | −9.4 | −5.3 | 258.5 | −15 |
| 1.4 | 0.185 | 2.211 | 408.8 | −23.9 | −20.9 | −9.5 | 378.4 | −22 |
| 1.6 | 0.277 | 1.933 | 593.9 | −43.7 | −39.8 | −14.9 | 539.2 | −24 |
| 1.8 | 0.394 | 1.719 | 837.8 | −71.7 | −67.3 | −21.4 | 749.1 | −20 |
| 2.0 | 0.540 | 1.547 | 1160.1 | −109.8 | −104.9 | −28.7 | 1026.5 | −10 |
| 2.2 | 0.719 | 1.406 | 1587.7 | −159.5 | −154.3 | −36.7 | 1396.7 | |
| 2.4 | 0.934 | 1.289 | 2155.0 | −222.1 | −216.7 | −45.1 | 1893.2 | |
| 2.6 | 1.187 | 1.190 | 2907.7 | −298.3 | −293.0 | −53.9 | 2560.9 | |
| 2.8 | 1.483 | 1.105 | 3921.8 | −389.9 | −384.7 | −62.8 | 3474.4 | |

self-consistency, since the potential energy will be shown below to depend weakly upon $u(r)$. This procedure leads to

$$u(r) = \frac{1}{(2\pi R)^{1/2}} \frac{\sin kr}{r}$$

with $k = \pi/R$. The minimum value of the kinetic energy is

$$\frac{T}{A} = \frac{\hbar^2}{2m} \frac{\pi^2}{R^2} \text{ with } 2R + c = a\sqrt{3}/2 .$$

The potential energy per nucleon

$$\frac{V}{A} = \frac{1}{2} \sum_{j \neq i} \langle ij \,|\, V_{12} \,|\, ij \rangle$$

is particularly simple in our case. Indeed, since the single particle wave functions have nonoverlapping supports, there is no exchange term. By repeated use of the multipole expansion formula for a Yukawa potential we find

$$\left\langle ij \left| \frac{e^{-\alpha|\vec{r}_1 - \vec{r}_2|}}{\alpha|\vec{r}_1 - \vec{r}_2|} \right| ij \right\rangle = \frac{e^{-\alpha|\vec{R}_i - \vec{R}_j|}}{\alpha|\vec{R}_i - \vec{R}_j|} I^2(\alpha, R),$$

where the function $I(\alpha, R)$ is given by

$$I(\alpha, R) = \int \theta(R - r) |u(r)|^2 \frac{sh(\alpha R)}{\alpha R} d^3r$$
$$= 1 + \frac{\alpha^2}{3!} \langle r^2 \rangle + \frac{\alpha^4}{5!} \langle r^4 \rangle + \ldots ,$$

with $\theta(x) = 1$ if $x > 0$ and 0 if $x \leq 0$. The first term in the previous expansion corresponds to the interaction of two point nucleons. It provides a very good approximation to the potential energy as can be checked in Table I. For this reason we have also assumed the nucleons to be pointlike when evaluating the potential energy due to the tensor force. Notice that since $\langle r^k \rangle \leq R^k$ we have $1 \leq I(\alpha R) \leq sh(\alpha R)/\alpha R$. This implies that for $\alpha = 0.7$ fm$^{-1}$ and $R = 0.3$ fm, the variation in the potential energy with $u(r)$ is less than 1.5 percent.

Results obtained for various values of the density are shown in Table I and compared with the results of Jastrow calculations.[5] Our energies are much higher than those of Ref. 5 even at large densities. This large difference confirms the validity of the simple argument given above against crystalline structure of nuclear matter at normal density. In Ref. 1 a significant binding energy was obtained. This is because the authors use the kinetic energy of a Fermi gas and the potential energy of a bcc lattice, which is not a consistent procedure. We have also performed variational calculations with sc, fcc, and hcp lattices. These calculations yield very similar results.

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