

The lattice energy, which had been omitted in a previous preliminary calculation (Buchler and Barkat 1971*a*), is now properly included in the usual Wigner-Seitz manner (Buchler and Barkat 1971*b*, and the present work).

### III. THE VARIATIONAL PROBLEM

The basic problem now consists in minimizing the *average* energy density,

$$\varepsilon \equiv E_{\text{cell}}/\Omega, \quad (12)$$

at constant average baryon density,

$$\mathfrak{N} = \Omega^{-1} \int_{\Omega} (\rho_n + \rho_p)(d\mathbf{r})^3, \quad (13)$$

with the constraint of charge neutrality,

$$Q \equiv \Omega^{-1} \int_{\Omega} (\rho_p - \rho_e)(d\mathbf{r})^3 = 0. \quad (14)$$

Instead of minimizing  $\varepsilon$  at constant  $\mathfrak{N}$ , it is equivalent and computationally simpler to minimize the quantity

$$J \equiv \varepsilon - \mu_n \mathfrak{N} - \mu_e Q \quad (15)$$

at fixed Lagrange parameter  $\mu_n$ , with  $\mathfrak{N}$  then becoming a calculated quantity. It will presently become obvious (relations [29], [30], [32]) that  $\mu_n$  is to be interpreted as the chemical potential (CP) of the neutrons, and  $\mu_e$  as the CP of the electrons. The quantity  $J$  can be written

$$J = \frac{1}{\Omega} \int_{\Omega} \{f(\rho, \rho_p, \rho_e) + \frac{1}{2}e(\rho_p - \rho_e)\Phi[\rho_p - \rho_e] - \xi \rho \nabla^2 \rho\} (d\mathbf{r})^3, \quad (16)$$

where  $f$  is a simple analytic function of the densities including everything except the direct Coulomb and the gradient terms.

Consider now a variation of the densities of the form

$$\rho(\mathbf{r}) \rightarrow \rho(\mathbf{r}) + \nu_1 \bar{\rho}(\mathbf{r}), \quad \rho_p(\mathbf{r}) \rightarrow \rho_p(\mathbf{r}) + \nu_2 \bar{\rho}_p(\mathbf{r}), \quad \rho_e(\mathbf{r}) \rightarrow \rho_e(\mathbf{r}) + \nu_3 \bar{\rho}_e(\mathbf{r}), \quad (17)$$

subject to the constraint

$$\mathbf{n} \cdot \nabla \bar{\rho} = \mathbf{n} \cdot \nabla \bar{\rho}_p = 0 \quad \text{at} \quad \mathbf{r} = R_c, \quad (18)$$

where  $\mathbf{n}$  is the normal to the surface of the cell. Setting the derivatives with respect to the  $\nu$ 's, the infinitesimal parameters, equal to zero, we obtain the Euler-Lagrange equations

$$\frac{\partial f}{\partial \rho} - 2\xi \nabla^2 \rho = 0, \quad (19)$$

$$\frac{\partial f}{\partial \rho_p} + e\Phi = 0, \quad (20)$$

$$\frac{\partial f}{\partial \rho_e} - e\Phi = 0, \quad (21)$$

which have to be satisfied everywhere except through possible surfaces of discontinuity  $S_i$  for the densities or their derivatives. The integration by parts leading to equation (19) yields the matching conditions

$$\rho \mathbf{n} \cdot \nabla \bar{\rho} \Big|_{S_i^-}^{S_i^+} = 0, \quad \bar{\rho} \mathbf{n} \cdot \nabla \rho \Big|_{S_i^-}^{S_i^+} = 0. \quad (22)$$

Since the variations  $\bar{\rho}$  and  $\nabla\bar{\rho}$  are arbitrary, these relations imply that both  $\rho$  and  $\mathbf{n}\cdot\nabla\rho$  have to be continuous everywhere. There is no such restriction on the derivatives of the proton and electron densities. Had we included a neutron proton gradient difference term of the form

$$-\theta[\nabla(\rho_n - \rho_p)]^2 \quad (23)$$

with  $\theta$  constant ( $\theta \approx \frac{1}{3}\xi$ , cf. Brueckner *et al.* 1969a, b; Baym *et al.* 1971) in the energy functional, it would have been required to also have  $\mathbf{n}\cdot\nabla\rho_p$  continuous everywhere. Such a term, if evaluated as a perturbation after the variational problem has been solved, contributes negligibly numerically. On the other hand, its proper inclusion in the variational problem can lead to numerical instability (Brueckner *et al.* 1969a) and it has not been included at this stage.

At the cell boundary, specializing to spherical symmetry, we have

$$\rho\mathbf{n}\cdot\nabla\bar{\rho} = \bar{\rho}\mathbf{n}\cdot\nabla\rho = 0, \quad r = R_c, \quad (24)$$

which is satisfied in view of the imposed boundary condition (18).

Variation with respect to the position of the surfaces  $S_i$  gives the condition that the integrand  $f$  be continuous across each  $S_i$ . The continuity of  $\rho_p$  and  $\rho_e$  everywhere, which is physically reasonable and which we shall assume, certainly satisfies this condition, although in principle we cannot rule out an arbitrary number of jumps in  $\rho_p$  and  $\rho_e$ , such that  $f$  remains continuous.

Variation with respect to the cell boundary yields the condition

$$J = \text{integrand (evaluated at } r = R_c \text{) of equation (16),} \quad (25)$$

which has the physical interpretation that the average pressure be equal to the pressure at the cell boundary. From relation (15), it is apparent that the integrand indeed is equal to minus the pressure given by

$$p = -\epsilon + \mu_n\rho_n + (\mu_n - \mu_e)\rho_p + \mu_e\rho_e = -\epsilon + \mu_n\rho_n + \mu_p\rho_p + \mu_e\rho_e, \quad (26)$$

with the separate nucleon and electron contributions equal to

$$p^{\text{nuc1}} = -\epsilon_N(\rho_n, \rho_p) + \rho_n \frac{\partial\epsilon_N}{\partial\rho_n} + \rho_p \frac{\partial\epsilon_N}{\partial\rho_p} - \xi\rho\nabla^2\rho + \frac{1}{2}e\rho_p\Phi - \frac{1}{3}C_x\rho_p^{4/3}, \quad (27)$$

$$p^{\text{el}} = -\epsilon_{e1}(\rho_e) + \rho_e \frac{\partial\epsilon_{e1}}{\partial\rho_e} - \frac{1}{2}e\rho_e\Phi - \frac{1}{3}C_x\rho_e^{4/3}. \quad (28)$$

In summary, the variational problem therefore leads to solving the coupled set of equations

$$2\xi\nabla^2\rho = \frac{\partial\epsilon_t}{\partial\rho_n} - \mu_n, \quad (29)$$

$$2\xi\nabla^2\rho = \frac{\partial\epsilon_t}{\partial\rho_p} - \mu_p + e\Phi; \quad (30)$$

or equivalently,

$$4\xi\nabla^2\rho = \frac{\partial\epsilon_t}{\partial\rho_n} + \frac{\partial\epsilon_t}{\partial\rho_p} - (\mu_n + \mu_p - e\Phi), \quad (29a)$$

$$0 = \frac{\partial\epsilon_t}{\partial\rho_n} - \frac{\partial\epsilon_t}{\partial\rho_p} - (\mu_n - \mu_p + e\Phi). \quad (30a)$$

together with

$$\nabla^2\Phi = -4\pi e(\rho_p - \rho_e) \quad (31)$$