Density-Functional Calculations of the Cohesive Energy of Condensed Matter in Very Strong Magnetic Fields

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The ground-state energies of atoms and of rhombohedral and body-centered tetragonal atomic lattices have been calculated by density-functional theory for magnetic flux densities of 10^{12}–10^{13} G. The cohesive energies derived are too small to support a finite–electric-field boundary condition at the polar cap in a pulsar magnetosphere.

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The polar-cap electric-field boundary condition in a pulsar magnetosphere with positive corotational charge density is determined by the cohesive energy of the surface atoms.[1] It is generally believed[2,3] that the surface electric field is finite. Variational calculations[4] of the ground-state energies of atoms and infinite linear molecular chains in very strong magnetic fields gave cohesive energies for the molecular chain, and therefore for a stable three-dimensional atomic lattice, adequate to support a finite electric field component $\mathbf{E}\cdot\mathbf{B}\neq 0$ at the neutron star surface. Recently, Müller[5] recalculated the variational models of Flowers *et al.*[4] and found the original cohesive energies to be spurious as a result of serious errors in some of the numerical methods used. To find the correct boundary condition, the ground-state energies of atoms and of rhombohedral and body-centered tetragonal atomic lattices have been calculated for very strong magnetic fields. There appear to be no previously published ground-state energies for such systems. The method adopted is that of density-functional theory.[6–8]

The infinite linear molecular chain is formed from nuclei spaced at intervals $2C$ on a line parallel with $\mathbf{B}$. Because of the axial symmetry of both atoms and molecules, self-consistent solutions of the Kohn-Sham equations[7] have been obtained[9] for these systems with no substantial approximation apart from the restriction to lowest Landau orbitals and the neglect of relativistic corrections. The ground-state energies are very much lower than those found by Flowers *et al.* and by Müller.

The classes of lattice which appear likely to have the optimum cohesive energy are determined by the cylindrical form of the atomic Landau orbitals. The cubic system has too much symmetry, while any class containing the symmetry element C_6 appears unsuitable becasue of the close proximity of the nuclei. Thus the classes selected are the body-centered tetragonal (D_{4h}) and rhombohedral (D_{3d}).

An elementary estimate of the rate of thermal emission of atoms at the surface, made by reference to terrestrial metals, shows that the cohesive energy necessary to support a finite–electric-field boundary condition is $E_c \gtrsim 2.8$ keV at a polar-cap surface temperature of 10^6 K. A surface temperature of 5×10^5 K appears to be the minimum consistent with heating of the polar cap by the reverse flow of electrons from bound-free transitions or pair creation.[10] Thus the cohesive energies found here, for the relevant magnetic flux densities,[2,3,11–13] are very clearly too small to allow a finite–electric-field boundary condition.

The energy functional of the atomic lattice is

$$E[n]=E_{\rm KS}-\frac{1}{2}\int d^3r\,d^3r'\frac{n(\mathbf{r})n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}+E_Z+E_{\rm xc}[n]-\int d^3r\,n(\mathbf{r})\frac{\delta E_{\rm xc}}{\delta n}. \quad (1)$$

The electron density is $n(\mathbf{r})$; E_Z is the internuclear potential energy, $E_{\rm xc}$ the exchange-correlation functional, and $E_{\rm KS}$ the ground-state eigenvalue of the potential[7]

$$U=V+\frac{\delta E_{\rm xc}}{\delta n}+\int d^3r'\frac{n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}, \quad (2)$$

in which V is the potential of the nuclei. We adopt a local-density approximation for $E_{\rm xc}$ in which the expression for the exchange-correlation energy per electron in a uniform charge-neutralized gas of density n is[9]

$$\epsilon_{\rm xc}=(2\pi n\ln n+13.7n-37.8n^2)-(0.0096\ln n+0.122), \quad (3)$$

expressed in field-dependent units of length and energy, $(\hbar c/eB)^{1/2}=2.566\times 10^{-10}B_{12}^{-1/2}$ cm and $e^2(\hbar c/eB)^{-1/2}=0.5612B_{12}^{1/2}$ keV, where B_{12} is the magnetic flux density in units of 10^{12} G. The first set of terms, the exchange energy, is identical with the high-field limit of Danz and Glasser.[14] The second set is an empirical correlation energy[9] chosen so that the exchange-correlation functional obtained from $\epsilon_{\rm xc}$ for each occupied self-consistent atomic orbital cancels, as far as possible, the Coulomb self-interaction of the orbital.[15]

The selected lattices can be formed by the assembly

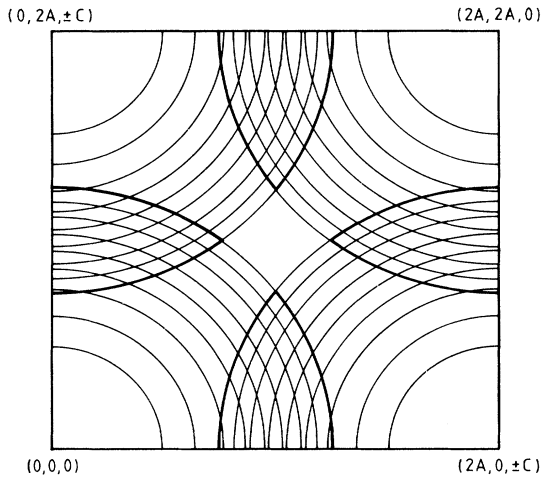

FIG. 1. The arrangement of parallel infinite linear molecular chains in the xy plane for the body-centered tetragonal lattice, with the Cartesian coordinates of nearest-neighbor atoms. The quadrants of circles are the maxima of the functions $\rho R_{0\nu}^2(\rho)$ which define the intersection regions of θ for each ν.

of parallel infinite linear molecular chains, nearest-neighbor separation $2A$, suitably displaced in the z direction. The body-centered tetragonal lattice is shown in Fig. 1 with the Cartesian coordinates of nearest-neighbor atoms. The eigenfunctions of U for the unperturbed molecular chain are[9]

$$\psi_{\nu s} = R_{0\nu}(\rho)(2\pi)^{-1/2} e^{-i\nu\theta} f_{\nu s}(k,z) \tag{4}$$

in cylindrical polar coordinates, where $R_{0\nu}$ is the lowest Landau orbital; $\nu = 0, 1, 2, \ldots, \nu_m$ is the zone number of the Bloch function $f_{\nu s}$. Zero-point motion of the nuclei is neglected. The electrons are completely spin-polarized (the cyclotron energy is $\hbar\omega_B = 11.58 B_{12}$ keV). Some eigenfunctions of the lattice U are of great complexity because of the substantial nonorthogonality of intersecting Landau orbitals (Fig. 1), but the deeply bound small-ν states, which do not intersect, are very well approximated by the $\psi_{\nu s}$. These properties are compatible with a local approximation in θ.

The potential U inside a cylindrical atomic volume of radius $\rho_0 > A$, length $2C$, is found from the charge density of nearest-neighbor atoms by Fourier-Bessel transforms (order 0,3 for rhombohedral, and 0,4 for body-centered tetragonal) and from a quadrupole approximation for more distant atoms. The eigenfunctions $f_{\nu s}(k,z,\theta)$ and eigenvalues $\epsilon_{\nu s}(k,\theta)$ of the potential

$$U_\nu(z,\theta) = \int_0^{\rho_0} \rho\, d\rho\, R_{0\nu}^2(\rho)\, U(\mathbf{r}) \tag{5}$$

are computed, from a trial density distribution, for a

TABLE I. The atomic ground-state energies E_a (Ref. 9) and the cohesive energies E_c of rhombohedral and body-centered tetragonal atomic lattices calculated for atomic numbers and magnetic flux densities relevant to the stellar surface in radio pulsars. The atom with $Z = 26$, $B_{12} = 1$, should have one electron in a two-node state (Ref. 9), not allowed for in calculating the quoted E_a. The bracketed E_c has been obtained by extrapolation in Z and B.

Z	B (10^{12} G)	E_a (keV)	E_c (keV) Body-centered tetragonal	E_c (keV) Rhombohedral
10	1	−10.70	0.12	0.07
	2	−14.16	0.20	0.14
	5	−20.24	0.48	0.45
	10	−26.34	0.69	0.78
14	1	−19.09	0.12	
	2	−25.37	0.21	
	5	−36.76	0.46	
	10	−48.29	0.62	
20	1	−35.48	0.12	
	2	−47.07	0.24	
	5	−68.37	0.54	
	10	−90.77	0.98	
26	1	(−56.01)	(0.12)	
	2	−74.49	0.29	0.19
	5	−108.18	0.60	0.59
	10	−143.52	0.92	0.75

number of discrete values of k and θ and used to obtain an estimate of E and an improved $n(\mathbf{r})$. The Fermi wave numbers $k_{F\nu s}(\theta)$ are found by requiring the electron chemical potential to be independent of ν and θ. Convergence to a self-consistent solution is rapid. There is no approximation in the limit of small ν where U_ν becomes θ independent. In the intersection region, where U is a slowly varying function of position, the method is equivalent to a local approximation in ρ and θ [$\rho R_{0\nu}^2$ has a sharp maximum at $\rho=(2\nu+1)^{1/2}$]. The intersection region of θ is defined, for each ν, by the intersection of a circle of radius $(2\nu+1)^{1/2}$ with circles of radius $(2\nu_m+1)^{1/2}$ centered on the nearest-neighbor axes (Fig. 1). Because of the lattice symmetry, intersection-region contributions to E_{KS} and the total electronic charge can be divided equally between the molecular chains concerned.

The atomic lattice energies found by variation of A, ν_m, and C have been subtracted from the atomic ground-state energies E_a of Ref. 9 to give cohesive energies (Table I). The optimum ν_m are such that the Landau orbitals just fill the xy plane (the density is one independent state per 2π area). As an example, the body-centered tetragonal lattice constants for $Z=26$ and $B_{12}=5$ are $A=6.4$, $C=12.0$, in the field-dependent units defined above. As a result of the subtraction made in deriving E_c, errors caused by the restriction to lowest Landau orbitals and neglect of relativistic corrections, which are greatest at small ν, should cancel almost completely. Changes in the exchange-correlation functional can cause substantial shifts in E_a, but not in E_c. A consequence of the local approximation in θ made in the lattice calculations is that, as for the Thomas-Fermi method,[16] the E_c are most probably overestimates of the true cohesive energies. In the limit of large A, the lattice energy approaches the known[9] infinite molecular chain energy.

The investigation of possible structures has not been exhaustive. Although structures of lower energy cannot be excluded, the smallness of the cohesive energies found here for both rhombohedral and body-centered tetragonal lattices points clearly to a zero surface electric-field boundary condition for pulsars.

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