MICROPHYSICS OF NEUTRON STAR OUTER ENVELOPES IN THE PERIODIZED, MAGNETIC THOMAS-FERMI MODEL

T. A. ENGSTROM, V. H. CREPSI AND B. J. OWEN
Department of Physics, Pennsylvania State University, University Park, PA

J. BRANNICK
Department of Mathematics, Pennsylvania State University, University Park, PA

XIAOZHE HU
Department of Mathematics, Tufts University, Medford, MA

ABSTRACT

Observations of several types of neutron stars indicate surface temperature inhomogeneities. In recent years magneto-thermal simulations have supported the idea that the magnetic field and anisotropic heat conduction play important roles in generating these inhomogeneities. Simulations rely on crustal microphysics input heretofore calculated at the level of a plasma model – neglecting lattice structure and electron polarizability. We focus on the low density outer envelope, treating both of these elements by a proper periodization of the magnetic Thomas-Fermi model. Our solution method involves a novel domain decomposition and we describe a scalable implementation using Hypre. The method may be seen as a prototype for the general class of problems involving nonlinear charge screening of periodic, quasi-low-dimensionality structures, e.g. liquid crystals. Findings include low density $c' < 0$ elastic instabilities for both bcc and fcc lattices, reminiscent of the situation in some light actinides, and phonon thermal conductivity three orders of magnitude larger than that derived from the plasma model. The former result suggests there is a symmetry-lowering transition to a tetragonal or orthorhombic lattice. The latter indicates transport anisotropy may be greatly reduced within $\sim 10$ meters of the surface, giving the effect of a “heat-spreader cladding” which may significantly increase the size of polar hot spots and alter pulse profiles.

Subject headings: conduction – magnetic fields – methods: numerical – stars: neutron

1. INTRODUCTION

In conventional solid state physics, the Thomas-Fermi model is regarded as an historical development and a pedagogical tool (although it remains a key ingredient of modern, orbital-free density functional theory). Conversely, in certain extreme conditions of solid state astrophysics, where order-of-magnitude estimates of thermodynamic quantities are sought, the failure to predict binding/condensation of atoms is not a serious deficiency due to matter being under high pressure, and appropriate \textit{ab initio} methods are in a state of infancy, the Thomas-Fermi model has not yet faded into obsolescence. In particular, magnetic Thomas-Fermi models first written down in the 1970s, and extended in many directions in the 1980-90s, continue to be relied upon for the equation of state of magnetized neutron star outer envelopes – see Haensel et al. (2007) chap. 4, the review by Lai (2001), and references within. Alternatively, the magnetized jellium model (where both nuclei and electrons are treated as uniform charge distributions) and magnetized Coulomb crystal model (point nuclei in a uniform electron background) have been studied – see Baiko (2009) for the latter – and we also acknowledge two approximate Kohn-Sham-DFT calculations for condensed matter at high field and zero pressure [Medin & Lai 2006; Jones 1986]. Magnetic Thomas-Fermi (MTF) models are aimed at matter composed of heavy atoms in a highly non-perturbative magnetic field, and are reasonably appropriate for the outer $\sim 10$ meters (in this paper, “outer envelopes”) of many neutron stars, where $\rho < 10^6$ g/cc and $B \sim 10^{12} - 10^{13}$ gauss. For a free electron, $10^{13}$ gauss corresponds to a magnetic length 65 times smaller than the Bohr radius, and zero-point cyclotron energy (or Zeeman energy) more than $1/10$ of the rest mass.

An under-appreciated property of the MTF model is that its regime of asymptotic exactness contains many field configurations for which Bloch’s theorem can be proved. (In other huge magnetic field regimes, use of periodic boundary conditions may not be so innocuous.) But as with its nonmagnetic counterpart, it has been standard practice to replace the properly periodized MTF model with an approximate version having spherical Wigner-Seitz cells and a vanishing normal derivative at the cell edge. Physics related to bulk phase stability is obviously out of reach of this approximation, due to the lack of an explicit lattice. Here we attempt to extract some of this physics by extending a novel domain decomposition approach invented by MacFarlane & Hubbard (1983). While M&H could not reach the threshold...
accuracy required to resolve energy differences between structures, we significantly improve their method by incorporating curved subdomain interfaces with the appropriate symmetry, and implement the improved method making use of the Hypre library of scalable, multigrid-preconditioned solvers (Falgout et al. 2006). We then calculate the equation of state, phase diagram, elastic constants, lattice thermal conductivity, and exchange correction in the periodized MTF model.

Among our findings is a type of lattice instability generally driven by the splitting of sharp features in the electronic density of states due to a symmetry-lowering. It is interesting that the MTF model, which has no “density of states,” should capture this kind of symmetry-lowering transition, and it is perhaps the simplest model that does so.

2. REGIME OF VALIDITY

We begin by recapitulating the MTF regime as it pertains to an isolated, heavy atom (Fushiki et al. 1992). Define the reduced field \( b = B/B_0 \) where \( B_0 = m^2 e^2 \hbar^2 c^{-3} = 2.4 \times 10^9 \) gauss. A strong field is next defined as one in which the magnetic length \( \ell = b^{-1/2} a_0 \) beats out the zero-field mean electron spacing \( Z^{-2/3} a_0 \) as the smallest length scale in the problem: \( b \gg Z^{4/3} \). Instead of the standard three-dimensional behavior \( k_F = (3\pi^2 n_e)^{1/3} \), the Fermi momentum follows the lowest Landau level expression \( k_{z,F} = 2\pi^2 \ell^2 n_e \) in a strong field \( B = B\hat{z} \), which modifies the usual \( n_e^{5/3} \) dependence of the kinetic energy density to \( n_e^3 \). MTF description additionally requires the electrostatic potential to vary slowly on the lengthscale \( k_{-1,b}^{-1} \), and simple scaling relations indicate this condition is met when \( b \ll Z^3 \). MTF theory is an exact limit of quantum mechanics for \( Z b Z^{-4/3} \to \infty \) while \( b Z^{-3} \to 0 \); in this regime, sphericity of the atom is not destroyed (Yngvason 1991; Lieb et al. 1992).

Extending MTF theory to bulk matter under pressure, one repeats the above arguments, replacing the characteristic size of an isolated atom with the Wigner-Seitz radius \( r_n = (3Z/4\pi n_e^{\text{avg}})^{1/3} \), and finds that the validity conditions put a restriction on the number of flux quanta penetrating the unit cell: \( Z^{2/3} \ll (r_n/e)^2 \ll Z \).

Like orbital-free density functional theory in general, the MTF model works with densities, not wavefunctions. Wavefunctions are implicit in that the amplitude of the underlying wavefunction determines the density, but the phase is not directly expressed. Therefore, the MTF model can’t be expected to capture some implications of the phase structure of the underlying wavefunction, in particular, issues with periodicity-breaking in a strong magnetic field. While this argument helps justify use of periodic boundary conditions (PBCs) for arbitrary field configurations in the MTF model, we can also show that PBCs are exact for a large number of field configurations satisfying \( Z^{2/3} \ll (r_n/e)^2 \). Consequently, the physical regime treated by the MTF model here is also amenable to wavefunction-based methods that require (or are greatly simplified by) PBCs, and which may be used to check the accuracy of MTF predictions. Consider the single-electron Hamiltonian

\[
H = \frac{1}{2m} \left( \mathbf{p} - \frac{e}{c} \mathbf{A} \right)^2 + V(\mathbf{r}),
\]

where \( V(\mathbf{r}) = V(\mathbf{r} + \mathbf{R}) \) and \( \mathbf{R} \) is any lattice vector. Magnetic translation operators \( T_\mathbf{R} \) can be constructed that commute with \( H \), but in general, they don’t commute with each other — the origin of Hofstadter periodicity breaking (Jain 2007; Kohmoto et al. 1993). In the symmetric gauge

\[
T_\mathbf{R} \mathcal{T}_\mathbf{R} = \mathcal{T}_\mathbf{R} T_\mathbf{R} \exp \left[ \frac{2\pi i}{\phi_0} \mathbf{B} \cdot (\mathbf{R} \times \mathbf{R}') \right],
\]

where \( \phi_0 = \hbar c/e \) is the flux quantum. Now restrict the magnetic field orientation to be along an irreducible lattice vector \( \mathbf{R}_|| \), where \( R_0 \sim r_n \). In other words, the field is oriented to a high symmetry direction in the crystal. Choose \( \mathbf{R}_|| \) as the primitive lattice vector \( \mathbf{a}_1 \). Any valid choice of the remaining primitive vectors \( \mathbf{a}_2 \) and \( \mathbf{a}_3 \) gives flux \( \phi = 0 \) through two elementary plaquettes (an elementary plaquette is defined by \( \mathbf{a}_1 \times \mathbf{a}_2 \times \mathbf{a}_3 \)) and in the MTF regime, the flux through the third plaquette automatically satisfies \( \phi/\phi_0 \gg Z^{2/3} \). Never is more than a small fractional adjustment of \( B \) required for \( \phi/\phi_0 \) to be integer-valued through this third plaquette; with this adjustment \( \{ T_{\mathbf{a}_1}, T_{\mathbf{a}_2}, T_{\mathbf{a}_3}, H \} \) form a commuting set and may be simultaneously diagonalized by the Bloch functions \( \psi_{k,n}(\mathbf{r}) = e^{ik\cdot \mathbf{a}_1 n} \psi_{k,n}(\mathbf{r}) \) where \( n \) is a magnetic subband index and \( |\psi_{k,n}| \) has the periodicity of the primitive lattice. (For \( \phi/\phi_0 \) rational-valued through each elementary plaquette, \( |\psi_{k,n}| \) is periodic over certain non-primitive cells; for irrational flux, \( |\psi_{k,n}| \) is incommensurate with \( V \).) Note that a change of basis takes the set of plaquette fluxes \( \{ 0, 0, \phi/\phi_0 \} \) into a different set of integer fluxes while the actual field configuration remains unchanged.

3. MODEL & DOMAIN DECOMPOSITION

The MTF model for a degenerate electron gas in the lowest Landau level interacting with a lattice of point nuclei is defined by the energy functional

\[
E[n_e] = E_{\text{kin}} + V_{\text{int}} + V_{\text{xc}} + V_{\text{ee}},
\]

where

\[
E_{\text{kin}} = \frac{2\pi^4}{3\beta^3} \frac{e^2}{a_0} \int d^3 r n_e^3,
\]

and the other terms have the usual meaning. One obtains the MTF equation by imposing the stationarity condition \( \delta(E - \mu \int d^3 r n_e) = 0 \) and combining the result with the Poisson equation \( \Delta \Phi = 4\pi e n_e \). While \( \Phi \) is the total electrostatic potential from electrons and nuclei, nuclear charge density is omitted from the right hand side of this Poisson equation and instead taken into account via the boundary conditions \( \Phi(\mathbf{r}) = Z e |\mathbf{r} - \mathbf{R}|^{-1} \) as \( |\mathbf{r} - \mathbf{R}| \to 0 \). It is convenient to make a change of variables defined by \( \mathbf{r} = \mathbf{r} + \mathbf{R}, \mathbf{R} = \mathbf{R} \mathbf{X} \) and \( \mu + e\Phi(\mathbf{r}) = Ze^2 u(\mathbf{X})/\sigma \), where \( \sigma = a_0 (Z^2/8\pi^3)^{1/5} \). Delaying further discussion of boundary conditions, we write down the startlingly concise PDE which is the result of these manipulations: \( \Delta u = \sqrt{u} \).

To solve the model, we use an improved version of MacFarlane & Hubbard’s domain decomposition method, hereafter IMH. The original method features subdomain interfaces that are easy to implement (boxes), but don’t respect the symmetry of the solution, and we have observed that this method generates large and unphysical
discontinuities in $\nabla u$ near the box corners. Use of curved interfaces is the main improvement in iMH. Noting the method can be generalized to any lattice, we restrict the present discussion to cubic Bravais lattices, for which a convenient choice of domain $\Omega$ is one octant of the conventional unit cell. Subdomain $\Omega_A$ is formed by centering a small sphere of radius $x_0$ on a lattice point, and taking the intersection with $\Omega$. There are $N$ identical copies of $\Omega_A$, one in each corner of $\Omega$ where a nucleus is located (two corners for bcc, four for fcc). A large has no physical significance, and we are interested in the $\epsilon$ of model. Since

$$y'' = \sqrt{2}y_k, \quad 0 \leq x \leq x_0,$$

(5)

$$y_k(0) = 1,$$

(6)

$$y_k(0) = \frac{2\xi}{x} + \frac{\epsilon_F}{Z} - \int_{V_0} d^3x \left( \frac{\sqrt{u_{k-1}}}{4\pi} - \frac{1}{V_0} \right) q(x),$$

(7)

and second half-step given by the nonlinear boundary value problem

$$\Delta u_k = \sqrt{u_k}, \text{ in } \Omega_B,$$

(8)

$$\hat{n} \cdot \nabla u_k = 0, \text{ on flat parts of } \partial \Omega_B,$$

(9)

$$u_k = \frac{y_k(x_0)}{x_0}, \text{ on curved parts of } \partial \Omega_B.$$  

(10)

In Equation [7] the $k^{th}$ derivative condition is obtained as a functional of the $k-1^{st}$ solution, extending the concept of “overlap” in domain decompositions. Information flow in iMH is represented schematically in Figure [1a]. The integral over the primitive cell volume $V_0$ involves a product of the density nonuniformity correction and the Ewald-type sum

$$q(x) = \frac{4\pi}{V_0} \sum_{G \not= 0} \frac{\cos(G \cdot x) e^{-G^2/4\nu^2}}{G^2} + \sum_x \frac{\text{erfc}(\eta|x + x|) - \pi}{\eta^2 V_0},$$

(11)

which can be obtained using a result due to Nijboer & De Wette [1957]. The Madelung constant is given by $\xi = \frac{2}{r_s} x_s \lim_{x \to -1} q(x) - x^{-1} = -0.8959293$ (bcc), 0.8958736 (fcc), while the Wigner-Seitz radius and Lagrange multiplier (Fermi energy) appear in dimensionless form $x_s = r_s/\sigma$ and $\epsilon_F = \mu \sigma/\epsilon^2$. In conventional units,

$$x_s = \frac{1.33b^{2/3}}{Z^{1/3}} \left( \frac{\text{M in amu}}{\rho \text{ in g/cc}} \right)^{1/3}.$$  

(12)

Decoupled from iMH is a normalization requirement $1 = (4\pi)^{-1} \int_{V_0} d^3x \sqrt{u}$ which completes the description of model. Since $\epsilon_F$ and $Z$ only appear together, as a ratio, for a given lattice the model is specified by three parameters: $x_0$, $x_s$ and $\epsilon_F/Z$. The Dirichlet radius $x_0$ has no physical significance, and we are interested in the

$$y(x) \mapsto F[u],$$

$$y(x) \mapsto G[y],$$

$$u(x) \mapsto F[u].$$

Figure 1. (a) Schematic of information flow in the iMH domain decomposition. (b) Fractional contribution of $F$ to the derivative condition $y'(0)$. As indicated in the schematic, $F$ is the contribution from the large subdomain and $G$ is the contribution from all small subdomains. Data shown are from the last iteration (converged and normalized) of the bcc lattice problem.

The limit $x_0 \to 0$, taken externally to the model ($x_0 \to x_s$ essentially recovers the spherical Wigner-Seitz cell approximation). Of the latter two parameters, only one is independent, as the other must be adjusted to its normalization value. Once a converged, normalized solution is in hand, the $T = 0$ Helmholtz free energy per nucleus is found by an integration over the primitive cell

$$U = \frac{Z^2 e^2}{\sigma} \left[ y'(0) \frac{1}{2} - \frac{1}{24\pi} \int_{V_0} d^3x u^{3/2} \right].$$

(13)

This expression excludes the energy stored in the magnetic field.

4. NUMERICAL IMPLEMENTATION

Starting with an initial guess $y_0(0)$ corresponding to the uniform electron gas, the initial value problem (Equations [17]) is integrated using a semi-implicit Euler method with adaptive stepsize and built-in stability checks [Press et al. 2007]. Having thus specified a Dirichlet value for the boundary value problem, we solve Equations [8-10] by Newton’s iteration with initial guess $u_0 = 1$. Each linear system in Newton’s iteration is solved by the finite volume method (FVM), through Hypre’s Struct interface, using either 600$^3$ or 640$^3$ grid-
points. Certain 7-point stencils are modified to implement the Neumann and curved Dirichlet boundaries using standard discretizations that preserve both the overall $O(h^2)$ accuracy of the FVM scheme and the discrete maximum principle (Morton & Mayers 2005). Each linear system is preconditioned by one V-cycle of *Hypre’s* SMG multigrid and then iterated with conjugate gradients until the relative residual norm $< 10^{-9}$. This high tolerance is required for Newton’s iteration to converge to the same solution regardless of whether weighted Jacobian or symmetric R/B Gauss-Seidel is used in the preconditioner. Newton’s iteration is terminated when the relative solution difference norm and relative nonlinear residual norm are both $< 10^{-8}$. Integrations must then be performed to update the derivative condition $y_0(0)$. In $\Omega_B$, we apply a low-order quadrature rule cell-wise over dual FVM cells, where the approximate solution is trilinear-accurate. Exceptions are the dual cells cut by a curved boundary; for $x_0/t_x = 0.08$ there are $\sim 4^3$ of these. Each cut cell is handled by simple Monte Carlo integration with a few thousand points, which gives sufficient accuracy without causing a bottleneck. We make use of *Hypre’s* internal ghost-zone updating routines for the dual-cell-wise integration, and note this is a scalable approach. A high-order quadrature rule is used for the $\Omega_A$ integration. Iteration of IMH proceeds as described, the only difference being that convergence is accelerated by using the initial guess $u_k = u_{k-1}$ for the $k^{th}$ Newton’s iteration. As a check, we also try $u_k = 1$ and find no dependence on which of these initial guesses is used. IMH is iterated until $||u_k - u_{k-1}||/||u_k|| < 10^{-9}$.

While the limit $x_0 \to 0$ is desired from a physical standpoint, it must be kept in mind that the Dirichlet boundaries can be represented as smoothly curved surfaces within the structured grid only for $x_0/h \gg 1$. Increasing $x_0$ increases the rate of information transfer from $\Omega_A$ to $\Omega_B$, but it also decreases the rate of information transfer in the reverse direction, illustrated by Figure 1(b). We therefore restrict our study of $x_0$-dependence to the compromise range where $x_0/t_x$ goes from 0.08 to 0.32. Over this range, one can discern no discontinuity in $\nabla u$ at the interface, as occurs in the original MacFarlane & Hubbard method, and the SMG-preconditioned solver yields consistent results. *Hypre’s* PMG preconditioner also yields consistent results for the larger values of $x_0/t_x$, and is much more efficient than SMG.

5. ELASTIC CONSTANTS

Elastic response of bcc and fcc lattices are obtained using finite strains (essentially a frozen phonon calculation at zero wavevector). It is implicitly assumed that the energy density $B^2/8\pi$ stored in the magnetic field has no dependence on the strains, i.e.,

$$c_{ij} = \frac{\partial^2(U/V_0)}{\partial e_i \partial e_j}, \quad (14)$$

in engineering (Voigt) notation. While it is common to choose $c' = c_{11} - 2c_{12}$ as one of the three independent elastic constants and calculate this quantity from a tetragonal (Bain) distortion, we instead choose to calculate $c_{11}$ directly from a uniaxial strain. The remaining two independent constants $c_{44}$ and $c_{12}$ are obtained from a symmetric shear deformation and the single-crystal bulk modulus $K = -\partial P/\partial (\ln V_0) = (c_{11} + 2c_{12})/3$, respectively. The problem in the uniaxially-deformed domain remains amenable to the method previously described, the only difference being insertion of one or more extra layers of gridpoints at a height $z$ well away from any curved boundaries. For the sheared case, the stencil and quadrature rule obviously must be modified, as must the domain itself, and owing to these complications we calculate $c_{44}$ for bcc only. Our modified 7-point stencil has discretization in the shear plane accurate to order $h^2(1 + (e_4/2)^2)$, where $e_4 \ll 1$ is the strain component associated with the deformation. Symmetry-lowering makes it necessary to increase the size of the domain to half of the conventional cell, and replace Neumann with periodic boundaries on surfaces normal to the shear plane. *Hypre’s* SMG solver has a power-of-two restriction on grid periods, so the sheared problems are computed using $1024^2 \times 513$ gridpoints. Cubic lattice stability requires that the Born conditions are met: $c'$, $c_{44}$, and $K$ must all be positive.

From the elastic constants, we wish to obtain the mean sound velocity $\bar{v}$ and thereby Debye temperature $\Theta = \hbar k_B (6\pi^2 n_i)^{1/3} \bar{v}$ and related thermal properties. For this purpose we use the venerable Voigt-Reuss-Hill-Gilvary (VRHG) approximation, which treats a polycrystalline material as an isotropic body with bulk and shear moduli given by Hill averages $K_H = (K_V + K_R)/2$ and $G_H = (G_V + G_R)/2$. The Voigt (theoretical max) and Reuss (theoretical min) moduli appearing in these expressions are obtained directly from the $c_{ij}$. Mean sound velocity is then found by averaging over longitudinal and transverse modes

$$\bar{v} = \left[ \frac{1}{3} \left( \frac{1}{l_i^2} + \frac{2}{l_t^2} \right) \right]^{-1/3}, \quad (15)$$

where

$$\bar{l}_i = \sqrt{\frac{K_H + \frac{3}{2}G_H}{\rho}}, \quad (16)$$

$$\bar{l}_t = \sqrt{\frac{G_H}{\rho}}. \quad (17)$$

For a large database of elastic constants for real cubic materials, whenever the anisotropy $(G_V - G_R)/(G_V + G_R)$ is less than 20 percent, the error in the VRHG estimate of $\bar{v}$ is less than 2 percent (Anderson 1963). For the MTF bcc solid, $(G_V - G_R)/(G_V + G_R)$ is less than 12 percent within the density range studied.

Lattice conductivity of the neutron star envelope limits transport anisotropy due to the strong magnetic field. Pérez-Azorín et al (2006) and Chugunov & Haensel (2007) have estimated phonon thermal conductivity from a hybrid ion plasma/Coulomb crystal model, using the anharmonic scattering approximation

$$\kappa_{ph} \sim \frac{\rho \bar{v}^3 r_s}{\gamma T}, \quad T \gtrsim \Theta, \quad (18)$$

derived from the phonon Boltzmann equation by Ziman (1960). Here we calculate $\kappa_{ph}$ in the MTF model, using Equation 18 with the Debye form of the Grüneisen parameter $\gamma_D = -\partial (\ln \Theta)/\partial (\ln V_0)$. 

For comparison with the non-periodized model and linear response theory, calculations are performed with $x_s$ in the range 1 to 2. An issue arises for $x_s > 1.73$, where an intermediate stage of Newton’s iteration generates an approximate solution $u_0$ that is not everywhere real. No results are presented in these cases. We first check that the asymptotic limits of $\varepsilon_F/Z$ and $y'(0)$ are consistent with the MTF “atom” at zero pressure, and that the nonuniformity correction $2\xi/x_s + \varepsilon_F/Z - y'(0)$ tends to zero in the high density limit, see Figure 2. Next we compute the equation of state and $c_{44}$ for lowest Landau level occupation, see for example, Baiko (2002).

Next we calculate an exchange correction to the equation of state and bcc-fcc energy difference to zeroth order in $\delta n_e = n_{TFD} - n_{TF}$, where $n_{TFD}$ and $n_{TF}$ are the self-consistent Thomas-Fermi-Dirac and Thomas-Fermi densities. A local density approximation for the exchange energy of a strongly magnetized electron gas was first given by Danz & Glasser (1971). To leading order in the low density expansion, their result agrees with that later obtained by Fushiki et al. (1989)

$$E_{ex} = \frac{b^2}{2\pi^3} \int d^3r \left( \frac{n_e}{n_s} \right)^2 \left[ 2 \ln \left( \frac{2n_e}{n_s} + \gamma - 3 \right) \right].$$

Here $\gamma = 0.5772...$ is the Euler constant and $n_s = 2^{-1/2} \pi^{-2} \ell^{-3}$ is the density at which the first excited Landau level starts to become populated. For the purpose of our crude zeroth-order calculation, this leading order term is sufficient and avoids the non-integrable divergence at the nuclei that one would get with higher order terms. Results for the exchange correction are shown in Figure 3. For high field strengths and low densities, the exchange correction slightly softens the equation of state and further increases the energetic favorability of fcc.

Elastic constants, given in Figure 4, are remarkably similar for bcc and fcc lattices. Both lattices have a $c' < 0$ instability at densities below $x_s \approx 1.5$. No $c_{44} > 0$ or $K < 0$ instabilities were found. The density range between fcc’s energetic favorability over bcc and the onset of its instability is very small, suggesting fcc is unlikely to appear at all in the equilibrium phase diagram. Instead, as $c'$ describes the response to a deformation involving a diagonal, zero-trace strain matrix, the instability suggests the true equilibrium structure is a crystal with orthorhombic or tetragonal symmetry. This type of lattice instability is common in terrestrial metals, and one can find an example of $c' < 0$ for both cubic phases in the light actinides uranium and neptunium (the equilibrium structures are orthorhombic), see Grimvall et al. (2012). We leave the search for the stable low density structure, i.e. mapping out Bain transformation paths, for future work. $c_{44}$ is the only elastic constant (indeed, the only fundamental physical quantity we have found) that has significant dependence on the Dirichlet radius $x_0$. For large $x_0$, $c_{44}$ is considerably smaller in magnitude than the other elastic constants, although still positive. At small $x_0$, $c_{44}$ is similar in magnitude to $c_{12}$ and the Cauchy relations $c_{44} = c_{14} = c_{12}/2$ derived for central force potentials (Phillips 2001) are reasonably well obeyed, as would be expected from Equations 3 and 4. This internal consistency suggests to us that the $c_{44}$ data obtained using small $x_0$ are the most accurate, and unless otherwise indicated, the remainder of the discussion will assume the small $x_0$ data. One might expect that at high density, the MTF solid becomes elastically similar to the Coulomb crystal – we find this is not the case. For an isotropic solid, $(c_{11} - c_{12})/2c_{44} = 1$. The bcc Coulomb
crystal is highly anisotropic (Kobyakov & Pethick 2014), having $(c_{11}-c_{12})/2c_{44} \approx 0.13$ (compare lithium and plutonium), whereas for the MTF bcc lattice, this quantity is an order of magnitude larger, and increasing with density, at $x_s=1.13$. We have checked the elastic constant results using several different strain magnitudes and find no inconsistencies.

Debye temperature, Grüneisen parameter (which expresses phonon anharmonicity), and lattice conductivity in the anharmonic scattering regime are plotted in Figure 5 over the density range where both bcc and fcc are stable. The Debye temperature is of the same order as observed, redshifted surface temperatures of many neutron stars (Chamel & Haensel 2008). We find the Grüneisen parameter in the MTF solid is more comparable to that of a terrestrial material (typical values being 1–2) than the ion plasma, where $T_P \sim \omega_P \sim n_i^{1/2}$, or $\gamma_P = 1/2$. Our most striking result is the lattice conductivity, which we find to be three orders of magnitude larger than in the hybrid ion plasma/Coulomb crystal. The difference is mostly attributable to the speed of sound, which appears cubed in Equation (18). Chugunov & Haensel assume a sound velocity $\bar{v} = \omega_P/3q_{BZ}$, where $\omega_P = (4\pi n_i Z^2 e^2/m_i)^{1/2}$ and $q_{BZ} = (6\pi^2 n_i)^{1/3}$, which at $\rho \sim 10^7$ g/cc, is an order of magnitude smaller than sound velocity in the MTF model. The cause of the $\bar{v}$ discrepancy is elucidated by a simple scaling argument, which is not only insensitive to the particular lattice structure, but indicates a discrepancy may persist to higher densities than those studied here. In the ion plasma, where there is no charge screening, $\bar{v} \sim n_e^{1/6}$. In the presence of a polarizable background, ion plasma oscillations are modulated by the static dielectric function according to $\omega(k)^2 = \omega_P^2/\epsilon(k)$. As $k \to 0$, this gives the Bohm-Staver sound velocity $\bar{v} \sim n_e^{1/4}$ for screening by a $d$-dimensional electron gas (Ashcroft & Mermin 1976), and $d = 1$ in the MTF model. This argument can be extended to a region in the $b$-$n_e$ plane where high density has forced the longitudinal electron motion to become relativistic but still only the lowest Landau level is occupied: $2^{-1} \omega e^2 / m_i < \omega \rho < 2^{-1} \pi^{-2} \omega^2 / 3$, where $a$ is the fine structure constant. In this region the Bohm-Staver sound velocity grows as $n_e^{-1/2}$, again faster than in the ion plasma. For reasons mentioned in the preceding paragraph, we have elected to use the $c_{44}$ data computed with $x_0/x_s = 0.08$ in the calculation of Figure 5. If one instead used the $c_{44}$ data computed with $x_0/x_s = 0.32$, the phonon conductivity obtained would be smaller only by a factor of three (from that obtained at $x_0/x_s = 0.08$).
The extent to which surface temperature inhomogeneities are smoothed out by the cladding should be determined from a self-consistent calculation of magnetothermal evolution, which is beyond the scope of this work. However, a crude estimate can be made based on a result due to Potekhin & Yakovlev (2001). These authors solved a 1D, plane-parallel envelope cooling model (which has since become a standard treatment) using anisotropic electron conductivity and a dipole field configuration. Figure 4 in their paper shows envelope temperature profiles for the case of fixed envelope-core boundary temperature. These temperature profiles have almost no dependence on the polar angle at high density – instead, the anisotropy is picked up over a density range corresponding roughly to the MTF regime (what Potekhin & Yakovlev call the “strongly-quantizing field” regime). When the boundary temperature is fixed to $10^6$ K, a field of $10^{12}$ gauss causes the poles to be a factor of three hotter than equatorial regions. Increasing the field strength to $10^{14}$ gauss makes the poles over an order of magnitude hotter than equatorial regions. Since the origin of this surface temperature anisotropy is, in large part, neglect of “isotropizing” phonon conductivity in the outer envelope, we estimate that including this contribution could produce surface temperature profiles which are a factor of three less anisotropic than they otherwise would be. This could have a substantial impact on pulse profiles and pulsed fractions. It also suggests that sources of anisotropy in the inner envelope and below may have to be stronger than previously believed, to overcome the heat spreading layer. More recent simulations (Pons et al. 2009) have more anisotropy in the inner layers, but this does not change the fact that much of the anisotropy is picked up at lower densities.

Magneto-thermal evolution of neutron stars, and related astrophysical manifestations, are strongly dependent not just on envelope microphysics, but also the field configuration (Perna et al. 2013, Viganò et al. 2013, 2014). In the previously standard picture of a poloidal (dipole) field, heat flow is dammed by the envelope in the equatorial regions, causing hot spots at the poles (Geppert et al. 2004). Perna et al. (2013) have found that a strong toroidal field component is required to account for the single-peaked pulse profiles and large pulsed fractions of several classes of neutron stars. There is also an older, generic argument for toroidal field geometry based on dynamo action in the proto-neutron star. In the (probably artificial, but instructive) limiting case of an almost purely toroidal field, phonon transport would appear to be the dominant mechanism by which the top and bottom of the envelope are thermally coupled – not just in the equatorial regions, but everywhere. For such field configurations, the accuracy of phonon conductivity

Figure 5. Lattice dynamical properties of the bcc $^{56}$Fe MTF solid for densities above the $\epsilon' < 0$ instability ($\epsilon'$ ranges from about 1.1 to 1.3). The elastic constant data corresponding to $Q_x/Q_z = 0.08$ were used in these calculations. Top: Debye temperature. Middle: Grüneisen parameter in the Debye model. Symbols are the same as above. $\gamma \approx 1-2$ is typical of terrestrial solids, whereas in the ion plasma $\gamma = 1/2$. Bottom: thermal conductivity of phonons in the anharmonic scattering regime. Symbol shape indicates field strength, as above, while open and filled symbols stand for $T = 10^6$ and $10^7$ K, respectively. The green dashed line labeled “CH6” is the conductivity calculated by Chugunov & Haensel (2007) for a hybrid ion plasma/Coulomb crystal with $B = 3 \times 10^{12}$ gauss and $T = 10^6$ K, using our Equation 18 times an enhancement factor $\exp(\beta T_p/T)$, where $T_p$ is an order of magnitude greater than $\Theta_m$. The green solid line labeled “CH7” is the same thing, but with $T = 10^7$ K. These enhancement factors are of order unity, and the three order of magnitude difference between Chugunov & Haensel’s result and ours is coming from the ratio $\omega_p^2/e^2$. At the highest densities considered here, $\omega_p$ is about 11 times larger in the MTF model than the value $2\pi e^2/\kappa_{ph}$ corresponding to Chugunov & Haensel’s hybrid model. As discussed in Section 6, the phonon conductivity has a smooth, power-law dependence on density (in the lowest Landau level model), and does not jump discontinuously to the hybrid model result.

7. DISCUSSION

Anisotropy of electron conductivity in magnetized neutron star envelopes may be as large as $\kappa_{||}/\kappa_{\perp} \sim 10^6$ (Potekhin 1999), while Pérez-Azorín et al. (2006) and Chugunov & Haensel (2007) found that including isotropic phonon conductivity from a hybrid ion plasma/Coulomb crystal reduces the total anisotropy to $\kappa_{||}/\kappa_{\perp} \sim \kappa_{ph}/\kappa_{ih} \sim 10^3$ (their Figures 6 and 5, respectively). Our result, which takes electron polarizability into account, suggests this is further reduced to $\kappa_{ph}/\kappa_{ih} \sim 1$ in the outer envelope. The effect is that of a “heat-spreader cladding,” which could be significant so long as transport in the outer envelope is not dominated by the Hall term, as in the case of magnetars ($B \gtrsim 10^{14}$ gauss) and very old neutron stars ($\gtrsim 10^5$ yrs). While many pulsars fit this description, x-ray emission from the surface is generally not seen; observable signatures of heat-spreading would be most likely to originate from the “Magnificent Seven” isolated neutron stars, a handful of x-ray pulsars (see Lin et al. (2014) for a new one and discussion of others), and central compact objects in supernova remnants. The latter have weak surface fields ($B \lesssim 10^{11}$ gauss) inferred from spin-down observations, but they could have a stronger internal field buried by fallback (Viganò & Pons 2012). See Perna et al. (2013) for more discussion of these types of stars.
input to simulations becomes crucial. The next generation of magneto-thermal evolution simulations can now make use of updated microphysics with enhanced phonon conductivity in the outer envelope where electron polarizability is non-negligible.

Our work (complementary to Kobyakov & Pethick [2014] which considered high density) suggests that the crystal lattice structure of a neutron star crust is more complicated than heretofore assumed. Even without invoking a multi-component accreted crust or interstitial neutrons, our results show that the equilibrium structure can have unexpectedly low symmetry. We briefly mention some possible consequences of a symmetry-lowering transition, such as that arising from the $c' < 0$ elastic instabilities we have found. Aside from obvious thermodynamic signatures such as latent heat, a low-symmetry structure should couple to the magnetic field direction. If the coupling is strong, one can imagine the transition being driven by a changing field, or conversely, the transition exerting a back-action on the crustal field, which could have non-local effects. Also, a $c' < 0$ driven transition could potentially be of a martensitic (shape memory) nature.

T.A.E. acknowledges an Academic Computing Fellowship from Pennsylvania State University. We thank George Pavlov for useful comments on the manuscript.

REFERENCES

Anderson, O.L. 1963, Journal of Physics and Chemistry of Solids, 24, 7
Ashcroft, N.W., & Mermin, N.D. 1976, Solid State Physics, (Belmont, CA: Brooks/Cole)
Baiko, D.A. 2002, Phys. Rev. E, 66, 5
Baiko, D.A. 2009, Phys. Rev. E, 80, 4
Banerjee, B., Constantinescu, D.H., & Rehák, P. 1974, Phys. Rev. D, 10, 8
Chamel, N., & Haensel, P. 2008, Living Rev. Relativity, 11, 10
Chugunov, A.I., & Haensel, P. 2007, MNRAS, 381, 1143
Danz, R.W., & Glasser, M.L. 1971, Phys. Rev. B, 4, 1
Falgout, R.D., Jones, J.E., & Yang, U.M. 2006, in Numerical Solution of Partial Differential Equations on Parallel Computers, ed. Bruaset, A.M., & Tveito, A. (Springer-Verlag Berlin Heidelberg), 51
Fushiki, I., Gudmundsson, E.H., & Pethick, C.J. 1989, ApJ, 342, 958
Fushiki, I., Gudmundsson, E.H., Pethick, C.J., & Yngvason, J. 1992, Annals of Physics, 216, 1
Geppert, U., Kükler, M., & Page, D. 2004, A&A, 426, 1
Grinwall, G. Magyari-Köpe, B., Oxolins, V., & Persson, K.A. 2012, Reviews of Modern Physics 84, 2
Haensel, P., Potekhin, A.Y., & Yakovlev, D.G. 2007, Neutron Stars 1: Equation of State and Structure, (New York, NY: Springer Science+Business Media, LLC)
Jain, J.K. 2007, Composite Fermions, (New York, NY: Cambridge University Press)
Jones, P.B. 1986, MNRAS, 218, 477
Kobyakov, D., & Pethick, C.J. 2014, Phys. Rev. Lett., 112, 11
Kohmoto, M., Halperin, B.I., & Wu, Y. 1993, Physica B, 184, 1
Lai, D. 2001, Reviews of Modern Physics, 73, 3
Lieb, E.H., Solovej, J.P., & Yngvason, J. 1992, Phys. Rev. Lett., 69, 5
Lin, L.L.C., Hui, C.Y., Li, K.T., et al. 2014, arXiv:1408.4741
MacFarlane, J.J., & Hubbard, W.B. 1983, ApJ, 272, 301
Medin, Z., & Lai, D. 2006, Phys. Rev. A, 74, 6
Morton, K.W., & Mayers, D. 2005, Numerical Solution of Partial Differential Equations, (2nd ed.; New York, NY: Cambridge University Press)
Nijboer, B.R.A., & De Wette, F.W. 1957, Physica, 23, 309
Pérez-Azorín, J.F., Miralles, J.A., & Pons, J.A. 2006, A&A, 451, 3
Perna, R., Viganò, D., Pons, J.A., & Rea, N. 2013, MNRAS, 434, 3
Phillips, R.B. 2001, Crystals, Defects and Microstructures: Modeling Across Scales, (Cambridge, United Kingdom: Cambridge University Press)
Pons, J.A., Miralles, J.A., & Geppert, U. 2009, A&A, 496, 1
Potekhin, A.Y. 1999, arXiv:astro-ph/9909100
Potekhin, A.Y., & Yakovlev, D.G. 2001, A&A, 374, 1
Press, W.H., Teukolsky, S.A., Vetterling, W.T., & Flannery, B.P. 2007, Numerical Recipes: The Art of Scientific Computing, (3rd ed.; New York, NY: Cambridge University Press)
Viganò, D., & Pons, J.A. 2012, MNRAS, 425, 4
Viganò, D., Rea, N., Pons, J.A., et al. 2013, MNRAS, 434, 1
Viganò, D., Perna, R., Rea, N., & Pons, J.A. 2014, arXiv:1406.0874
Yngvason, J. 1991, Letters in Mathematical Physics, 22, 2
Ziman, J.M. 1960, Electrons and Phonons: The Theory of Transport Phenomena in Solids, (Oxford: Clarendon Press)