

taken to be half the nearest-neighbour distance.  $E_{\text{MTZ}}$  is taken as the effective energy zero in the metal.

The actual construction of a muffin-tin potential is based on the MATTHEISS (1964) prescription of overlapping Hartree-Fock-Slater neutral atom charge densities. The total charge density  $f(\mathbf{r})$  can be written as:

$$f(\mathbf{r}) = f_0(\mathbf{r}) + \sum_{i \neq 0} f(\mathbf{r} - \mathbf{R}_i), \quad (6)$$

where  $\mathbf{R}_i$  is the position of an atom neighbouring the central atom  $i = 0$ . For liquid iron we assumed that the atoms were arranged in the bcc structure with a lattice parameter  $a$  corresponding to the density of the liquid, i.e.

$$\begin{aligned} \Omega_0 &= \frac{1}{2}a^3, \\ R_{\text{MT}} &= (\frac{1}{4}\sqrt{3})a. \end{aligned} \quad (7)$$

The coordination number of normal liquid iron near its melting point is  $\approx 9$  (WASEDA and SUZUKI, 1970; RUPPERSBERG and SEEMAN, 1966), which is not very different from the corresponding value of 8 for the bcc lattice. The total charge density should not be very sensitive to small changes in the coordination number or indeed to changes in the positions of atoms further away than the nearest neighbours. The electron-ion potential is obtained by solving the appropriate Poisson equation. Some average of the electron exchange interaction has to be included, and this has been done using a form of the Slater free-electron approximation; for details see DREIRACH *et al.* (1972) and the references therein.

The Fermi energy  $E_F$  can be calculated at each density using the method given by DREIRACH (1971). We write

$$E_F = E_b + \frac{\hbar^2}{2m^*} K_F^2, \quad (8)$$

where  $E_b$  is the energy of the bottom of the conduction band,  $m^*$  is a constant effective mass which is independent of density.  $K_F$  is the Fermi radius given by the familiar free-electron result,

$$K_F^3 = 3\pi^2 Z / \Omega_0. \quad (9)$$

Here  $Z$  is the number of "valence" electrons which we have taken to be constant and equal to one for iron. A discussion of the physics behind this choice is given by DREIRACH *et al.* (1972). Eq. (8) assumes that the width of the conduction band,  $E_F - E_b$ , scales with

density  $\Omega_0^{-1}$  like a simple parabolic band. The energy of the bottom of the band can be calculated from a knowledge of the  $s$  phase shifts of the corresponding muffin-tin potential, while the effective mass  $m^*$  was evaluated from band structure data on solid iron (WOOD, 1962).

We calculated muffin-tin potentials at several densities using the method outlined above. The phase shifts  $\eta_l$  were calculated for several energies by numerically integrating the radial Schrödinger equation inside the muffin-tin sphere. In table 1, we list the calculated val-

TABLE 1

Parameters entering the evaluation of the scattering cross-section at different densities. Here  $\Omega/\Omega_0$  is the ratio of atomic volumes, with  $\Omega_0$  the atomic volume of normal liquid iron. The muffin-tin zero  $E_{\text{MTZ}}$  is measured with respect to atomic zero. The energies  $E_b$ ,  $E_r$  and  $E_F$  are measured with respect to  $E_{\text{MTZ}}$

Density (g/cm <sup>3</sup> )	$\Omega/\Omega_0$	$E_{\text{MTZ}}$ (Ry)	$E_b$ (Ry)	$E_r$ (Ry)	$E_F$ (Ry)	$\Gamma$ (Ry)
6.86	1	-1.420	0.060	0.527	0.632	0.070
7.92	0.866	-1.626	0.141	0.66	0.77	0.110
8.82	0.778	-1.794	0.220	0.77	0.896	0.150
9.00	0.763	-1.828	0.237	0.79	0.922	0.155
9.40	0.730	-1.903	0.276	0.838	0.98	0.180

ues of some relevant parameters which determine the scattering cross section for the conduction electrons. Although we do not use the "resonance" formulae (4) and (5) in the actual calculation of the resistivity, it is instructive to look at how the position and width of the  $d$  resonance changes with the variation of density because these have major influence on the resistivity. As the density increases, the muffin-tin zero  $E_{\text{MTZ}}$  gets progressively lower, and this is simply due to the increasing overlap of the neighbouring atomic charge densities or potentials. The energy of the bottom of the band  $E_b$  and the resonance energy  $E_r$  both increase on decreasing the atomic volume. The width  $\Gamma$  of the resonance is a strong function of density and increases rapidly with increasing density. This in turn implies that the  $d$  band in the corresponding metal will broaden with an increase in density.

To calculate the resistivity, we need to know the liquid structure factor  $a(q)$  at each density. There is little experimental information about this, but it is possible, however, to make reasonable estimates of the behaviour of  $a(q)$  using the hard-sphere model (ASHCROFT and LEKNER, 1966). In this model, the structure

factor has a simple analytic form which depends on only two parameters, the packing fraction  $p$  and the hard sphere diameter  $R$ . These parameters are related to each other as

$$R^3 = \frac{6\Omega_0 p}{\pi}. \quad (10)$$

For most liquid metals under normal pressure and at temperatures near the melting point, a good approximation to the experimental structure factor can be obtained using a value of  $p$  equal to 0.45. The same choice for iron reproduces the observed  $a(q)$  of WASEDA and SUZUKI (1970) quite closely.

We estimated the variation of  $a(q)$  with density by making use of the thermodynamic relation (ASHCROFT and LEKNER, 1966)

$$a(0) = \frac{(1-p)^4}{(1+2p)^4} = \frac{K_B T \beta}{\Omega_0}, \quad (11)$$

where  $K_B$  is Boltzmann's constant,  $T$  is the absolute temperature and  $\beta$  is the isothermal compressibility.

If we want to calculate the electrical resistivity of iron in the Earth's core, we must take into account the variation of both the temperature and the density, i.e., we should know the relevant equation of state. Given such information, we can calculate the compressibility  $\beta$ , solve for  $p$  in eq. (11) and hence construct the appropriate structure factor.

HIGGINS and KENNEDY (1971) have recently attempted to analyse the temperature, pressure and density distributions in the Earth's core. They find that the pressure-temperature conditions approximate the melting curve for iron. We have used their data to calculate the packing fraction for several densities.

#### 4. Results for the resistivity of liquid iron

The resistivity was calculated by performing the integral in eq. (1) and using the full  $t$  matrix of eq. (3). For pure iron at 1620 °C, we obtained a value of 172  $\mu\Omega \cdot \text{cm}$  for the resistivity, which is in reasonable agreement with the experimental value of 139  $\mu\Omega \cdot \text{cm}$ . This calculation employed the experimental structure factor of WASEDA and SUZUKI (1970). The results for the resistivity at different densities and temperatures, calculated using the procedure for the structure factor outlined above, are listed in table 2. We predict a decrease in resistivity as the pressure and temperature

increase. The trends in these results are in qualitative agreement with those of KEELER and ROYCE (1971), who carried out shock wave experiments on the resistivity of *solid* iron.

TABLE 2

Calculated values of the resistivity of pure iron for various points on the melting point curve

Density (g/cm <sup>3</sup> )	Temperature (°C)	Pressure (Mbar)	Resistivity $\mu\Omega \cdot \text{cm}$
8.0	2400	0.15	138
8.5	2800	0.25	134
9.0	3000	0.46	124
9.5	3300	0.69	98
10.0	3400	0.77	63

KEELER and ROYCE (1971) have also measured the electrical conductivity of pure iron at pressures of  $\approx 1$  Mbar and at temperatures above 3000 °C. They give a value for the resistivity of iron of about 57  $\mu\Omega \cdot \text{cm}$  at 1.4 Mbar, this pressure corresponding to that at the core-mantle interface. Since our calculations are based on the HIGGINS and KENNEDY (1971) temperature-density relation for the melting curve of iron, our results should not be compared *directly* with these high-temperature shock-wave data of KEELER and ROYCE (1971). Nevertheless, if we take the density of iron at the interface to be 10 g/cm<sup>3</sup> (as quoted by KEELER and ROYCE, 1971), then according to the melting curve given by HIGGINS and KENNEDY (1971) the corresponding pressure and temperature would be about 0.77 Mbar and 3400 °C, respectively. Our calculated value of the resistivity under these conditions is 63  $\mu\Omega \cdot \text{cm}$  which is close to the shock-wave result, although the latter corresponds to a pressure of 1.4 Mbar and a temperature of 3500 °C.

#### 5. Discussion

The magnetohydrodynamic theories of the origin of the geomagnetic field require that the magnetic Reynolds number should be much larger than unity. The accepted figure is about 100, and this imposes a lower limit on the magnitude of the electrical conductivity of the outer liquid core. This limit is about  $3 \times 10^3 \Omega^{-1} \cdot \text{cm}^{-1}$  (e.g., KEELER and ROYCE, 1971, and references therein). In other words, the resistivity should be less than about 330  $\mu\Omega \cdot \text{cm}$ . Clearly our calculated figure easily satisfies this requirement. Even allowing for in-