were taken to be

$$V_{xc}^{+}(r_s)=\mu_{xc}(r_s)+\tfrac{1}{3}A(r_s)\left[\frac{\rho^{+}-\rho^{-}}{\rho}\right],$$

$$V_{xc}^{-}(r_s)=\mu_{xc}(r_s)+\tfrac{1}{3}A(r_s)\left[\frac{\rho^{-}-\rho^{+}}{\rho}\right],$$

where ρ^{+} and ρ^{-} are the spin-up and spin-down electron charge densities, respectively, ρ is the total electron charge density,

$$\mu_{xc}(r_s)=\beta(r_s)\,V_{KS}(r_s)$$

and

$$A(r_s)=S(r_s)\,V_{KS}(r_s)\ .$$

Here $V_{KS}(r_s)$ is the Kohn–Sham $\alpha=\frac{2}{3}$ exchange potential.

$$\beta(r_s)=1+C_p x\ln(1+1/x)$$

and

$$S(r_s)=1+\frac{C_p}{2}y\ln(1+1/y)\ ,$$

where

$$x=\frac{r_s}{r_p}\ ,\quad y=\frac{r_s}{2^{4/3}r_p}$$

and

$$r_s=(3/4\pi\rho)^{1/3}\ .$$

Following Janak,[15] we set $C_p=0.045$ and $r_p=21.0$.

(iv) Semirelativistic, soft-core calculation with different values for α for the spin-up and spin-down bands, $\alpha\uparrow=0.728$ and $\alpha\downarrow=0.708$, as obtained from the results of Gopinathan *et al.*[16] This will be referred to as the GWB model.

B. Self-consistent APW method

The APW method that we have used to calculate spin-polarized energy bands and the Fermi surface roughly follows the approach by Connolly.[3] All calculations were carried out self-consistently within the muffin-tin approximation. The lattice constant corresponding to normal spacing was taken to be $a=3.5235$ Å, which is also the value chosen by Connolly. After each iteration the fractions of occupied spin-up and spin-down states were determined as well as the Fermi energy; these values were used in the construction of the exchange potential for the succeeding iteration.

In order to compare with pressure measurements, calculations were also made for a lattice spacing reduced by 2.5% with the NR model and by 2.5 and 5% for the vBH form of exchange and correlation. If one assumes the compressibility is constant (5.5×10^{-4} kbar^{-1}),[17] these values correspond to pressures of 135 and 270 kbar, respectively, and were thought to be large enough to give changes greater than the errors of the calculation and small enough that gross distortions in the energy bands were not expected.

For the nonrelativistic calculations the initial configurations for the spin-up and spin-down electrons were chosen as $3d^5 4s^1$ and $3d^4$, respectively, while for the relativistic calculations the initial configurations were chosen somewhat arbitrarily as $3d^{4.5}4s^{0.5}$ and $3d^4 4s^1$ for spin-up and spin-down, respectively. In all of our calculations for nickel a final spin-polarized (magnetic) system was obtained. It would be interesting to make a test of our method by carrying out similar calculations for copper. (Wang and Callaway,[5] using a nonrelativistic Hamiltonian and a slightly different value for the lattice constant, appear to have started with the same configuration for both the spin-up and spin-down states and obtained final values for the exchange splitting in nickel which were similar to ours.)

Initially the calculations were carried out self-consistently using about five iterations at six points in $\frac{1}{48}$th of the Brillouin zone and subsequently four or five more iterations at 20 points in $\frac{1}{48}$th of the Brillouin zone. It was assumed that convergence had been attained when the changes in energy levels in successive iterations were approximately 2 mRy. When we began calculating cross-sectional areas of the Fermi surface and their changes with pressure, however, we discovered inconsistencies in the values calculated. We were finally able to conclude that these errors were primarily the result of lack of convergence in our calculation. In order to discuss this, we must first describe our treatment of the constant potential outside the muffin tins.

For the standard APW calculation the constant potential outside the muffin-tin spheres is set equal to zero and all the energy levels are shifted accordingly. In the spin-polarized calculations, however, spin-up and spin-down bands are calculated separately and in each case the potential outside the muffin tin is set equal to zero. The energies of the two sets of bands, corresponding to what we call Potential 1 and Potential 2, are shifted independently and these shifts must be reconciled in order to properly position the Fermi energy. We chose to leave the energy bands calculated from Potential 1 (spin-down bands for the von Barth–Hedin form for exchange and correlation) unshifted and to shift the bands corresponding to Potential 2 by an amount $|V_{0\uparrow}|-|V_{0\downarrow}|$, where $V_{0\uparrow}$ and $V_{0\downarrow}$ are the values of the constant potentials outside the muffin tin for the spin-up and spin-down bands, respectively. After each iteration this shift was made and then the Fermi level was determined.

The lack of convergence manifested itself particularly in the amount of the shift. Therefore, although the bands corresponding to Potential 1 appeared to be converged to better than 1 mRy, this was not the case for the Potential 2 bands. We found it necessary to iterate for the 20-point mesh a total of about 15 times in order to obtain satisfactory convergence, that is changes in all energy levels of less than 0.5 mRy for successive iterations.

After the energy bands had been converged from the 20-point mesh, a final calculation was made at 89 points in $\frac{1}{48}$ of the Brillouin zone. The Fermi surface was obtained by interpolation from this 89-point mesh except for the two small pieces, the necks at L and the hole pockets at X. In these cases the energies were calculated at $\vec{k}$ values appropriate to the 240-point mesh. Even after all this there remained small discrepancies in the values of Fermi surface areas due to numerical errors from integration and interpolation. These were most notable for the smaller cross sections and thus our results for the changes in such Fermi-surface cross sections with lattice spacing are only semiquantitative.

C. Interpolation procedures– Fermi-surface calculations

Subsequent to the final iteration, energy values were interpolated by the linear tetrahedron method,[18] starting with 89 first-principles APW points in $\frac{1}{48}$ of the Brillouin zone, to determine the density of states and its angular-momentum components, the magnetic moment per atom, Fermi-surface cross-sectional areas, and cyclotron masses. These quantities were also calculated by a Slater–Koster (SK) fit to the APW energies and the results were essentially the same as those obtained from the tetrahedron scheme. Both schemes for interpolation are described below.

In the tetrahedron approach the Brillouin zone is subdivided into tetrahedra, the corners of which correspond to $\vec{k}$ vectors at which energies have been determined from the APW calculations. Within each tetrahedron each band is interpolated linearly. That is, $\epsilon_j(\vec{k}) = \epsilon_{j0} + \vec{a}_j \cdot \vec{k}$, where $\epsilon_j(\vec{k})$ is the energy of the jth band at point $\vec{k}$, and ϵ_{j0} and the three components of $\vec{a}_j$ are parameters obtained from the known values of $\epsilon_j(\vec{k})$ at the corners of the tetrahedron. This form of interpolation is well suited to the computation of densities of states and similar functions because a single analytic expression exists for the contribution from each tetrahedron.[18] This approach can also be conveniently used for determination of the shape of the Fermi surface. The simple linear formula for each tetrahedron, together with an appropriate scheme for selecting the correct tetrahedron in the fundamental Brillouin zone corresponding to an arbitrary $\vec{k}$ vector provides an efficient algorithm for specifying $E(\vec{k})$ for all $\vec{k}$. The linear expressions for adjacent tetrahedra become identical at their common cell boundaries, and therefore the interpolated band structure is continuous from one cell to the next. Once $\epsilon_j(\vec{k})$ is determined for all bands j it is a straightforward matter to determine the extremal cross-sectional areas of the Fermi surface and the corresponding cyclotron masses.

TABLE II. Density-of-states decomposition.

Calculation	Densities of states (Ry spin)$^{-1}$				
	$N_s(E_F)$	$N_p(E_F)$	$N_d(E_F)$	$N_f(E_F)$	$N_{\mathrm{total}}(E_F)$
$a_0\uparrow$ NR[a]	0.1695	0.3107	1.5262	0.0006	2.2191
$a_0\downarrow$ NR[a]	0.0838	0.1708	19.1683	0.0521	19.688
$a_0\uparrow$ SR[a]	0.1832	0.3942	1.5955	0.0070	5.3379
$a_0\downarrow$ SR[a]	0.1065	0.2081	20.0850	0.0429	20.6680
$a_0\uparrow$ vBH[a]	0.1913	0.4098	1.7130	0.0074	2.5762
$a_0\downarrow$ vBH[a]	0.1017	0.1983	21.3050	0.0430	21.8732
$a_0\uparrow$ vBH[b]	0.2751	0.4396	(1.1470[c]– 2.542[d])		2.116
$a_0\downarrow$ vBH[b]	0.2249	0.2058	(14.435[c]– 6.080[d])		20.940
0.975 $a_0\uparrow$ vBH[a]	0.1660	0.2967	1.785	0.0062	2.4487
0.975 $a_0\downarrow$ vBH[a]	0.0924	0.1844	19.420	0.0419	19.9543
0.950 $a_0\uparrow$ vBH[a]	0.1321	0.3119	1.6735	0.0076	2.3270
0.950 $a_0\downarrow$ vBH[a]	0.0849	0.1743	17.490	0.0414	18.000

[a]Tetrahedron interpolation from 89-point mesh.
[b]Slater–Koster interpolation from 20-point mesh.
[c]T_{2g} symmetry.
[d]E_g symmetry.