A linearised relativistic augmented-plane-wave method utilising approximate pure spin basis functions†

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Abstract. We describe a fully relativistic augmented-plane-wave (APW) method where the basis functions are pure spin functions in the large component. This feature allows spin-mixing interactions to be separated and treated more efficiently than in the standard relativistic APW method. These basis functions are constructed by solving an approximate relativistic radial equation. In addition, the energy derivative is used in the construction of the basis functions so that one obtains adequate variational freedom solving a linear secular equation. Both the utility and the limitations of the technique are discussed.

The desirability of computationally fast approximate methods for solving the single-particle Dirac equation in a crystal potential is apparent. Recently a number of authors have suggested similar techniques based on approximating the solution of the Dirac equation in the central field (Rosicky *et al* 1976, Koelling and Harmon 1977, Wood and Boring 1978, Takeda 1978, 1979). At their lowest level these approximations can be directly incorporated into non-relativistic molecular and energy band computations by simply performing a different radial solution. At this level, one is omitting spin–orbit coupling but including scalar particle corrections as would be done with the Klein–Gordon equation. In this note, we discuss the implementation of the Koelling–Harmon method for the central-field Dirac equation in the linearised APW band structure method (Anderson 1975, Koelling and Arbman 1975). The formal basis of the technique is the variational solution of the Dirac single-particle equation in the periodic potential. We first discuss the construction of approximate basis functions using a muffin-tin approximation for the crystal potential. The use of these basis functions in the full Dirac equation with a non-muffin-tin potential is then considered. Finally we review our experience with the technique and discuss a situation where the procedure breaks down.

It will be useful to rederive the results of Koelling and Harmon here to place them in context for discussing the limitations of the procedure used. We will always measure energies relative to the rest-mass energies so that the single-particle Hamiltonian can be written as

$$H = c\boldsymbol{\alpha} \cdot \boldsymbol{p} + (\beta - 1)mc^2 + V(r) \tag{1}$$

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where $V(r)$ is the crystal potential and the notation is standard. The procedure is to take the radial equations for the relativistic $\kappa = l$ $(j = l - \frac{1}{2})$ and $\kappa = -l - 1$ $(j = l + \frac{1}{2})$ orbitals which are uncoupled for a spherical potential, and transform to the equations for the average and the difference. We then assume the difference for the large component (but not the small) to be negligible so that we need only solve for the average. With this average function, basis functions are constructed which are then used with the full Dirac formalism.

The radial Dirac equation can be written

$$\frac{dP_\kappa}{dr} = -\kappa P_\kappa + 2McQ_\kappa \tag{2a}$$

$$\frac{dQ_\kappa}{dr} = (1/c)(V - \epsilon)P_\kappa + \kappa Q_\kappa \tag{2b}$$

$$M \equiv m + (1/2c^2)(\epsilon - V_{\mathrm{MT}}) \tag{2c}$$

where P and Q are the large and small component radial solutions multiplied by the radius r. We use only the spherical component of the potential, V_{MT}, at this point. We now consider the average and difference functions $\bar{P}_l, \bar{Q}_l, \delta P_l, \delta Q_l$, defined by

$$(2l + 1)\bar{P}_l \equiv lP_l + (l + 1)P_{-l-1} \tag{3a}$$

$$(2l + 1)\bar{Q}_l \equiv lQ_l + (l + 1)Q_{-l-1} \tag{3b}$$

$$\delta P_l \equiv P_{-l-1} - P_l \tag{3c}$$

$$\delta Q_l \equiv Q_{-l-1} - Q_l. \tag{3d}$$

The equations satisfied by these quantities are

$$\frac{d}{dr}\bar{P}_l - \frac{1}{r}\bar{P}_l = 2Mc\bar{Q}_l + \frac{l(l+1)}{(2l+1)}\frac{1}{r}\delta P_l \tag{4a}$$

$$\frac{d}{dr}\bar{Q}_l + \frac{1}{r}\bar{Q}_l = \frac{1}{c}(V - \epsilon)\bar{P}_l - \frac{l(l+1)}{(2l+1)}\frac{1}{r}\delta Q_l \tag{4b}$$

$$\frac{d}{dr}(\delta P_l) = \left(\frac{2l+1}{r}\right)\bar{P}_l + 2Mc\delta Q_l \tag{4c}$$

$$\frac{d}{dr}(\delta Q_l) = \frac{1}{c}(V_{\mathrm{MT}} - \epsilon)\delta P_l - \left(\frac{2l+1}{r}\right)\bar{Q}_l. \tag{4d}$$

From here forward we will drop the subscript l (and the bar over $\bar{P}, \bar{Q}$) for convenience. If we now assume that $(d/dr)(\delta P) \simeq 0$, equation (4c) yields

$$\partial Q \approx -(\tfrac{1}{2}Mc)[(2l + 1)/r]P \tag{5}$$

which can be substituted into equation (4b). The resulting equation plus equation (4a) with $\delta P \simeq 0$ gives the result of Koelling and Harmon which was derived somewhat differently: the elimination method with the same criterion was applied to the second-order equation before unfolding back to two coupled first-order equations. We will use

$$\phi_{lms} = \frac{1}{r}\begin{bmatrix} P_l Y_{lm}\chi_s \\ i\hat{r} \cdot \sigma[-Q_l + (P_l/2Mcr)\sigma \cdot L] Y_{l,m}\chi_s \end{bmatrix} \tag{6}$$

as our l, m, s, component of the basis functions where χ_s is the two-component spinor and P and Q satisfy the radial equations of Koellin and Harmon

$$\frac{dP}{dr} - \frac{1}{r}P = 2McQ \tag{7a}$$

$$\frac{dQ}{dr} + \frac{1}{r}Q = \left[\frac{l(l+1)}{2Mcr^2} + \frac{(V - \epsilon)}{c}\right]P \tag{7b}$$

The second term in the lower component of equation (6) is the result of using equation (5). It is easily verified that using the muffin-tin full Dirac Hamiltonian (equation (1) with $V(r)$ replaced by $V_{MT}(r)$), one gets

$$H_{MT}\phi_{lms} = \epsilon\phi_{lms} + H_0^{so}\phi_{lms} \tag{8a}$$

$$H_0^{so} \equiv \frac{1}{(2Mc)^2}\frac{1}{r^2}\frac{dV_{MT}(r)}{dr}\begin{bmatrix} P\boldsymbol{\sigma}\,.\,\boldsymbol{L}Y_{lm}\chi_s \\ 0 \end{bmatrix}. \tag{8b}$$

It should be noted that H_0^{so} is a spin–orbit coupling operator and that the last term in equation (8a) is a measure of the extent to which the ϕ_{lms} fails to be a true solution of the spherical potential Dirac equation. Further, the spin and orbital wavefunctions are separated in the upper components of ϕ_{lms}. This is a useful feature of the method as it allows the spin mixing interactions to be separated and treated in a final variation. It is useful to impose the normalisation condition

$$\int_0^R dr\,(P_l^2 + Q_l^2) = 1 \tag{9}$$

to complete the specification of each angular momentum component.

The method we consider is an augmented-plane-wave (APW) method (Slater 1937). Thus, in the interstitial region we use basis functions which are plane waves.

$$P(k_n s; r) \equiv \begin{bmatrix} \chi_s \\ [(\boldsymbol{\sigma}\,.\,\boldsymbol{k}_n)/(W_n + mc^2)]\chi_s \end{bmatrix} \Omega^{-1/2}\exp(\mathrm{i}\boldsymbol{k}_n\,.\,\boldsymbol{r}) \tag{10a}$$

$$\boldsymbol{k}_n = \boldsymbol{k} + \boldsymbol{G}_n \tag{10b}$$

$$W_n^2 = m^2c^4 + k_n^2c^2 \tag{10c}$$

where Ω is the crystal volume and $\boldsymbol{G}_n$ is a reciprocal-lattice vector. Note that we omit the relativistic normalisation factor as we will have to renormalise anyway due to the augmentation. Furthermore it will be quite adequate to make the approximation $W_n + mc^2 \simeq 2mc^2$.

There is a great deal of latitude in the way one chooses to augment the plane waves. The original Slater APW formulation required that one use solutions $\phi_{lms}(\epsilon)$ where ϵ equalled the eigenvalue. Although strictly correct, this results in a non-linear secular equation. One can view the ϵ_l (one for each angular momentum) as non-linear variational parameters and greatly facilitate the solution of the problem, but the final result is the same as the standard prescription (Harmon and Koelling 1974). Alternatively, one can formulate a discrete set which forms the basis for expansion of the ϕ_{lms} at the eigenvalue (Bross 1964, Koelling 1970). Done carefully, this can produce a secular problem which can be solved by a single diagonalisation (Bross *et al* 1970, Takeda and Kübler 1979, Williams *et al* 1979). It has been shown that over surprisingly large energy ranges, using only the function $\phi_{lms}(\epsilon_l)$ and its first energy derivative, denoted $\dot{\phi}_{lms}(\epsilon_l)$, provides

adequate variational freedom.

$$\phi_{lms}(r) \simeq \frac{1}{r}\left[\begin{matrix} P_l Y_{lm}\chi_s \\ i(\boldsymbol{\sigma}\cdot\hat{r})[-\dot{Q}_l + (1/2Mcr)\dot{P}_l\boldsymbol{\sigma}\cdot\boldsymbol{L}]Y_{lm}\chi_s \end{matrix}\right] \tag{11}$$

where $\dot{P}_l$ and $\dot{Q}_l$ satisfy

$$\frac{d}{dr}\dot{P}_l - \frac{1}{r}\dot{P}_l = \frac{2Mc}{r}\dot{Q}_l + \frac{1}{c}Q_l \tag{12a}$$

$$\frac{d}{dr}\dot{Q}_l + \frac{1}{r}\dot{Q}_l = \left[\frac{l(l+1)}{2Mcr^2} + \frac{1}{c}(V_{MT} - \epsilon)\right]\dot{P}_l - \frac{1}{c}P_l \tag{12b}$$

with the requirement that

$$\int_0^R dr(P_l\dot{P}_l + Q_l\dot{Q}_l) = 0. \tag{12c}$$

Higher-order terms have been omitted in equations (11) and (12b). The muffin-tin Dirac Hamiltonian now gives

$$H_{MT}\dot{\phi}_{lms} = \epsilon\dot{\phi}_{lms} + \phi_{lms} + H_1^{so}\dot{\phi}_{lms} \tag{13a}$$

$$H_1^{so}\dot{\phi}_{lms} = \frac{1}{(2Mcr)^2}\frac{dV_{MT}}{dr}\left(\dot{P}_l - \frac{P_l}{4Mc^2}\right)\left[\begin{matrix}\boldsymbol{\sigma}\cdot\boldsymbol{L}Y_{lm}\chi_s \\ 0\end{matrix}\right] \tag{13b}$$

omitting terms of order $(1/m^3)$.

The APW within the muffin-tin spheres of radius R is now

$$P(\boldsymbol{k}_n s; r) = \sum_{lm}(A_{lm}(\boldsymbol{k}_n)\,\phi_{lms}(r) + B_{lm}(\boldsymbol{k}_n)\,\dot{\phi}_{lms}(r)) \tag{14}$$

where A and B are determined from the requirement that the large component and its spatial derivative be continuous across the muffin-tin sphere boundary. The lower components of the basis function will then have a discontinuity across the sphere boundary of order $(\Delta V_{MT} + k_n^2/2m - \epsilon_l)/mc^2$ which can be neglected. ΔV_{MT} is the discontinuity of the muffin-tin potential at R. The resulting variational solution if carried to full convergence would have a discontinuity of order $\Delta V_{MT}/mc^2$ for a muffin-tin calculation and would be continuous for the general potential. Utilising the Rayleigh expansion of the interstitial plane wave, one finds

$$A_{lm}(\boldsymbol{k}_n) = 4\pi R^2\Omega^{-1/2}i^l Y_{lm}^*(\hat{\boldsymbol{k}}_n)a_l(k_n) \tag{15a}$$

$$a_l(k_n) = \frac{\dot{g}_l(d/dr)j_l(k_nR) - (d\dot{g}_l/dr)j_l(k_nR)}{R^2(\dot{g}_l\,dg_l/dr - g_l\,d\dot{g}_l/dr)} \tag{15b}$$

$$B_{lm}(\boldsymbol{k}_n) = 4\pi R^2\Omega^{-1/2}i^l Y_{lm}(\hat{\boldsymbol{k}}_n)b_l(k_n) \tag{15c}$$

$$b_l(k_m) = \frac{j_l(k_nR)(dg_l/dr) - g_l(d/dr)j_l(k_nR)}{R^2(\dot{g}_l\,dg_l/dr - g_l\,d\dot{g}_l/dr)} \tag{15d}$$

where $g_l = (1/r)P_l$ and is evaluated for $r = R$. The basis set is now specified once one specifies the $\{\epsilon_l\}$ for the ϕ and $\dot{\phi}$. In the typical case, one sets all $\{\epsilon_l\}$ equal to common energy central in the range of energies being examined, although this was not done for Pb.

Because we fix the $\{\epsilon_l\}$, we have a fixed basis set. Thus the variational procedure will

yield a linear secular equation. Although we have constructed the basis functions using approximate relativistic kinematics and a muffin-tin approximation to the potential, they are to be used with the full non-muffin-tin Dirac equation (1). Although there is some arbitrariness in the choice of variational functional because of the matching boundary, we will adopt the one used by Loucks (1965) in constructing the first fully relativistic APW method, which is given by

$$E[\psi] = \left(\int_{I+II} d^3r\psi^+ H\psi + i \int_{r=R} d^2r[\psi_{II}^+ \hat{r} . \alpha\psi_r - \psi_I^+ \hat{r} . \alpha\psi_{II}]\right)\Big/ \int_{I+II} d^3r\psi^+ \psi \qquad (16)$$

where region I is within the muffin-tin spheres and region II is the interstitial region. We expand

$$\phi = \sum_{ns} C_{ns} P(k_n, s; r) \qquad (17)$$

and perform the standard Rayleigh–Ritz variation to obtain the standard secular equation of the form

$$\mathbf{Hc} = E\mathbf{Sc}. \qquad (18)$$

The matrix elements $H_{n's', ns}$ and $S_{n's', ns}$ can be obtained in a straightforward fashion. Because the basis functions are continuous in the large component and very nearly so in the small component, the surface term of equation (16) will be of negligible size. One also may make a number of approximations in the evaluation of the volume integrals. The interstitial volume integral can be treated as though the plane waves were Pauli spinors. This is the same approximation used in the RAPW and relativistic Green function methods. Further, one may neglect the terms involving $\sigma . L$ in the small component. The approximations mentioned above may be relaxed without fundamentally complicating the method. We have found, however, that they have no significance in practice. (For simplicity we do not include them in the subsequent discussion.) The essence of the method is that one *temporarily* neglects matrix element of the spin–orbit operators H_0^{so} and H_1^{so} of equations (8) and (13). When this is done, one gets precisely the spin-diagonal non-relativistic form of Koelling and Arbman (1975)—their equations (13) and (16)—except that the radial solutions have been obtained from the 'semi-relativistic' radial equations. One can now solve this spin–orbit-less problem and include a majority of the relativistic effects since the spin–orbit coupling often has little effect away from the high symmetry points and lines. This has been done for a number of systems (Harmon *et al* 1978, Liu *et al* 1979; Koelling 1979) with excellent results. The non-muffin-tin components of the potential can be included at this step even when spin–orbit coupling is to be included later. This has been done for the RAPW method (Elyashar and Koelling 1976). In the process of attaining self-consistency the crystal potential in equation (1) is expressed as a functional of the charge density determined by solving equation (1) in the previous iteration. Since the charge density is often affected little by the spin–orbit coupling one can perform the self-consistency iterations at this level of approximation with little loss of accuracy. This approach works well even in the case of the heavy metal Th (Koelling 1979). The saving in computational effort is considerable, especially since one is able to avoid the doubling in size of the matrix and the complex matrix elements which occur when the spin–orbit interaction is included.

The primary spin–orbit effect enters through the matrix elements of H_0^{so} and H_1^{so}.

Defining

$$\xi^l \equiv \int_0^R dr P_l^2 \left(\frac{1}{2Mc}\right)^2 \frac{1}{r} \frac{dV_{MT}}{dr} \tag{19a}$$

$$\dot{\xi}^l \equiv \int_0^R dr P_l \dot{P}_l \left(\frac{1}{2Mc}\right)^2 \frac{1}{r} \frac{dV_{MT}}{dr} \tag{19b}$$

$$\ddot{\xi}^l \equiv \int_0^R dr \dot{P}_l^2 \left(\frac{1}{2Mc}\right)^2 \frac{1}{r} \frac{dV_{MT}}{dr} \tag{19c}$$

one has

$$H_{n's', ns} \approx H_{n', n}^{SR} \delta_{s, s'} + H_{n's', ns}^{so} \tag{20a}$$

$$S_{n's', ns} \simeq S_{n', n}^{SR} \delta_{s, s'} \tag{20b}$$

$$H_{n's', ns}^{so} \approx 4\pi \sum_{lmm'} R_{n'n}^l \left[\chi_{s'}^+ \int Y_l^{m'*} \boldsymbol{\sigma} \cdot \boldsymbol{L} Y_l^m \, d^2\hat{r} \chi_s\right] Y_l^{m'}(\boldsymbol{k}_{n'}) Y_l^m(\hat{\boldsymbol{k}}_n) \tag{20c}$$

$$R_{n'n}^l \equiv (4\pi R^4/\Omega)\{a_l(k_{n'}) a_l(k_n) \xi^l + [a_l(k_{n'}) b_l(k_n) + b_l(k_{n'}) a_l(k_n)] \dot{\xi}_l + b_l(k_{n'}) b_l(k_n) \ddot{\xi}_l\}. \tag{20d}$$

Terms of higher order in M^{-1} which we have shown to be insignificant even in Pb are omitted in equations (20a–d). This secular equation is to be solved by a two-step process much in the same way as the standard RAPW equations are solved (Koelling 1974). One first solves the problem for H^{SR} and S^{SR} to obtain a set of solutions C_n^{SR} and ϵ_j^{SR}. Then one uses the new basis set

$$\phi_{js} \equiv \sum_n C_n^{SR}(e_j^{SR}) P(k_n s; r) \tag{21}$$

for $\epsilon_j^{SR} \leqslant \epsilon_{max}$ and solves a second secular equation. Although the spin–orbit terms have been ignored as though they were a perturbation, they are in fact treated here variationally rather than perturbatively. This can be done by working with ϕ_{js} in either the APW or the angular momentum representation. We have done both. The angular momentum representation is useful since one often wants to use that representation elsewhere. Further, it is more efficient when the number of APWs increases for the more open structures.

The method outlined above, which we denote SO-LAPW, makes possible drastic reductions in computation effort compared with the standard RAPW method. A comparison between the results of the two methods for Pd is presented in table 1. Except for the uppermost level at K, the results agree to within 1 mRy, with the SO-LAPW giving the higher value. This is precisely what one would expect, considering that the approximate relativistic form of the basis function restricts the variational freedom. The 6 mRyd difference for the sixth band at K results at least partially because that band is so high in energy. This has two effects: (i) the solution is far from the energy ($\epsilon_l = 0.2$ Ryd) for which the basis functions were constructed so the linear energy derivative does not provide adequate variational freedom; (ii) the higher bands will more easily couple into this band for the second spin–orbit variation, so truncation errors occur. There is the additional feature that this is the top of the plane-wave-like band and so will contain an appreciable amount of p character. This should be kept in mind as we turn to our discussion of Pb and the limitations of the SO-LAPW.

A case where the technique begins to break down is Pb. In setting up the basis functions, the assumption was made that the large components of the $j = l \pm \frac{1}{2}$ radial functions were equal to an average radial function given by equation $(7a)$. The first place this will break down is for p states in heavy metals, for the following reasons. Since these penetrate nearer the nucleus than higher l functions, they sample the deep nuclear potential and spend an appreciable fraction of their time moving at relativistic speeds.

Table 1. Pd eigenvalue comparison (all energies in mRyd).

k point	SO-LAPW ($\epsilon_l = 0.2$)	RAPW
Γ_6^+	11	11
Γ_8^+	312	312
Γ_7^+	335	335
Γ_8^+	444	443
K	184	183
	227	226
	388	387
	463	462
	522	522
	1068	1062
L	142	141
	306	305
	331	331
	525	524
	539	539
Δ	172	171
$(\pi/a00)$	230	229
	388	387
	422	421
	424	423
	486	485

(The s states are not a problem because they do not have a spin–orbit coupling.) In addition, the $P_{1/2}$ relativistic function as a finite amplitude at the nucleus as opposed to the $P_{3/2}$ and higher l functions which vanish at the nucleus. The semi-relativistic approximation orbital P_1 is unfortunately required to vanish in the SO-LAPW method. In figure 1, the fully relativistic 6p radial functions for Pb are displayed for an energy roughly 2 ev above the Fermi energy. Clearly the approximation $P_{1/2} \approx P_{3/2}$ (where the subscript denotes the total angular momentum j) can be expected to be fairly crude in this case. In table 2, selected eigenvalues are shown which indicate that the use of the restricted basis functions, which are formed with $P_{l=1}$, yields errors of order 20–40 mRyd for states of $P_{1/2}$ character. Again, the SO-LAPW values lie *above* the RAPW values, indicative of incomplete variational freedom. To ensure that the discrepancy does not arise from any of the terms omitted, we repeated the calculation including them—but not changing the basis functions. The results were changed by less than one mRyd, indicating that it is truly a restriction in the variational freedom by the formation of the κ-independent basis functions that limits the accuracy.

A closer examination of figure 1 can be quite revealing in this regard. P_1 is only a

mediocre function to use in trying to resolve the difference between the fully relativistic functions and the spin–orbit averaged one. Its nodes do not line up well with the points where the three functions are identical, for example. That the difficulty should be with the $P_{1/2}$ states clearly relates to the fact that $|P_{1/2} - P_1| \approx 3|P_{3/2} - P_1|$. This is interesting since one would expect instead a factor of two from equation (3). If that were the case, one could expect a considerable improvement in the precision of the basis function.
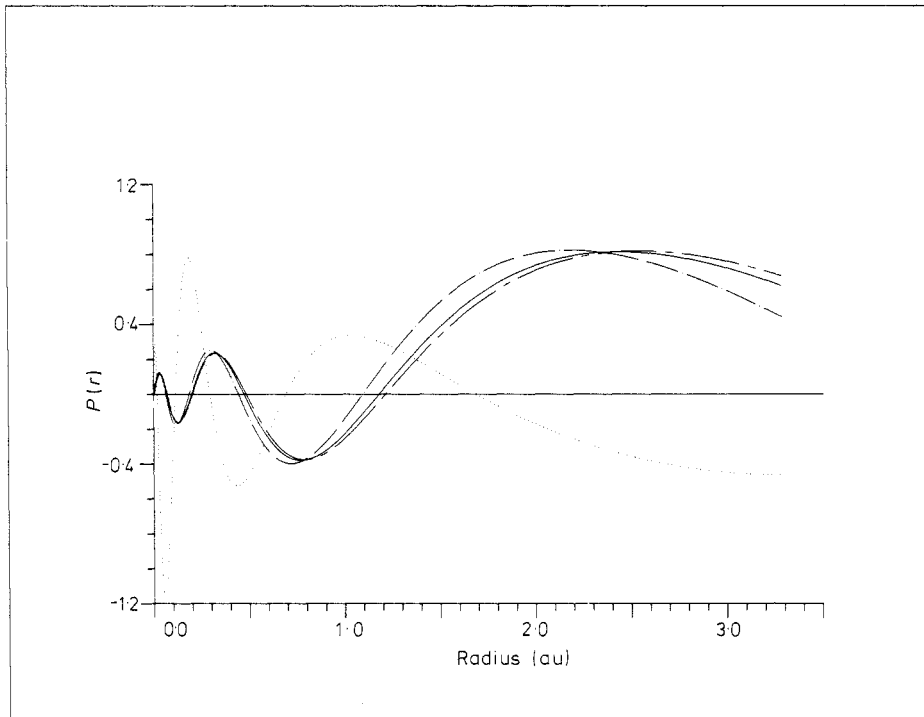

Figure 1. Pb p orbitals for $\epsilon = 0.6$ Ry. The full curve is the semi-relativistic approximation p orbital, the broken curve is the relativistic $P_{3/2}$ orbital, the chain curve is the relativistic $P_{1/2}$ orbital and the dotted curve is the semi-relativistic orbital energy derivative, $\dot{P}_1$. Note that the nodes of $\dot{P}_1$ do not line up well with the points where $P_{1/2}, P_{3/2}$ and P_1 are identical. The finite amplitude of $P_{1/2}$ at $r = 0$ is not large enough to show clearly on the scale of this figure.

This is yet another manifestation of the breakdown of the approximation $\delta P = 0$ in equation (4). We have not been able as yet to discover a simple approximate form for δP which could be used in calculating the average function. Of course one could solve by an iterative technique, but then it would be more efficient to merely solve the radial Dirac equations and perform the average directly.

To conclude, we point out that this technique works quite well with a considerably reduced computational requirement except for the p states of heavy atoms. Thus it is appropriate to all of the transition and actinide metals and only begins to break down for the Hg, Tl, Pb, Bi corner of the periodic table. The method allows one to manipulate the inclusion of spin–orbit coupling to his best advantage. It is quite acceptable as a fast and only slightly approximate scheme.

Table 2. Comparison of muffin-tin SO-LAPW eigenvalues (in mRyd) with their RAPW counterparts for Pb, using $E_0 = 0.25$ Ryd, $E_{l \neq 0} = 0.75$ Ryd. The largest errors occur for the lower member of pairs which are degenerate when spin–orbit effects are ignored (denoted by braces). We note that the Fermi energy is approximately 0.4 Ryd.

Eigenvalues	LAPW	RAPW	Error
Γ_6^+	-0.466	-0.466	0
Γ_6^-	$0.829 \rbrace$	$0.786 \rbrace$	$45 \rbrace$
Γ_8^-	$1.037 \rbrace$	$1.031 \rbrace$	$6 \rbrace$
X_6^+	-0.078	-0.077	$-1\dagger$
X_6^-	0.162	0.151	11
X_6^-	$0.529 \rbrace$	$0.492 \rbrace$	$37 \rbrace$
X_7^-	$0.610 \rbrace$	$0.608 \rbrace$	$2 \rbrace$
X_6^+	0.791	0.786	5
X_7^-	0.927	0.927	0
W_6	-0.068	-0.068	0
W_7	$0.269 \rbrace$	$0.251 \rbrace$	$18 \rbrace$
W_6	$0.345 \rbrace$	$0.343 \rbrace$	$2 \rbrace$
W_7	0.429	0.426	3
L_6^+	-0.186	-0.183	$-3\dagger$
L_6^-	0.086	0.077	9
L_6^-	$0.775 \rbrace$	$0.749 \rbrace$	$26 \rbrace$
L_4^-, L_5^-	$0.899 \rbrace$	$0.895 \rbrace$	$4 \rbrace$
L_6^-	1.073	1.073	0

† These eigenvalues illustrate a case in which SO-LAPW eigenvalues lie *below* their RAPW counterparts. This results from $\dot{P}_2$, which is evaluated far from the eigenvalue in question, having one less node than P_2 making it difficult to maintain orthogonality to the 5d core states. Lowering E_2 makes the eigenvalues coincide.

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