# Relativistic Method of Desclaux

The total energy of the system is:

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Where

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P and Q are the Dirac spinors, and

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And

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Where kappa is the relativistic quantum number

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is the orbital quantum number and is the total angular momentum of the electron.

The radial equations are solutions to:

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Where the potential and exchange terms are given by

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The functions Y are given by Grant (1961).

## Solution of the radial equations

We now consider the solution of the pair of differential equations 8 and 9, in which Y(r), X(P,Q)(r) are known functions, and epsilon is an eigenvalue to be determined. We will here, without confusion, omit the suffix A.

For the same reasons as in the non-relativistic problem it is convenient to make the change of variable

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And to tabulate all of the functions on the same grid of points, equally spaced in the new variable t. Making this transformation, the new equations become

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These first-order differential equations are of the form:

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Assuming a uniform mesh,

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And defining and applying the finite-difference approximation for the derivative, we obtain

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And introducing the discrete approximation to the second derivative:

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And rearranging terms,

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And finally

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## Starting the integration

Applying a one-sided derivative approximation to the first point,

Assuming a uniform mesh,

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And defining and applying the finite-difference approximation for the derivative, we obtain

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Applying a finite difference derivative for u,

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We arrive at an expression for the first point in the integration:

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If we take the boundary condition that y0 = 0 then the expression reduces to

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## Beginning inward integration

Here we may make use of the asymptotic forms:

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Where

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