```
      for L := 0 step 1 until Lmax do
      if abs(F[L]-Fapprox[L]) > epsilon × abs(F[L]) then
      begin
        for k := 0 step 1 until Lmax do Fapprox[k] := F[k];
        nu1 := mu1 := nu;  nu := nu + 10;
        if nu < 300 then go to L0 else
        begin
          outstring (1, 'convergence difficulty in Coulomb');
          go to L5
        end
      end
    end;
    t1 := 6.2831853072 × eta;
    comment The constant 2π in the preceding statement must be
      supplied more accurately if more than 11 significant digits are
      desired in the final results;
    if abs(t1) < 1 then
    begin
      t2 := s := 1;   L := 1;
L4: L := L + 1;
      t2 := t1 × t2/L;   s := s + t2;
      if abs(t2) > epsilon × abs(s) then go to L4;
      s := sqrt(1/s)
    end
    else
      s := sqrt(t1/(exp(t1)-1));
    F[0] := s × F[0];
    for L := 1 step 1 until Lmax do
    begin
      s := (L-.5) × sqrt(L↑2+eta2) × s/(L×(L+.5));
      F[L] := s × F[L]
    end;
L5: end Coulomb;
```

comment The procedure *Coulomb* was tested on the CDC 3600 computer, with the procedure *minimal* in single precision (unless stated otherwise). The tests included the following:

(i) Generation of $\Phi_L(\eta, \rho) = [C_L(\eta)\rho^{L+1}]^{-1}F_L(\eta, \rho)$, $L = 0(1)21$, to 8 significant digits (d=8) for $\eta = 0, -5(2)5$, $\rho = .2, 1(1)5$. The results were in complete agreement with values tabulated in [4].

(ii) Computation of $F_0(\eta, \rho)$, $F_0'(\eta, \rho) = (d/d\rho)F_0(\eta, \rho)$ to 6 significant digits for $\eta = 0(2)12$, $\rho = 0(5)40$, using $F_0' = (\rho^{-1}+\eta)F_0 - (1+\eta^2)^{\frac{1}{2}}F_1$. Comparison with [5] revealed frequent discrepancies of one unit in the last digit. In addition, beginning with $\eta = 8$, the results became progressively worse for $\rho = 30, 35, 40$, being correct to only 2–3 digits when $\eta = 12$, $\rho = 40$. With the procedure *minimal* in double precision, however, these errors disappeared.

(iii) Computation to 8 significant digits of $F_0(\eta, \rho)$, $F_0'(\eta, \rho)$ for $\rho = 2\eta$, $\rho = .5(.5)20(2)50$. The results agreed with those published in [1] for $\rho \leqq 16$, but became increasingly inaccurate for larger values of ρ. Complete agreement was observed, however, when the procedure *minimal* was operating in the double-precision mode;

References:

1. Abramowitz, M., and Rabinowitz, P. Evaluation of Coulomb wave functions along the transition line. *Phys. Rev. 96* (1954), 77–79.
2. Abramowitz, M., and Stegun, I. A. (Eds.). *Handbook of Mathematical Functions*. NBS Appl. Math. Ser. 55, U. S. Gov't. Printing Off., Washington, D. C., 1964.
3. Gautschi, W. Computational aspects of three-term recurrence relations. *SIAM Rev.*, to appear.
4. National Bureau of Standards. *Tables of Coulomb Wave Functions, Vol. I*. Appl. Math. Ser. 17, U. S. Gov't. Printing Office, Washington, D. C., 1952.
5. Tubis, A. Tables of nonrelativistic Coulomb wave functions. LA-2150, Los Alamos Scientific Lab., Los Alamos, New Mexico, 1958.

CERTIFICATION OF ALGORITHM 257 [D1] HAVIE INTEGRATOR [Robert N. Kubik, *Comm. ACM 8* (June 1965), 381]

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Havie Integrator was coded in CDC 3600 Fortran. This routine and a Fortran-coded Romberg integration routine based upon Algorithm 60, Romberg Integration [*Comm. ACM 4* (June 1961), 255] were tested with five and four integrands, respectively.

The results of these tests are tabulated below. (The Algol-coded Havie routine was transcribed and tested for the two integrands used by Kubik, with identical results in both cases.)

In the following table, *A* is the lower limit of the interval of integration, *B* is the upper limit, *EPS* the convergence criterion, *VI* the value of the integral and *VA* the value of the approximation.

Integrand	*A*	*B*	*EPS*	*VI*	*Routine*	*VA*	*Number of Function Evaluations*
$\cos x$	0	$\pi/2$	10^{-6}	1.0	Havie	0.9999999981	17
					Romberg	1.000000000	17
e^{-x^2}	0	4.3	10^{-6}	0.886226924	Havie	0.886226924	17
					Romberg	0.886336925	65
$\ln x$	1	10	10^{-6}	14.0258509	Havie	14.02585084	65
					Romberg	14.02585085	65
$\left(\frac{(x)^{1/2}}{e^{x-4}+1}\right)$	0	20	10^{-6}	5.7707276	Havie	5.770724810	32,769
					Romberg	5.770724810	16,385
$\cos(4x)$	0	π	10^{-6}	0.0	Havie	3.1415926536	3[a]

[a] Since in the Havie procedure, the sample points of the interval, chosen for function evaluation, are determined by halving the interval and are, therefore, function-independent, there are functions for which the convergence criterion is satisfied before the requisite accuracy is obtained. An example is the integrand $f(x) = \cos(4x)$ integrated over the interval $[0, \pi]$. The value obtained from the routine is $= \pi$. The true value of the integral is 0.

This inherent limitation applies to all integration algorithms that obtain sample points in a fixed manner.

REMARK ON ALGORITHM 286 [H] EXAMINATION SCHEDULING [J. E. L. Peck and M. R. Williams, *Comm. ACM 9* (June 1966), 433].

The 6th and 7th lines from the end of the procedure should be corrected by the insertion of a **begin end** pair so that they read

```
if row [i] < 0 then
  begin outinteger (1, i); outinteger (1, row [i]); outinteger
    (1, w[i])
  end
```

1966 Algorithms Index will appear in the December issue of *Communications*.