Note

Application of the El-Gendi Method to the Schrödinger Integral Equation

Radial wave functions $u_l(r)$ and scattering phase shifts $\delta_l(k)$ of short range local interactions $V(r)$ are most frequently determined at positive energies k^2 (in the center of mass frame) by solving numerically the partial-wave Schrödinger differential equation

$$\frac{d^2 u_l}{dr^2} + \left[k^2 - \frac{l(l+1)}{r^2} - V(r)\right] u_l = 0 \tag{1}$$

under the boundary conditions

$$
\begin{aligned}
u_l(r) &\sim \alpha_l(k)\, r^{l+1} \qquad \text{as} \quad r \to 0 \\
&\sim kr[j_l(kr) - \tan \delta_l(k)\, n_l(kr)] \qquad \text{as} \quad r \to \infty,
\end{aligned}
\tag{2}
$$

where j_l and n_l are the spherical Bessel and Neumann functions, respectively. A previous paper [1] contains results obtained by solving this boundary value problem via the standard fourth-order Runge-Kutta method [2] and Numerov's method [2]. It was found that both methods yield reliable phase shifts when they employ a step length $h \leqslant 0.01$ and matching points determined from the condition $kr \geqslant 25$. However, both methods exhibited instability at very low energies with $l > 1$.

An alternative approach, also investigated in Ref. [1], is to transform the differential equation (1) and its associated boundary conditions (2) into the integral equation [3]

$$u_l(r) = krj_l(kr) + \int_0^\infty G_l(r, r')\, V(r')\, u_l(r')\, dr' \tag{3}$$

in which the Green's function takes the form

$$
\begin{aligned}
G_l(r, r') &= krr' j_l(kr)\, n_l(kr') \qquad \text{for} \quad r \leqslant r' \\
&= krr' j_l(kr')\, n_l(kr) \qquad \text{for} \quad r \geqslant r'.
\end{aligned}
\tag{4}
$$

By comparing the second of the boundary conditions (2) with the integral equation (3) when $r \geqslant r'$ we obtain the phase shift formula

$$\tan \delta_l(k) = - \int_0^\infty r\, j_l(kr')\, V(r')\, u_l(r')\, dr'. \tag{5}$$

122

The infinite upper limits of the integrals in Eqs. (3) and (5) can be removed by using the substitution

$$r = x/(1 - x), \tag{6}$$

which maps the interval $0 \leqslant r \leqslant \infty$ on to the interval $0 \leqslant x \leqslant 1$, to obtain

$$u_l(r) = krj_l(kr) + \int_0^1 \frac{1}{(1 - x')^2} G_l(r, r') V(r') u_l(r') \, dx' \tag{7}$$

and

$$\tan \delta_l(k) = -\int_0^1 \frac{x}{(1 - x)^3} j_l(kr) V(r) u_l(r) \, dx \tag{8}$$

in which the local interaction $V(r)$ vanishes when x (or x') equals unity.

In Ref. [1] the standard numerical approach for solving Fredholm integral equations of the second kind was now followed: the integrals on the right-hand sides of Eqs. (7) and (8) were replaced by a quadrature formula in order to reduce the former equation to a closed system of simultaneous linear algebraic equations for the radial wave function by restricting r to the pivotal points of the numerical integration. The solution of these linear equations was then substituted into the quadrature approximation representing the right-hand side of Eq. (8) in order to compute the phase shift $\delta_l(k)$. It was also clearly pointed out in Ref. [1] that care must be exercised when setting up the quadrature approximation to Eq. (7) because of the discontinuity in $\partial G_l/\partial r'$ at $r' = r$ (i.e., at $x' = x$).

The only Newton–Cotes integration formula which is always unaffected by the discontinuity in $\partial G_l/\partial r'$ is the composite trapezoidal rule. The application of the composite version of a higher-order formula to Eq. (7) could result in the possibility of an undefined error term in the quadrature approximation. Reference [1] contains results of calculations performed with the trapezoidal rule and Simpson's rule; both methods have been found to be completely stable at all energies for any value of the orbital angular momentum, with the trapezoidal rule exhibiting the faster rate of convergence with respect to the number of pivotal points employed (due to the discontinuity in $\partial G_l/\partial r'$ having some affect on Simpson's rule). The application of Gauss–Legendre quadrature formulas is also discussed in Ref. [1] where it is considered more appropriate to employ the transformation

$$r = (1 + x)/(1 - x), \tag{9}$$

which maps the interval $0 \leqslant r \leqslant \infty$ on to the interval $-1 \leqslant x \leqslant 1$, rather than Eq. (6) so that Eqs. (3) and (5) become respectively

$$u_l(r) = krj_l(kr) + \int_{-1}^1 \frac{2}{(1 - x')^2} G_l(r, r') V(r') u_l(r') \, dx' \tag{10}$$

and

$$\tan \delta_l(k) = -2 \int_{-1}^1 \frac{(1 + x)}{(1 - x)^3} j_l(kr) V(r) u_l(r) \, dx. \tag{11}$$

As the use of an n-point Gauss–Legendre formula normally requires the integrand to be differentiable at least $2n$ times [4] within the open interval $(-1, 1)$, there is the possibility of an undefined error term arising when such a formula is employed to approximate the integral in Eq. (10), because of the discontinuity in $\partial G_l/\partial r'$. However, it is shown in Ref. [1] that Gauss–Legendre formulas yield stable results at all energies for any value of l, their rate of convergence being approximately the same as that for the composite version of Simpson's rule.

The *El-Gendi* method [5] is intended for application to Fredholm integral equations with kernels $K(x, x')$ possessing a discontinuous first derivative at $x' = x$ within the open interal $-1 < x' < 1$. Equation (10) must first be rewritten in the form

$$u_l(r) = krj_l(kr) + \int_{-1}^{x} K_l^{(1)}(x, x')\, u_l(r')\, dx'$$

$$+ \left(\int_{-1}^{1} - \int_{-1}^{x} \right) K_l^{(2)}(x, x')\, u_l(r')\, dx' \tag{12}$$

in which

$$K_l^{(1)}(x, x') = \frac{2}{(1 - x')^2}\, krr'j_l(kr')\, n_l(kr)\, V(r') \tag{13a}$$

and

$$K_l^{(2)}(x, x') = \frac{2}{(1 - x')^2}\, krr'j_l(kr)\, n_l(kr')\, V(r'). \tag{13b}$$

This modified form of the partial-wave Schrödinger integral equation is then approximated by a closed system of simultaneous linear algebraic equations formed by applying a Clenshaw–Curtis type of quadrature formula [6] at the N Chebyshev points

$$x_n = \cos\left(\frac{n\pi}{N-1}\right), \qquad [n = 0, 1, 2,..., N-1]. \tag{14}$$

(Full details of the El-Gendi method are presented in Ref. [5].) The scattering phase shift is calculated by substituting the solution of these linear equations into the quadrature formula approximating the right-hand side of Eq. (11). Furthermore, the method provides the radial wave function as a finite Chebyshev series.

An ALGOL 60 program, employing the El-Gendi method, has been developed to compute radial wave functions and scattering phase shifts of local interactions of the form

$$V(r) = \sum_t A_t \exp(-\mu_t r)/r + \sum_t B_t \exp(-\rho_t r) \tag{15}$$

($\mu_t > 0$, $\rho_t > 0$) for any value of the orbital angular momentum l ($= 0, 1, 2, 3,...$) over any (user) specified range of positive energies k^2. Table 1 displays the approximate times taken, per k value, on a CDC 7600 computer by this program to set up and solve the equations of the method in terms of the number of Chebyshev points used. By comparing these times with the corresponding times presented in Ref. [1] it is observed

TABLE I

Approximate Times (in Seconds) Taken on a CDC 7600 Computer by an ALGOL 60 Program to
Set Up and Solve the Equations of the El-Gendi Method, per k value[a]

l	$N = 20$	$N = 30$	$N = 40$	$N = 50$
0	0.37	0.94	1.80	3.04
1	0.39	0.96	1.85	3.11
2	0.51	1.27	2.40	4.03
3	0.62	1.54	2.91	4.93

[a] N is the number of Chebyshev points used. The dependence on l is due to the Green's function (4).

that, for a given number of pivotal points and a specified value of l, the composite trapezoidal rule is approximately three times faster than the El-Gendi method due to the more complicated nature of the weights and pivotal points involved in the latter method.

Tables II and III contain S-, P-, D-, and F-wave phase shifts, computed via the El-Gendi method, of the static electron-hydrogen potential

$$V(r) = -2(1 + 1/r) \exp(-2r). \qquad (16)$$

These results are in close agreement at most energies with the phase shifts determined from the methods investigated in Ref. [1]. It is observed that the excellent stability

TABLE II

S- and P-Wave Phase Shifts (in Degrees) for the e^--H Interaction (16)[a]

k	$\delta_0(k)$				$\delta_1(k)$			
	$N = 20$	$N = 30$	$N = 40$	$N = 50$	$N = 20$	$N = 30$	$N = 40$	$N = 50$
0.1	41.3816	41.3805	41.3803	41.3802	0.0153559	0.0153548	0.0153548	0.0153548
0.5	59.8551	59.8547	59.8546	59.8546	1.49127	1.49141	1.49141	1.49141
1.0	51.8859	51.8827	51.8827	51.8827	6.38640	6.38696	6.38698	6.38698
1.5	44.9365	44.9491	44.9490	44.9491	10.5659	10.5495	10.5500	10.5500
2.0	39.8425	39.8199	39.8165	39.8168	12.7865	12.8239	12.8265	12.8263
2.5	35.854	35.903	35.904	35.905	13.9522	13.8745	13.8679	13.8674
3.0	32.961	32.804	32.812	32.811	14.089	14.239	14.239	14.242
3.5	30.050	30.310	30.293	30.288	14.477	14.256	14.262	14.265
4.0	28.315	28.158	28.174	28.183	14.065	14.112	14.109	14.100
4.5	26.70	26.41	26.42	26.40	13.52	13.84	13.82	13.83
5.0	24.48	24.89	24.83	24.85	13.87	13.47	13.55	13.53

[a] N is the number of Chebyshev points used in the El-Gendi method.

TABLE III

D- and F-Wave Phase Shifts (in Degrees) for the e^--H Interaction (16)[a]

k	$\delta_2(k)$				$\delta_3(k)$			
	$N = 20$	$N = 30$	$N = 40$	$N = 50$	$N = 20$	$N = 30$	$N = 40$	$N = 50$
0.1	3.79845×10^{-5}	3.79785×10^{-5}	3.79791×10^{-5}	3.79792×10^{-5}	9.48324×10^{-8}	1.00166×10^{-7}	1.00152×10^{-7}	1.00151×10^{-7}
0.5	0.0794436	0.0796581	0.0796587	0.0796587	0.0045820	0.0046509	0.0046536	0.0046537
1.0	1.02151	1.02063	1.02061	1.02062	−0.709924	0.178818	0.178914	0.178912
1.5	2.80950	2.82786	2.82647	2.82750	0.80549	0.81067	0.81226	0.81224
2.0	4.5879	4.6173	4.6149	4.6151	1.7528	1.7469	1.7505	1.7506
2.5	5.9322	5.9839	5.9930	5.9935	2.6145	2.7368	2.7106	2.7108
3.0	6.937	6.946	6.957	6.954	3.433	3.580	3.543	3.545
3.5	7.366	7.602	7.592	7.590	4.26	4.19	4.21	4.22
4.0	7.93	7.96	7.98	8.00	4.22	4.77	4.80	4.74
4.5	8.23	8.24	8.26	8.24	5.06	5.07	5.12	5.12
5.0	7.98	8.37	8.34	8.36	5.56	5.40	5.44	5.31

[a] N is the number of Chebyshev points used in the El-Gendi method.

properties of the three quadrature methods of Ref. [1] are also present in the El-Gendi method with the sole exception of the F-wave solution at $k = 1$ obtained with 20 Chebyshev points. For $l = (0, 1, 2)$ there is more rapid convergence at low energies ($k < 2$), with respect to the number of pivotal points employed (but *not* necessarily in terms of computer time), with the El-Gendi method than with the composite trapezoidal rule, but at medium and high energies the latter converges more rapidly than the former (particularly in terms of computer time).

Thus, the numerical results presented in this note and in Ref. [1] demonstrate that the El-Gendi method should be employed for the calculation of phase shifts at low energies, where the use of only 30 Chebyshev points may yield results of sufficient accuracy. However, the composite trapezoidal rule is recommended for the determination of phase shifts with good overall accuracy when averaged over all energies and all orbital angular momenta, where the use of 40 to 50 pivotal points appears to be adequate.

Appendix

Both this note and Ref. [1] contain details (including numerical results) of various methods for computing radial wave functions and scattering phase shifts of *short-range* local interactions, particularly of the form given by Eq. (15). Some of these methods have also been employed to determine S-, P-, D-, and F-wave phase shifts of the [12, 6] Lennard–Jones potential

$$V(r) = 1/r^{12} - 2/r^6, \tag{17}$$

which has a longer range than any potential of the type (15). The results obtained from a 50-point trapezoidal rule solution of Eqs. (7) and (8) [for the interaction (17)] are in close agreement at most energies with those yielded by the Numerov method solution of Eq. (1) using a step length $h = 0.01$ and matching points determined from the condition $kr \approx 25$. However, attempts to obtain an El-Gendi solution of Eq. (12) for the potential [17] failed because of ill-conditioning irrespective of the number of Chebyshev points employed. It thus appears that the El-Gendi method can be applied to the partial-wave Schrödinger integral equation only when $V(r)$ has a short range. (The method has been used successfully with neutron–proton interactions of the form (15), consisting of sums of two or more Yukawa potentials, which contained repulsive cores and attractive outer regions.)

References

1. M. S. STERN, *J. Computational Physics*, **25** (1977), 56–70.
2. F. SCHEID, "Theory and Problems of Numerical Analysis," pp. 193-234, McGraw–Hill, New York, 1968.
3. T. Y. WU AND T. OHMURA, "Quantum Theory of Scattering," pp. 45–46, Prentice–Hall, Engelwood Cliffs, N.J., 1962).

4. A. RALSTON, "A First Course in Numerical Analysis," pp. 76–158, McGraw–Hill, New York, 1965).
5. S. E. EL-GENDI, *Comput. J.* **12**_(1969), 282–287.
6. C. W. CLENSHAW AND A. R. CURTIS, *Numer. Math.* **2** (1960), 197–205.

M. S. STERN

Department of Applied Mathematics and Computing Science, University of Sheffield, Sheffield S10 2TN, England