THEORETICAL CHEMISTRY INSTITUTE

THE UNIVERSITY OF WISCONSIN

THE QUANTUM CORRECTIONS TO THE TRANSPORT

COLLISION INTEGRALS

by

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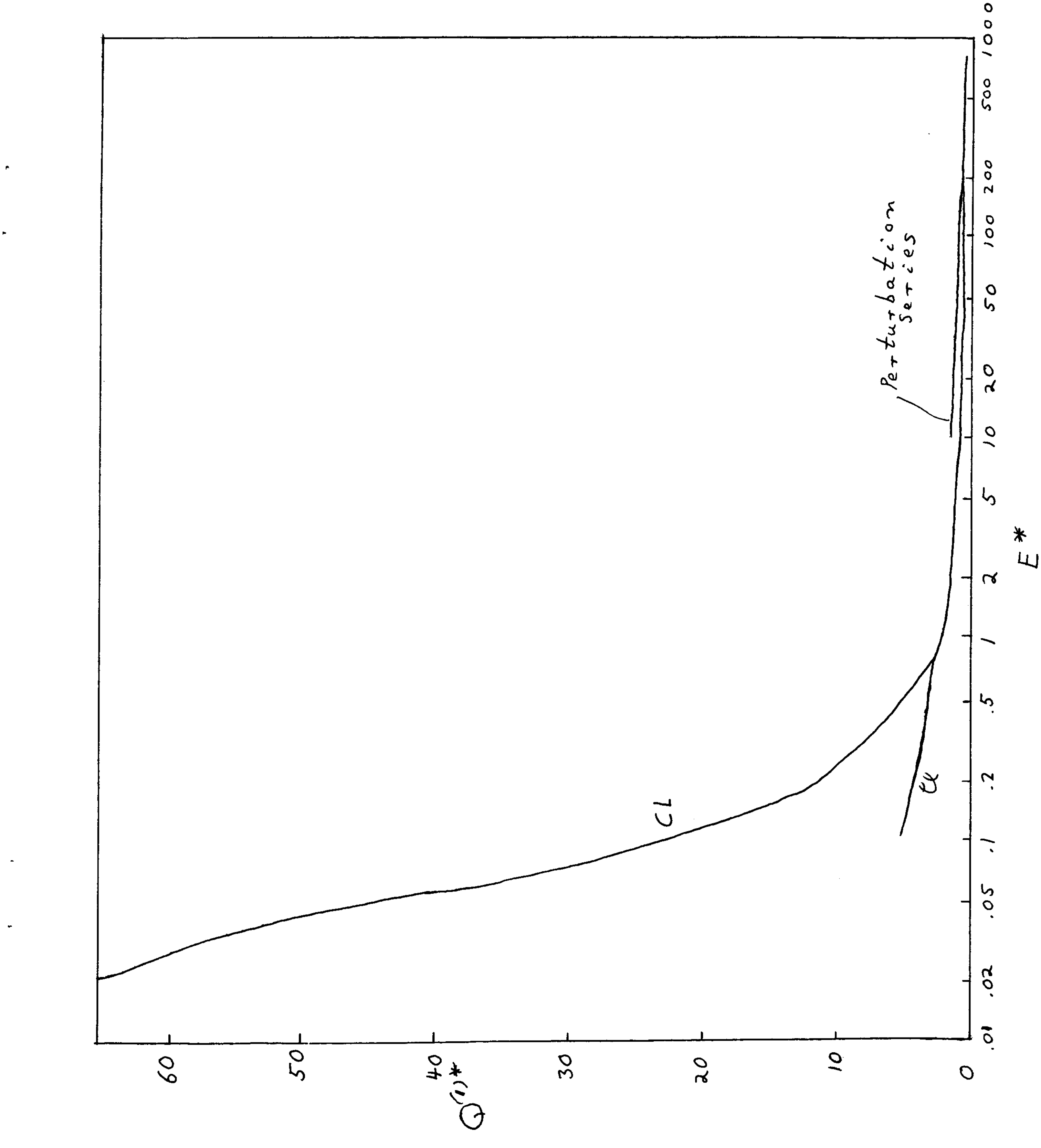
Part 2 Pages 92 - 180

MADISON, WISCONSIN

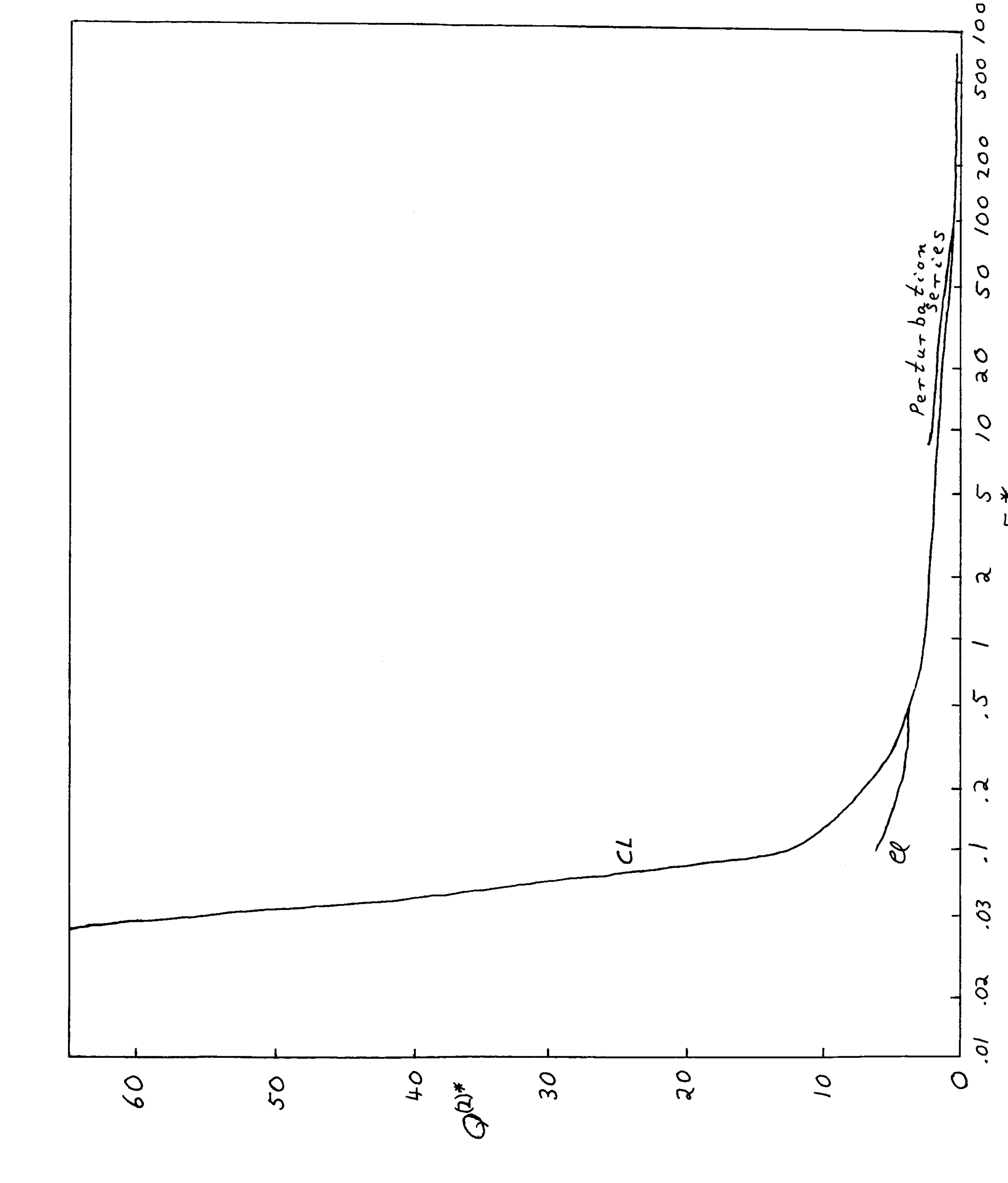
$\Omega_{\ell\ell}^{(1)*}$ and $\Omega_{CL}^{(1)*}$ for the Lennard-Jones Potential as Functions of E^* showing the High Reduced Energy Behavior of the Perturbation Series.



$Q^{(1)*}$
60
50
40
30
20
10
0
.01
.02
.05
.1
.2
.5
1
2
5
10
20
50
100
200
500
1000
E^*
CL
Perturbation Series

Figure 6.3-1

$\Omega^{(2)*}_{cl}$ and $\Omega^{(2)*}_{CL}$ for the Lennard-Jones Potential as Functions of E^* showing the High Reduced Energy Behavior of the Perturbation Series.



$Q^{(2)*}$
0
10
20
30
40
50
60
E^*
.01
.02
.03
.1
.2
.5
1
2
5
10
20
50
100
200
500
1000
CL
el
Perturbation series

Figure 6.3-2

$\Omega_{el}^{(1,1)*}$ and $\Omega_{CL}^{(1,1)*}$ for the Lennard-Jones Potential as Functions of T^* showing the High Reduced Temperature Behavior of the Perturbation Series.

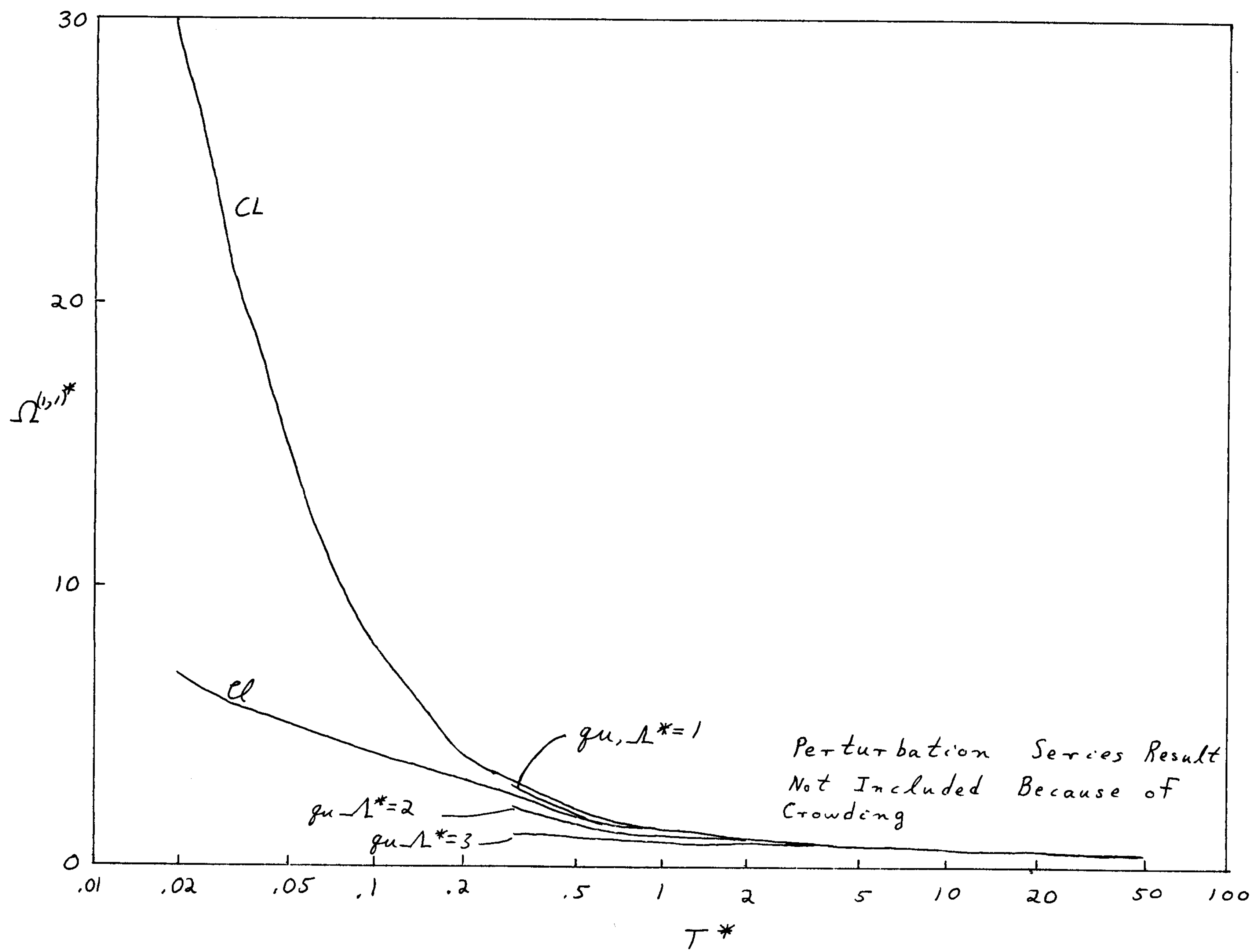

30
20
10
0
$\Omega^{(1,1)*}$
CL
Cl
qu, $\Lambda^*=1$
qu $\Lambda^*=2$
qu $\Lambda^*=3$
Perturbation Series Result
Not Included Because of
Crowding
.01
.02
.05
.1
.2
.5
1
2
5
10
20
50
100
T^*

Figure 6.3-3

$\Omega_{cl}^{(2,2)*}$ and $\Omega_{CL}^{(2,2)*}$ for the Lennard-Jones Potential as Functions of T^* showing the High Reduced Temperature Behavior of the Perturbation Series.

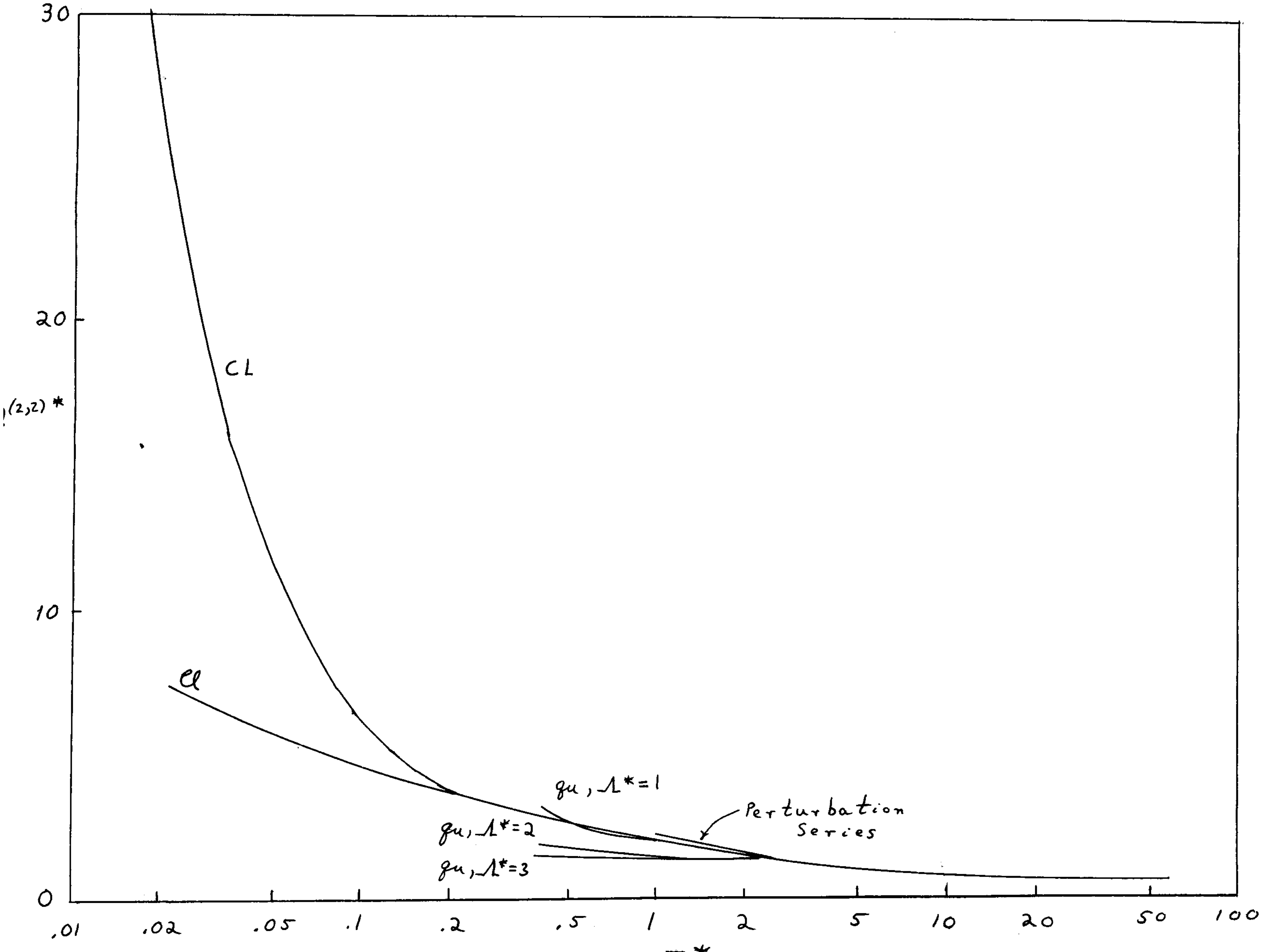

30
20
10
0
$\Omega^{(2,2)*}$
CL
Cl
qu, $\Lambda^*=1$
qu, $\Lambda^*=2$
qu, $\Lambda^*=3$
Perturbation Series
.01
.02
.05
.1
.2
.5
1
2
5
10
20
50
100
T^*

Figure 6.3-4

The following tables are the results of calculations using the Lennard-Jones potential.

The first two tables give $Q^{(1)*}$ and $Q^{(2)*}$ (the classical and the quantum corrections) as functions of log E^*. For $Q^{(2)*}$ the third quantum correction is not given, and the column labeled "IV" is the integral approximation to the fourth quantum correction (see Section 2 of Chapter II).

The last six tables give $\Omega^{(\ell,s)*}$ as a function of T^* for (ℓ,s) equal to (1,1), (1,2), (1,3), (2,2), (2,3), and (2,4). In the cases where $\ell = 2$, only the integral approximation is given to the fourth quantum correction.

The accuracy of these tables is in general about .1 per cent. The $Q_{CL}^{(\ell)*}$ are probably even more accurate. The low reduced temperature values of the omega integrals are probably in error by about 2 per cent.

TABLE I

$Q^{(1)*}$

$\log E^*$	CL	I	II	III	IV
-1.70	65.517				
-1.55	47.723				
-1.25	25.610				
-0.95	13.870				
-0.80	10.183	.47971	1.9029×10^{2}	2.5803×10^{1}	-5.0135×10^{9}
-0.75	9.1688	.42574	2.2468×10^{2}	7.4080×10^{1}	-5.6722×10^{9}
-0.65	7.4072	.33902	2.6518×10^{2}	1.7063×10^{2}	-7.1315×10^{9}
-0.55	5.9468	.22320	3.4208×10^{2}	8.3700×10^{1}	-9.6783×10^{9}
-0.50	5.3062	.16683	2.9971×10^{2}	$+2.6205 \times 10^{1}$	-1.1643×10^{10}
-0.45	4.7283	.10281	$+2.5097 \times 10^{2}$	-2.1290×10^{1}	-1.4242×10^{10}
-0.35	3.7420	.07706	-1.2790×10^{2}	-1.1627×10^{2}	-1.9669×10^{10}
-0.25	3.0152	.40551	-8.6473×10^{2}	-2.1125×10^{2}	$+7.2150 \times 10^{10}$
-0.20	2.8676	.58736	-6.5233×10^{1}	-2.5875×10^{2}	6.6123×10^{10}
-0.15	2.7297	.75831	$+7.8361 \times 10^{1}$	-3.0624×10^{2}	6.0099×10^{10}
-0.05	2.4614		2.4614		2.3189×10^{10}
+0.05	2.2196		+1.6611		2.3875×10^{8}
0.10	2.0338		-1.5581×10^{-1}		6.9006×10^{1}

$\log E^*$	CL	II	IV
0.15	1.8685	-2.6760×10^{-1}	-1.4668×10^{1}
0.25	1.5811	-1.7875×10^{-1}	-7.8820
0.35	1.3831	-1.1689×10^{-1}	-1.0956
0.40	1.2946	-7.3292×10^{-2}	-2.9775×10^{-1}
0.45	1.2199	-5.9323×10^{-2}	$+5.0089\times10^{-1}$
0.55	1.1111	-2.8885×10^{-2}	1.0098×10^{-1}
0.65	1.0310	-2.2680×10^{-2}	3.9070×10^{-2}
0.70	.99745	-1.8665×10^{-2}	2.3950×10^{-2}
0.75	.96742	-1.4687×10^{-2}	7.5070×10^{-3}
0.85	.91639	-8.8918×10^{-3}	5.0925×10^{-3}
0.95	.87413	-5.6675×10^{-3}	4.0330×10^{-3}
1.00	.85533	-4.4628×10^{-3}	2.9868×10^{-3}
1.05	.83767	-3.7427×10^{-3}	2.1452×10^{-3}
1.15	.80509	-2.4644×10^{-3}	1.1599×10^{-3}
1.25	.77529	-1.6031×10^{-3}	6.8208×10^{-4}
1.30	.76119	-1.2897×10^{-3}	5.2235×10^{-4}
1.35	.74752	-1.0376×10^{-3}	3.8243×10^{-4}

$\log E^*$	CL	II	IV
1.45	.72130	-6.5822×10^{-4}	2.3298×10^{-4}
1.55	.69629	-4.4181×10^{-4}	1.4455×10^{-4}
1.60	.68416	-3.5842×10^{-4}	1.0084×10^{-4}
1.65	.67226	-2.9092×10^{-4}	8.1361×10^{-5}
1.75	.64907	-1.9115×10^{-4}	5.5000×10^{-5}
1.85	.62661	-1.2446×10^{-4}	3.3826×10^{-5}
1.90	.61565	-9.9875×10^{-5}	2.6631×10^{-5}
1.95	.60485	-7.9817×10^{-5}	2.0774×10^{-5}
2.05	.58374	-5.2142×10^{-5}	1.0158×10^{-5}
2.15	.56325	-3.1263×10^{-5}	7.2955×10^{-6}
2.20	.55324	-2.4513×10^{-5}	5.8352×10^{-6}
2.25	.54338	-1.9154×10^{-5}	4.6741×10^{-6}
2.35	.52410	-1.1542×10^{-5}	3.0345×10^{-6}
2.45	.50541	-8.6507×10^{-6}	1.8302×10^{-6}
2.50	.49628	-4.9997×10^{-6}	1.3838×10^{-6}
2.55	.48729	-3.6098×10^{-6}	1.0428×10^{-6}
2.65	.46974	-1.5895×10^{-6}	7.7702×10^{-7}
2.75	.45274	-3.0268×10^{-7}	5.3922×10^{-7}
2.80	.44445	$+1.3351\times10^{-7}$	4.2263×10^{-7}

TABLE II

$Q^{(2)*}$

$\log E^*$	CL	I	II	IV
-1.70	87.034			
-1.55	60.141			
-1.25	28.200			
-0.95	12.759			
-0.80	8.4917	1.5056	7.8594×10^{2}	1.7068×10^{8}
-0.75	7.4163	1.7129	6.8280×10^{2}	2.7020×10^{8}
-0.65	5.7112	1.1746	$+5.1562\times10^{2}$	6.1877×10^{8}
-0.55	4.5391	.31137	-2.9054×10^{2}	1.5268×10^{9}
-0.50	4.1106	.28372	-1.0855×10^{3}	2.4341×10^{9}
-0.45	3.8044	.95770	-1.6862×10^{3}	3.8015×10^{9}
-0.35	3.4834	1.8292	-2.9997×10^{2}	$+5.0192\times10^{9}$
-0.25	3.3981	1.1415	$+2.0105\times10^{3}$	-3.5584×10^{10}
-0.20	3.3232	1.7836	1.5090×10^{3}	-9.7362×10^{9}
-0.15	3.2470	2.3009	1.0074×10^{3}	$+6.7351\times10^{8}$
-0.05	3.0621		4.2396	1.0281×10^{10}
+0.05	2.7958		2.7241	7.3209×10^{8}
0.10	2.7756		1.0234	-6.2042

$\log E^*$	CL	II	IV
0.15	2.6515	$+4.6885\times10^{-1}$	-3.4404
0.25	2.3240	-1.1307×10^{-1}	-1.8815
0.35	1.9853	-2.3123×10^{-1}	-3.2255×10^{-1}
0.40	1.8255	-1.9225×10^{-1}	-1.0812×10^{-1}
0.45	1.6816	-1.5307×10^{-1}	$+1.0632\times10^{-2}$
0.55	1.4637	-8.4659×10^{-2}	3.5898×10^{-2}
0.65	1.3072	-6.4123×10^{-2}	4.9257×10^{-3}
0.70	1.2442	-5.2101×10^{-2}	4.0352×10^{-3}
0.75	1.1899	-4.0413×10^{-2}	3.0002×10^{-3}
0.85	1.1034	-2.3222×10^{-2}	1.4725×10^{-3}
0.95	1.0384	-1.3652×10^{-2}	1.0249×10^{-3}
1.00	1.0114	-1.0916×10^{-2}	8.8908×10^{-4}
1.05	.98708	-8.1791×10^{-3}	7.0952×10^{-4}
1.15	.94462	-4.7941×10^{-3}	5.0867×10^{-4}
1.25	.90803	-2.6726×10^{-3}	3.0250×10^{-4}
1.30	.89134	-1.9463×10^{-9}	2.0959×10^{-4}
1.35	.87547	-1.3880×10^{-3}	1.5206×10^{-4}

$\log E^*$	CL	II	IV
1.45	.84563	-1.8628×10^{-4}	8.7062×10^{-5}
1.55	.81769	-2.3376×10^{-4}	4.8089×10^{-5}
1.60	.80424	-1.0624×10^{-4}	3.7560×10^{-5}
1.65	.79107	-1.3997×10^{-5}	2.9620×10^{-5}
1.75	.76541	$+9.8158\times10^{-5}$	1.6322×10^{-5}
1.85	.74052	1.5059×10^{-4}	1.1183×10^{-5}
1.90	.72832	1.6290×10^{-4}	8.5882×10^{-6}
1.95	.71627	1.6886×10^{-4}	6.5510×10^{-6}
2.05	.69262	1.7628×10^{-4}	3.9722×10^{-6}
2.15	.66954	1.5494×10^{-4}	2.3770×10^{-6}
2.20	.65822	1.4639×10^{-4}	1.7120×10^{-6}
2.25	.64703	1.3704×10^{-4}	1.3440×10^{-6}
2.35	.62506	1.1759×10^{-4}	8.5792×10^{-7}
2.45	.60363	9.7705×10^{-5}	5.7452×10^{-7}
2.50	.59312	9.0334×10^{-5}	4.5932×10^{-7}
2.55	.58274	8.2311×10^{-5}	3.6955×10^{-7}
2.65	.56240	6.8118×10^{-5}	2.0462×10^{-7}
2.75	.54261	5.6206×10^{-5}	1.3718×10^{-7}
2.80	.53292	5.0998×10^{-5}	1.0561×10^{-7}

TABLE III

$\Omega^{(1,1)*}$

T^*	CL	I	II	III	IV
0.02	28.257				
0.03	21.373				
0.04	17.130				
0.05	14.251				
0.06	12.272				
0.07	10.751				
0.08	9.5675				
0.09	8.6219				
0.10	7.8506				
0.2	3.9507	9.9686×10^{-2}	-4.8373×10^{1}	-7.9376×10^{1}	2.0534×10^{10}
0.3	3.0200	1.0271×10^{-1}	-5.1749×10^{1}	-6.9994×10^{1}	2.1519×10^{10}
0.4	2.5089	8.9023×10^{-2}	-3.7843×10^{1}	-5.0717×10^{1}	1.7136×10^{10}
0.5	2.1799	6.8690×10^{-2}	-2.6556×10^{1}	-3.5942×10^{1}	1.2887×10^{10}
0.6	1.9490	4.3348×10^{-2}	-1.8879×10^{1}	-2.5845×10^{1}	9.6522×10^{9}
0.7	1.7780	3.0105×10^{-2}	-1.3748×10^{1}	-1.9012×10^{1}	7.3142×10^{9}
0.8	1.6466	2.3469×10^{-2}	-1.0264×10^{1}	-1.4313×10^{1}	5.6323×10^{9}
0.9	1.5427	2.9292×10^{-2}	-7.8422	-1.1009×10^{1}	4.4096×10^{9}
1.0	1.4588	1.8793×10^{-2}	-6.1150	-8.6310	3.5065×10^{9}

T^*	CL	I	II	III	IV
1.2	1.3321	1.1933×10^{-2}	-3.9164	-5.5712	2.3134×10^{9}
1.4	1.2413	7.2880×10^{-3}	-2.6533	-3.7933	1.6001×10^{9}
1.6	1.1732	5.3418×10^{-3}	-1.8792	-2.6946	1.1501×10^{9}
1.8	1.1204	3.7191×10^{-3}	-1.1949	-1.7169	7.4248×10^{8}
2.	1.0782	2.5862×10^{-3}	-1.0421	-1.4977	6.4995×10^{8}
3.	.95092	9.1452×10^{-4}	-3.4647×10^{-1}	-4.9512×10^{-1}	2.1974×10^{8}
4.	.88498	4.7478×10^{-4}	-1.5634×10^{-1}	-2.2065×10^{-1}	9.9040×10^{7}
5.	.84295	2.1584×10^{-4}	-8.4004×10^{-2}	-1.1675×10^{-1}	5.2762×10^{7}
6.	.81292	1.1970×10^{-4}	-5.0532×10^{-2}	-6.9064×10^{-2}	3.1353×10^{7}
7.	.78982	8.2451×10^{-5}	-3.2897×10^{-2}	-4.4179×10^{-2}	2.0122×10^{7}
8.	.77117	6.3678×10^{-5}	-2.2704×10^{-2}	-2.9946×10^{-2}	1.3673×10^{7}
9.	.75559	4.3032×10^{-5}	-1.6389×10^{-2}	-2.1226×10^{-2}	9.7095×10^{6}
10.	.74223	3.8615×10^{-5}	-1.2259×10^{-2}	-1.5587×10^{-2}	7.1410×10^{6}
15.	.69483	9.0881×10^{-6}	-4.0700×10^{-3}	-4.7208×10^{-3}	2.1727×10^{6}
20.	.66404	4.0923×10^{-6}	-1.8976×10^{-3}	-2.0136×10^{-3}	9.2887×10^{5}
25.	.64135	2.0100×10^{-6}	-1.0646×10^{-3}	-1.0378×10^{-3}	4.7938×10^{5}
30.	.62346	1.0267×10^{-6}	-6.7049×10^{-4}	-6.0320×10^{-4}	2.7890×10^{5}
40.	.59625	5.0055×10^{-7}	-3.2939×10^{-4}	-2.5588×10^{-4}	1.1844×10^{5}
50.	.57600	2.0745×10^{-7}	-1.9278×10^{-4}	-1.3148×10^{-4}	6.0904×10^{4}

TABLE IV

$\Omega^{(1,2)*}$

T^*	CL	I	II	III	IV
0.02	22.695				
0.03	16.226				
0.04	12.660				
0.05	10.391				
0.06	8.8129				
0.07	7.6531				
0.08	6.7683				
0.09	6.0754				
0.10	5.5209				
0.2	3.0137	1.4718×10^{-1}	-7.1415×10^{1}	-8.6806×10^{1}	2.5635×10^{10}
0.3	2.3505	9.6452×10^{-2}	-3.9423×10^{1}	-5.0662×10^{1}	1.8161×10^{10}
0.4	1.9719	5.4732×10^{-2}	-2.0287×10^{1}	-2.7592×10^{1}	1.0976×10^{10}
0.5	1.7259	3.1742×10^{-2}	-1.1067×10^{1}	-1.5671×10^{1}	6.6526×10^{9}
0.6	1.5549	1.9286×10^{-2}	-6.4567	-9.4017	4.1727×10^{9}
0.7	1.4304	1.2274×10^{-2}	-3.9967	-5.9330	2.7197×10^{9}
0.8	1.3367	8.1396×10^{-3}	-2.6003	-3.9107	1.8372×10^{9}
0.9	1.2639	5.5929×10^{-3}	-1.7636	-2.6749	1.2811×10^{9}
1.0	1.2061	3.9619×10^{-3}	-1.2388	-1.8882	9.1844×10^{8}
1.2	1.1202	2.1434×10^{-3}	-6.6560×10^{-1}	-1.0162	5.0606×10^{8}
1.4	1.0597	1.2559×10^{-3}	-3.9101×10^{-1}	-5.9332×10^{-1}	3.0050×10^{8}
1.6	1.0146	7.8289×10^{-4}	-2.4604×10^{-1}	-3.6890×10^{-1}	1.8923×10^{8}
1.8	.97966	5.1270×10^{-4}	-1.6350×10^{-1}	-2.4110×10^{-1}	1.2492×10^{8}

T^*	CL	I	II	III	IV
2.0	.95160	3.4950×10^{-4}	-1.1357×10^{-1}	-1.6410×10^{-1}	8.5702×10^{7}
3.0	.86483	7.7433×10^{-5}	-2.8836×10^{-2}	-3.6188×10^{-2}	1.9362×10^{7}
4.0	.81706	2.5947×10^{-5}	-1.1545×10^{-2}	-1.2099×10^{-2}	6.5523×10^{6}
5.0	.78492	1.1000×10^{-5}	-5.9537×10^{-3}	-5.1223×10^{-3}	2.7945×10^{6}
6.0	.76090	5.4278×10^{-6}	-3.5899×10^{-3}	-2.5253×10^{-3}	1.3845×10^{6}
7.0	.74180	2.9782×10^{-4}	-2.3995×10^{-3}	-1.3848×10^{-3}	7.6183×10^{-5}
8.0	.72598	1.7673×10^{-6}	-1.7225×10^{-3}	-8.2137×10^{-4}	4.5307×10^{5}
9.0	.71251	1.1139×10^{-6}	-1.3019×10^{-3}	-5.1751×10^{-4}	2.8605×10^{5}
10.0	.70078	7.3646×10^{-7}	-1.0225×10^{-3}	-3.4205×10^{-4}	1.8937×10^{5}
15.0	.65798	1.4885×10^{-7}	-4.2916×10^{-4}	-6.9073×10^{-5}	3.8430×10^{4}
20.0	.62943	4.7640×10^{-8}	-2.4108×10^{-4}	-2.2098×10^{-5}	1.2325×10^{4}
25.0	.60813	1.9648×10^{-8}	-1.5582×10^{-4}	-9.1113×10^{-6}	5.0892×10^{3}
30.0	.59123	9.5189×10^{-9}	-1.0936×10^{-4}	-4.3554×10^{-6}	2.4676×10^{3}
40.0	.56544	3.0295×10^{-9}	-6.2466×10^{-5}	-1.4044×10^{-6}	7.8614×10^{2}
50.0	.54625	1.2468×10^{-9}	-4.0288×10^{-5}	-5.7787×10^{-7}	3.2373×10^{2}

TABLE V

$\Omega^{(1,3)*}$

T^*	CL	I	II	III	IV
.02	18.282				
.03	12.959				
.04	9.8964				
.05	8.0652				
.06	6.8063				
.07	5.8948				
.08	5.2122				
.09	4.6878				
.10	4.2765				
0.2	2.5560	1.3596×10^{-1}	-5.7721×10^{1}	-7.0588×10^{1}	2.4415×10^{10}
0.3	1.9908	5.6691×10^{-2}	-1.9460×10^{1}	-2.7471×10^{1}	1.1691×10^{10}
0.4	1.6733	2.3851×10^{-2}	-7.3043	-1.1259×10^{1}	5.3574×10^{9}
0.5	1.4731	1.1014×10^{-2}	-3.1602	-5.1285	2.6164×10^{9}
0.6	1.3384	5.5631×10^{-3}	-1.5404	-2.5688	1.3744×10^{9}
0.7	1.2431	3.0303×10^{-3}	-8.2645×10^{-1}	-1.3914	7.7058×10^{8}
0.8	1.1727	1.7567×10^{-3}	-4.7932×10^{-1}	-8.0335×10^{-1}	4.5671×10^{8}
0.9	1.1189	1.0723×10^{-3}	-2.9646×10^{-1}	-4.8884×10^{-1}	2.8368×10^{8}
1.0	1.0764	6.8330×10^{-4}	-1.9352×10^{-1}	-3.1077×10^{-1}	1.8335×10^{8}
1.2	1.0137	3.0785×10^{-4}	-9.4029×10^{-2}	-1.3953×10^{-1}	8.4401×10^{7}

T^*	CL	I	II	III	IV
1.4	.96930	1.5455×10^{-4}	-5.2439×10^{-2}	-6.9875×10^{-2}	4.3036×10^{7}
1.6	.93593	8.4275×10^{-5}	-3.2486×10^{-2}	-3.8035×10^{-2}	2.3745×10^{7}
1.8	.90968	4.9048×10^{-5}	-2.1827×10^{-2}	-2.2106×10^{-2}	1.3948×10^{7}
2.0	.88829	3.0087×10^{-5}	-1.5622×10^{-2}	-1.3546×10^{-2}	8.6197×10^{6}
3.0	.81934	4.4420×10^{-6}	-5.1642×10^{-3}	-1.9936×10^{-3}	1.3015×10^{6}
4.0	.77899	1.1161×10^{-6}	-2.6884×10^{-3}	-5.0015×10^{-4}	3.3076×10^{5}
5.0	.75075	3.7850×10^{-7}	-1.6924×10^{-3}	-1.6946×10^{-4}	1.1294×10^{5}
6.0	.72910	1.5563×10^{-7}	-1.1789×10^{-3}	-6.9634×10^{-5}	4.6649×10^{4}
7.0	.71160	7.3191×10^{-8}	-8.7486×10^{-4}	-3.2734×10^{-5}	2.2011×10^{4}
8.0	.69693	3.8003×10^{-8}	-6.7832×10^{-4}	-1.6991×10^{-5}	1.1457×10^{4}
9.0	.68433	2.1291×10^{-8}	-5.4314×10^{-4}	-9.5167×10^{-6}	6.4309×10^{3}
10.0	.67329	1.2668×10^{-8}	-4.4579×10^{-4}	-5.6614×10^{-6}	3.8323×10^{3}
15.0	.63258	1.7068×10^{-9}	-2.0951×10^{-4}	-7.6233×10^{-7}	5.1873×10^{2}
20.0	.60518	4.0970×10^{-10}	-1.2230×10^{-4}	-1.8293×10^{-7}	1.2480×10^{2}
25.0	.58466	1.3518×10^{-10}	-8.0052×10^{-5}	-6.0345×10^{-8}	4.1234×10^{1}
30.0	.56836	5.4573×10^{-11}	-5.6294×10^{-5}	-2.4360×10^{-8}	1.6662×10^{1}
40.0	.54349	1.3031×10^{-11}	-3.1909×10^{-5}	-5.8157×10^{-9}	3.9833
50.0	.52518	4.3038×10^{-12}	-2.0337×10^{-5}	-1.9206×10^{-9}	1.3165

TABLE VI

$\Omega^{(2,2)*}$

T^*	CL	I	II	IV
0.02	24.725			
0.03	16.266			
0.04	11.920			
0.05	9.3650			
0.06	7.7317			
0.07	6.6300			
0.08	5.8568			
0.09	5.2967			
0.1	4.8791			
0.2	3.3020	-3.3308×10^{-1}	3.2177×10^{2}	-1.5882×10^{9}
0.3	2.8651	-2.3241×10^{-1}	2.0205×10^{2}	-1.0941×10^{8}
0.4	2.5480	-1.3612×10^{-1}	1.1268×10^{2}	2.2984×10^{8}
0.5	2.2951	-8.0375×10^{-2}	6.4693×10^{1}	2.4455×10^{8}
0.6	2.0916	-4.9393×10^{-2}	3.9026×10^{1}	1.9671×10^{8}
0.7	1.9274	-3.1682×10^{-2}	2.4695×10^{1}	1.4814×10^{8}
0.8	1.7942	-2.1130×10^{-2}	1.6296×10^{1}	1.1009×10^{8}
0.9	1.6850	-1.4581×10^{-2}	1.1145×10^{1}	8.2156×10^{7}
1.0	1.5950	-1.0364×10^{-2}	7.8599	6.1976×10^{7}
1.2	1.4564	-5.6349×10^{-3}	4.2141	3.6675×10^{7}

T^*	C_L	I	II	III	IV
1.4	1.3560	-3.3132×10^{-3}	2.4459		2.2843×10^{7}
1.6	1.2807	-2.0706×10^{-3}	1.50[illegible]2		1.4885×10^{7}
1.8	1.2224	-1.3587×10^{-3}	9.7749×10^{-1}		1.0082×10^{7}
2.0	1.1760	-9.2765×10^{-4}	6.5839×10^{-1}		7.0571×10^{6}
3.0	1.0389	-2.0646×10^{-4}	1.3532×10^{-1}		1.6888×10^{6}
4.0	.96999	-6.9336×10^{-5}	4.0984×10^{-2}		5.8740×10^{5}
5.0	.92684	-2.9433×10^{-5}	1.5280×10^{-2}		2.5457×10^{5}
6.0	.89622	-1.4536×10^{-5}	6.4343×10^{-3}		1.2746×10^{5}
7.0	.87275	-7.9810×10^{-6}	2.9086×10^{-3}		7.0661×10^{4}
8.0	.85382	-4.7383×10^{-6}	1.3606×10^{-3}		4.2257×10^{4}
9.0	.83798	-2.9876×10^{-6}	6.3717×10^{-4}		2.6793×10^{4}
10.0	.82437	-1.9758×10^{-6}	2.8702×10^{-4}		1.7799×10^{4}
15.0	.77568	-3.9967×10^{-7}	-5.6741×10^{-6}		3.6489×10^{3}
20.0	.74362	-1.2797×10^{-7}	5.0030×10^{-5}		1.1761×10^{3}
25.0	.71975	-5.2793×10^{-8}	9.2043×10^{-5}		4.8713×10^{2}
30.0	.70077	-2.5581×10^{-8}	1.1350×10^{-4}		2.3666×10^{2}
40.0	.67170	-8.1433×10^{-9}	1.2567×10^{-4}		7.5587×10^{1}
50.0	.64995	-3.3518×10^{-9}	1.2248×10^{-4}		3.1173×10^{1}

TABLE VII

$\Omega^{(2,3)*}$

T^*	CL	I	II	III	IV
0.02	18.794				
0.03	11.949				
0.04	8.6886				
0.05	6.8601				
0.06	5.7473				
0.07	5.0325				
0.08	4.5527				
0.09	4.2171				
0.10	3.9731				
0,2	3.0192	-3.2139×10^{-1}	2.8470×10^{2}		-4.1963×10^{8}
0.3	2.5951	-1.4431×10^{-1}	1.1528×10^{2}		4.2453×10^{8}
0.4	2.2663	-6.2502×10^{-2}	4.7730×10^{1}		3.3110×10^{8}
0.5	2.0121	-2.9304×10^{-2}	2.1790×10^{1}		2.0046×10^{8}
0.6	1.8181	-1.4940×10^{-2}	1.0894×10^{1}		1.1859×10^{8}
0.7	1.6694	-8.1890×10^{-3}	5.8713		7.1738×10^{7}
0.8	1.5540	-4.7687×10^{-3}	3.3628		4.4825×10^{7}
0.9	1.4629	-2.9205×10^{-3}	2.0238		2.8948×10^{7}
1.0	1.3900	-1.8660×10^{-3}	1.2682		1.9277×10^{7}

T^*	CL	I	II	III	IV
1.2	1.2813	-8.4391×10^{-4}	5.4730×10^{-1}		9.2633×10^{6}
1.4	1.2052	-4.2479×10^{-4}	2.5897×10^{-1}		4.8641×10^{6}
1.6	1.1491	-2.3209×10^{-4}	1.3036×10^{-1}		2.7418×10^{6}
1.8	1.1062	-1.3528×10^{-4}	6.8132×10^{-2}		1.6369×10^{6}
2.0	1.0722	-8.3079×10^{-5}	3.6111×10^{-2}		1.0246×10^{6}
3.0	.97066	-1.2308×10^{-5}	-1.1555×10^{-3}		1.6056×10^{5}
4.0	.91732	-3.0977×10^{-6}	-2.9297×10^{-3}		4.1545×10^{4}
5.0	.88233	-1.0515×10^{-6}	-2.2037×10^{-3}		1.4337×10^{4}
6.0	.85654	-4.3265×10^{-7}	-1.5049×10^{-3}		5.9635×10^{3}
7.0	.83619	-2.0356×10^{-7}	-1.0174×10^{-3}		2.8277×10^{3}
8.0	.81940	-1.0573×10^{-7}	-6.8982×10^{-4}		1.4773×10^{3}
9.0	.80510	-5.9252×10^{-8}	-4.6706×10^{-4}		8.3163×10^{2}
10.0	.79265	-3.5263×10^{-8}	-3.1208×10^{-4}		4.9672×10^{2}
15.0	.74708	-4.7542×10^{-9}	1.8163×10^{-5}		6.7695×10^{1}
20.0	.71643	-1.1415×10^{-9}	1.0457×10^{-4}		1.6342×10^{1}
25.0	.69341	-3.7670×10^{-10}	1.2981×10^{-4}		5.4103
30.0	.67505	-1.5465×10^{-10}	1.3482×10^{-4}		2.1892
40.0	.64663	-3.6324×10^{-11}	1.2704×10^{-4}		5.2423×10^{-1}
50.0	.62604	-1.1094×10^{-11}	1.1485×10^{-4}		1.7258×10^{-1}

TABLE VIII

$\Omega^{(2,4)*}$

T^*	CL	I	II	III	IV
0.02	14.640				
0.03	9.2820				
0.04	6.7947				
0.05	5.4620				
0.06	4.6938				
0.07	4.2236				
0.08	3.9184				
0.09	3.7076				
0.10	3.5529				
0.2	2.8211	-2.4052×10^{-1}	1.9359×10^{2}		4.8130×10^{8}
0.3	2.3727	-6.9844×10^{-2}	5.1479×10^{1}		4.6480×10^{8}
0.4	2.0348	-2.2452×10^{-2}	1.5888×10^{1}		2.1197×10^{8}
0.5	1.7907	-8.3786×10^{-3}	5.7507		9.4881×10^{7}
0.6	1.6152	-3.5491×10^{-3}	2.3563		4.5021×10^{7}
0.7	1.4869	-1.6643×10^{-3}	1.0579		2.2827×10^{7}
0.8	1.3908	-8.4687×10^{-4}	5.0647×10^{-1}		1.2299×10^{7}
0.9	1.3169	-4.6057×10^{-4}	2.5246×10^{-1}		6.9881×10^{6}
1.0	1.2588	-2.6464×10^{-4}	1.2782×10^{-1}		4.1566×10^{6}

T^*	CL	I	II	III	IV
1.2	1.1737	-9.9630×10^{-5}	2.9431×10^{-2}		1.6472×10^{6}
1.4	1.1147	-4.2955×10^{-5}	4.8577×10^{-4}		7.3633×10^{5}
1.6	1.0713	-2.0524×10^{-5}	-8.0975×10^{-3}		3.6142×10^{5}
1.8	1.0380	-1.0629×10^{-5}	-1.0084×10^{-2}		1.9112×10^{5}
2.0	1.0114	-5.8732×10^{-6}	-9.8595×10^{-3}		1.0737×10^{5}
3.0	.92934	-5.7954×10^{-7}	-5.1492×10^{-3}		1.1131×10^{4}
4.0	.88387	-1.0935×10^{-7}	-2.6042×10^{-3}		2.1524×10^{3}
5.0	.85284	-2.9687×10^{-8}	-1.4079×10^{-3}		5.9298×10^{2}
6.0	.82935	-1.0177×10^{-8}	-7.9852×10^{-4}		2.0527×10^{2}
7.0	.81051	-4.1039×10^{-9}	-4.6169×10^{-4}		8.3350×10^{1}
8.0	.79474	-1.8650×10^{-9}	-2.6172×10^{-4}		3.8076×10^{1}
9.0	.78118	-9.2893×10^{-10}	-1.3579×10^{-4}		1.9042×10^{1}
10.0	.76929	-4.9753×10^{-10}	-5.2679×10^{-5}		1.0232×10^{1}
15.0	.72536	-4.4711×10^{-11}	1.0869×10^{-4}		9.2846×10^{-1}
20.0	.69551	-8.0511×10^{-12}	1.4006×10^{-4}		1.6800×10^{-1}
25.0	.67305	-2.1254×10^{-12}	1.4163×10^{-4}		4.4482×10^{-2}
30.0	.65511	-7.1511×10^{-13}	1.3493×10^{-4}		1.4997×10^{-2}
40.0	.62768	-1.2823×10^{-13}	1.1759×10^{-4}		2.6065×10^{-3}
50.0	.60784	-3.4146×10^{-14}	1.0290×10^{-4}		7.1968×10^{-4}

CHAPTER VII

CONCLUDING REMARKS

It is the purpose of this thesis to evaluate the quantum effects on a system under such conditions that these quantum effects just begin to become important. The particular quantum effects studied are the transport collision integrals which are based on the interaction between two particles.

Perhaps the most imporant feature of this work is the introduction of the concept of the classical limit and the distinction between this and the classical result. The coreless square well potential was studied to demonstrate this difference because the integrals involved are known. This is the exception rather than the rule. As things turned out, smoothness of the potential function was traded for ease of manipulation which resulted in inconclusive results. The numerical results[34] for the phase shift using the Lennard-Jones (12-6) potential amply substantiate the expression for this classical limit.

Numerically the $Q^{(\ell)*}$ series are probably more significant than the $\Omega^{(\ell,s)*}$ series. They show in great detail the effect of the inner region. The quantum corrections to the $\Omega^{(\ell,s)*}$ are unfortunately large over an extended reduced temperature range because of the very large quantum corrections to the $Q^{(\ell)*}$ for reduced energies below .8 .

The perturbation expansion series is an excellent check on the high reduced energy and temperature behavior of the Lennard-Jones results. The comparison of the two results also gives a bit of insight into the nature of the two expansions.

It is hoped by the author that the results obtained here will afford a little more insight into the quantum effects on the transport coefficients in those situations where the quantum effects are small; that a greater understanding of semiclassical approaches to this problem has been achieved; and finally, that the concept of the classical limit will prove advantageous in future calculations of the transport properties.

APPENDIX I. Detailed Development of $Q^{(1)}$ and $Q^{(2)}$ for Monotonic Potentials.

This appendix is a copy of a reprint of a publication containing the formal development of the series for $Q^{(1)}$ and $Q^{(2)}$ for monotonic potentials from the series for the phase shift. This appendix includes the details of the derivation of Section 1 of Chapter II.

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Quantum Corrections to the Transport Cross Sections*

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By a method developed earlier, the second quantum correction to the phase shift in a collision between particles with spherically symmetric potentials is obtained. This expression, along with the classical limit and the first quantum correction developed earlier, is used to obtain the classical limit and the first and second quantum corrections to the transport cross sections $Q^{(1)}$ and $Q^{(2)}$. In these expressions the potential function is not restricted to monotonic functions; the results apply to a potential with an attractive minimum.

IN an earlier paper[1] expansions of the phase shifts for a binary collision as series in powers of Planck's constant were obtained. These expansions enable one to describe quantum effects in any process involving collisions between molecules with spherically symmetric potentials as perturbations on the classical limit. In the previous paper explicit expressions were obtained for the classical limit and for the first quantum correction to the phase shift. In this paper an explicit expression for the second quantum correction is obtained. These quantities are then used to obtain corresponding series expressions for the cross sections[2] $Q^{(1)}$ and $Q^{(2)}$ which arise in the theory of the transport coefficients.

1. SECOND QUANTUM CORRECTION TO THE PHASE SHIFT

The calculation of the phase shift η_l is based on the differential relation[3]

$$d\eta_l/dE=\pi[\rho(E)-\rho^{(0)}(E)], \tag{1}$$

where $\rho(E)$ is the density of states (per unit energy interval) and $\rho^{(0)}(E)$ is the density in the absence of an intermolecular potential. According to Eq. (50) of Ref. 1, the density of states may be expanded in the form

$$\rho(E)=\pi^{-1}\sum_{N,j}\mathfrak{h}^{N-2}\int_0^\infty dr\mathfrak{W}_{Nj}(r,L)\times\left(\frac{r}{L}\right)^{2j+1}g^{(j)}\left[(E-\varphi)\left(\frac{r}{L}\right)^2-1\right], \tag{2}$$

where

$$\mathfrak{h}=\hbar/(2\mu)^{\frac{1}{2}}.$$

μ is the reduced mass of the two colliding particles, $g(x)$ is the function[4]

$$g(x)=x^{-\frac{1}{2}} \qquad x\geq 0,$$

$$g(x)=0 \qquad x<0.$$

$g^{(j)}(x)$ is the jth derivative of $g(x)$, φ is the intermolecular potential, and L is defined as

$$L=(l+\tfrac{1}{2})\mathfrak{h},$$

where l is the angular momentum quantum number. The $\mathfrak{W}_{Nj}(r,L)$ are functions defined in the previous paper through a set of recursion relations. It is also shown that the resulting expansion for the phase shift is of the form

$$\eta_l=\sum_j \mathfrak{h}^{2j-3}\eta_l^{(j)}, \tag{3}$$

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[1] C. F. Curtiss and R. S. Powers, Jr., J. Chem. Phys. 40, 2145 (1964).

[2] J. O. Hirschfelder, C. F. Curtiss, and R. B. Bird, *Molecular Theory of Gases and Liquids* (John Wiley & Sons, Inc., New York, 1954), p. 675.

[3] Reference 2, p. 72.

[4] More precisely the function $g(x)$ should be defined as

$$g(x)=\lim_{\epsilon\to 0}\mathrm{Re}(x+i\epsilon)^{-\frac{1}{2}}.$$

and that explicitly,

$$\eta_l^{(1)}=\int dr\left[(E-\phi)^{\frac{1}{2}}-\left(E-\frac{L^2}{r^2}\right)^{\frac{1}{2}}\right], \tag{4}$$

$$\eta_l^{(2)}=\frac{1}{24}\int dr(E-\phi)^{-\frac{1}{2}}\left[\frac{3}{r^2}-\frac{\phi'''}{\phi'}+\left(\frac{\phi''}{\phi'}\right)^2\right], \tag{5}$$

where ϕ is the effective potential

$$\phi=\varphi+(L^2/r^2). \tag{6}$$

For the evaluation of the second quantum correction to the phase shift, it is necessary to obtain explicit expressions for the $\mathcal{W}_{5j}$. From the recursion relations of the previous paper, it is found that

$$\begin{aligned}
\mathcal{W}_{52}&=\tfrac{9}{64}(1/r^4),\\
\mathcal{W}_{53}&=\tfrac{1}{24}(1/r^3)\phi'-\tfrac{1}{48}(1/r^2)\phi''-\tfrac{1}{120}\phi^{(\mathrm{IV})},\\
\mathcal{W}_{54}&=\tfrac{1}{96}(1/r^2)\phi'^2+\tfrac{1}{80}\phi'\phi'''+\tfrac{1}{80}\phi''^2,\\
\mathcal{W}_{55}&=-\tfrac{11}{720}\phi'^2\phi'',\\
\mathcal{W}_{56}&=\tfrac{1}{576}\phi'^4.
\end{aligned} \tag{7}$$

With these coefficients one finds that the second quantum correction to the phase shift is

$$\begin{aligned}
\eta_l^{(3)}=\int_0^\infty dr(E-\phi)^{-\frac{1}{2}}
&\times\left[-\frac{5}{16r^5\phi'}-\frac{9\phi''}{64r^4\phi'^2}+\frac{\phi'''}{24r^3\phi'^2}-\frac{\phi''^2}{16r^3\phi'^3}\right.\\
&-\frac{\phi^{(\mathrm{IV})}}{96r^2\phi'^2}+\frac{\phi''\phi'''}{24r^2\phi'^3}-\frac{\phi''^3}{32r^2\phi'^4}-\frac{\phi^{(\mathrm{VI})}}{576\phi'^2}\\
&+\frac{29}{2880}\frac{\phi''\phi^{(\mathrm{V})}}{\phi'^3}+\frac{47}{2880}\frac{\phi'''\phi^{(\mathrm{IV})}}{\phi'^3}-\frac{53}{1440}\frac{\phi''^2\phi^{(\mathrm{IV})}}{\phi'^4}\\
&\left.-\frac{7}{144}\frac{\phi''\phi'''^2}{\phi'^4}+\frac{7}{72}\frac{\phi''^3\phi'''}{\phi'^5}-\frac{7}{192}\frac{\phi''^5}{\phi'^6}\right].
\end{aligned} \tag{8}$$

This expression along with the expressions for $\eta_l^{(1)}$ and $\eta_l^{(2)}$ obtained previously are used in the next sections to obtain the first and second quantum corrections to $Q^{(1)}$ and $Q^{(2)}$.

2. CROSS SECTIONS $Q^{(N)}$

The expressions for the transport coefficients which arise in the kinetic theory involve certain moments of the collisional cross section, primarily $Q^{(1)}$ and $Q^{(2)}$. The quantum mechanical expression for these moments is

$$Q^{(N)}=\frac{2\pi}{E}\mathfrak{h}^2\sum_{l=0}^{\infty}\mathcal{R}_l^{(N)}\sin^2\chi_N;\qquad N=1,2, \tag{9}$$

where

$$\chi_N=\eta_{l+N}-\eta_l \tag{10}$$

and

$$\begin{aligned}
\mathcal{R}_l^{(1)}&=2(l+1),\\
\mathcal{R}_l^{(2)}&=(l+1)(l+2)/(l+\tfrac{3}{2}).
\end{aligned} \tag{11}$$

The coefficients $\mathcal{R}_l^{(N)}$ may be written in terms of $\mathfrak{h}$ and L. In particular it is readily shown that

$$\mathcal{R}_l^{(N)}=(2/N)(L/\mathfrak{h})g^{(N)}, \tag{12}$$

where

$$g^{(1)}=1+(\mathfrak{h}/2L) \tag{13}$$

and

$$g^{(2)}=\frac{1+2(\mathfrak{h}/L)+\frac{3}{4}(\mathfrak{h}/L)^2}{1+(\mathfrak{h}/L)}. \tag{14}$$

In terms of these quantities the expression for $Q^{(N)}$, Eq. (9) becomes

$$Q^{(N)}=\frac{4\pi\mathfrak{h}}{NE}\sum_{l=0}^{\infty}Lg^{(N)}\sin^2\chi_N. \tag{15}$$

The phase shift η_{l+N} can be written as a Taylor series in the form

$$\eta_{l+N}=\eta_l+\frac{N}{1!}\frac{\partial\eta_l}{\partial l}+\frac{N^2}{2!}\frac{\partial^2\eta_l}{\partial l^2}+\cdots.$$

Thus,

$$\chi_N=\sum_{j=1}^{\infty}\frac{N^j}{j!}\frac{\partial^j\eta_l}{\partial l^j} \tag{16}$$

or, since η_l is expressed in terms of $L=(l+\frac{1}{2})\mathfrak{h}$, χ_N may be written as

$$\chi_N=\sum_{j=1}^{\infty}\frac{N^j}{j!}\mathfrak{h}^j\frac{\partial^j\eta_l}{\partial L^j}. \tag{17}$$

Further, since the η_l are expanded in power series in $\mathfrak{h}$, Eq. (3),

$$\chi_N=\sum_{i=0}^{\infty}\mathfrak{h}^i\chi_{Ni}, \tag{18}$$

where

$$\chi_{Ni}=\sum_{K=1}^{1+\frac{1}{2}i}\frac{N^{i-2K+3}}{(i-2K+3)!}\frac{\partial^{i-2K+3}}{\partial L^{i-2K+3}}\eta_l^{(K)}. \tag{19}$$

It follows from the series form of the χ_N, Eqs. (18) and (19), and the standard expansions of the sine and cosine that

$$\sin^2\chi_N=\sum_n\mathfrak{h}^n s_n^{(N)}, \tag{20}$$

where

$$\begin{aligned}
s_0^{(N)}&=\sin^2\chi_{N0},\\
s_1^{(N)}&=\chi_{N1}\sin2\chi_{N0},\\
s_2^{(N)}&=\chi_{N1}^2\cos2\chi_{N0}+\chi_{N2}\sin2\chi_{N0},\\
s_3^{(N)}&=2\chi_{N1}\chi_{N2}\cos2\chi_{N0}+(\chi_{N3}-\tfrac{2}{3}\chi_{N1}^3)\sin2\chi_{N0},\\
s_4^{(N)}&=(\chi_{N2}^2+2\chi_{N1}\chi_{N3}-\tfrac{1}{3}\chi_{N1}^4)\cos2\chi_{N0}\\
&\quad+(\chi_{N4}-2\chi_{N1}^2\chi_{N2})\sin2\chi_{N0}.
\end{aligned} \tag{21}$$

We note from Eq. (19) that

$$\chi_{N0}=N(\partial\eta_l^{(1)}/\partial L). \tag{22}$$

In a similar manner we define

$$\psi_{N0}=N(\partial\eta_l^{(2)}/\partial L) \qquad \varphi_{N0}=N(\partial\eta_l^{(3)}/\partial L). \tag{23}$$

In terms of these quantities the $s_n^{(N)}$ of Eq. (21) become

$$\begin{aligned}
s_0^{(N)}&=\sin^2\chi_{N0},\\
s_1^{(N)}&=\tfrac{1}{2}N\chi_{N0}'\sin 2\chi_{N0},\\
s_2^{(N)}&=\tfrac{1}{4}N^2\chi_{N0}'\cos 2\chi_{N0}+(\tfrac{1}{6}N^2\chi_{N0}''+\psi_{N0})\sin 2\chi_{N0},\\
s_3^{(N)}&=N\chi_{N0}'(\tfrac{1}{6}N^2\chi_{N0}''+\psi_{N0})\cos 2\chi_{N0}\\
&\quad+(\tfrac{1}{24}N^3\chi_{N0}'''+\tfrac{1}{2}N\psi_{N0}'-\tfrac{1}{12}N^3\chi_{N0}'^3)\sin 2\chi_{N0},\\
s_4^{(N)}&=[(\tfrac{1}{6}N^2\chi_{N0}''+\psi_{N0})^2-\tfrac{1}{48}N^4\chi_{N0}'^4\\
&\quad+N\chi_{N0}'(\tfrac{1}{24}N^3\chi_{N0}'''+\tfrac{1}{2}N\psi_{N0}')]\cos 2\chi_{N0}\\
&\quad+[\tfrac{1}{120}N^4\chi_{N0}^{(\mathrm{IV})}+\tfrac{1}{6}N^2\psi_{N0}''+\varphi_{N0}\\
&\quad-\tfrac{1}{2}N^2\chi_{N0}'^2(\tfrac{1}{6}N^2\chi_{N0}''+\psi_{N0})]\sin 2\chi_{N0}.
\end{aligned} \tag{24}$$

The $g^{(N)}$ may also be written in a series form

$$g^{(N)}=\sum_K(\mathfrak{h}/L)^K g_K^{(N)}, \tag{25}$$

where

$$g_0^{(1)}=1,\quad g_1^{(1)}=\tfrac{1}{2},\quad g_j^{(1)}=0 \qquad j\geq 2; \tag{26}$$

and

$$g_0^{(2)}=1,\quad g_1^{(2)}=1,\quad g_j^{(2)}=(-1)^{j+1}/4 \qquad j\geq 2. \tag{27}$$

It should be noted, however, that the series expansion of $g^{(2)}$ is valid only for $L>\mathfrak{h}$ or $l>\frac{1}{2}$, i.e., it is valid for all (integer) l except $l=0$.

In the evaluation of certain integrals and the correction terms in the Euler–MacLaurin expansion (which is introduced later), it is convenient to make use of an expansion of the $s_n^{(N)}$ in powers of L. For this purpose we write

$$s_n^{(N)}=\sum_m L^m s_{nm}^{(N)}, \tag{28}$$

where

$$s_{nm}^{(N)}=(1/m!)[(d^m/dL^m)s_n^{(N)}]_{L=0}. \tag{29}$$

From the definition of χ_{N0}, Eq. (22), and the explicit expression for $\eta_l^{(1)}$, Eq. (4), one finds on differentiation that

$$\begin{aligned}
\chi_{N0}&=-N\left\{L\int dr\left[\frac{1}{r^2}(E-\phi)^{-\frac{1}{2}}-\frac{1}{r^2}\left(E-\frac{L^2}{r^2}\right)^{-\frac{1}{2}}\right]\right\}\\
&=N\left[\tfrac{1}{2}\pi-L\int dr\frac{1}{r^2(E-\phi)^{\frac{1}{2}}}\right].
\end{aligned} \tag{30}$$

A comparison of this expression with the usual integral expression for angle of deflection χ shows that under conditions such that only one classical turning point exists:

$$\chi_{N0}=\tfrac{1}{2}N\chi. \tag{31}$$

If three classical turning points exist, the integral of Eq. (30) is an integral over the entire classical region, i.e., an integral between the two inner turning points plus the integral from the third turning point to infinity. Clearly, for any intermolecular potential with a hard core the angle of deflection χ at $L=0$, a head on collision, is π. Thus

$$\chi_{N0}(0)=\tfrac{1}{2}N\pi. \tag{32}$$

With this result, it is found by explicit differentiation of the expressions for the $s_n^{(N)}$, that

$$\begin{aligned}
s_{00}^{(N)}&=\sin^2\tfrac{1}{2}N\pi,\\
s_{01}^{(N)}&=0,\\
s_{02}^{(N)}&=(\chi_{N0}'(0))^2\cos N\pi,\\
s_{03}^{(N)}&=(\chi_{N0}'(0))(\chi_{N0}''(0))\cos N\pi,\\
s_{04}^{(N)}&=[-\tfrac{1}{3}(\chi_{N0}'(0))^4+\tfrac{1}{4}(\chi_{N0}''(0))^2\\
&\quad+\tfrac{1}{3}(\chi_{N0}'(0))(\chi_{N0}'''(0))]\cos N\pi,\\
s_{10}^{(N)}&=0,\\
s_{11}^{(N)}&=N(\chi_{N0}'(0))^2\cos N\pi,\\
s_{12}^{(N)}&=\tfrac{3}{2}N(\chi_{N0}'(0))(\chi_{N0}''(0))\cos N\pi,\\
s_{13}^{(N)}&=N[\tfrac{1}{2}(\chi_{N0}''(0))^2+\tfrac{2}{3}(\chi_{N0}'(0))(\chi_{N0}'''(0))\\
&\quad-\tfrac{2}{3}(\chi_{N0}'(0))^4]\cos N\pi,\\
s_{20}^{(N)}&=\tfrac{1}{4}N^2(\chi_{N0}'(0))^2\cos N\pi,\\
s_{21}^{(N)}&=[\tfrac{5}{6}N^2(\chi_{N0}'(0))(\chi_{N0}''(0))\\
&\quad+2\chi_{N0}'(0)\psi_{N0}(0)]\cos N\pi,\\
s_{22}^{(N)}&=[\tfrac{5}{12}N^2(\chi_{N0}''(0))^2+\tfrac{7}{12}N^2(\chi_{N0}'(0))(\chi_{N0}'''(0))\\
&\quad+\chi_{N0}''(0)\psi_{N0}(0)+2\chi_{N0}'(0)\psi_{N0}'(0)-\tfrac{1}{2}N^2(\chi_{N0}'(0))^4]\\
&\quad\times\cos N\pi,\\
s_{30}^{(N)}&=[\tfrac{1}{6}N^3(\chi_{N0}'(0))(\chi_{N0}''(0))+N(\chi_{N0}'(0))\psi_{N0}(0)]\\
&\quad\times\cos N\pi,\\
s_{31}^{(N)}&=[\tfrac{1}{6}N^3(\chi_{N0}''(0))^2+\tfrac{1}{4}N^3(\chi_{N0}'(0))(\chi_{N0}'''(0))\\
&\quad+N(\chi_{N0}''(0))(\psi_{N0}(0))+2N(\chi_{N0}'(0))(\psi_{N0}'(0))\\
&\quad-\tfrac{1}{6}N^3(\chi_{N0}'(0))^4]\cos N\pi,\\
s_{40}^{(N)}&=[(\tfrac{1}{6}N^2\chi_{N0}''(0)+\psi_{N0}(0))^2-\tfrac{1}{48}N^4(\chi_{N0}'(0))^4\\
&\quad+N(\chi_{N0}'(0))(\tfrac{1}{24}N^3\chi_{N0}'''(0)+\tfrac{1}{2}N\psi_{N0}'(0))]\cos N\pi.
\end{aligned} \tag{33}$$

In the next two sections we consider the explicit evaluation of the series expressions for $Q^{(1)}$ and $Q^{(2)}$.

3. EXPANSION OF THE CROSS SECTION $Q^{(1)}$

The Euler–MacLaurin approximation may be used to transform the sum over l to an integral over l plus correction terms. In addition, one transforms the integration over l to an integration over L. It is to be noted, however, that the lower limit of integration is $l=0$ or $L=\frac{1}{2}\mathfrak{h}$. Explicitly one finds that

$$Q^{(1)}=\frac{4\pi}{E}\left\{\int_{\frac{1}{2}\mathfrak{h}}^{\infty} Lg^{(1)}\sin^2\chi_1 dL\right.$$
$$+\tfrac{1}{2}\left[Lg^{(1)}\sin^2\chi_1\big|_{L=\frac{1}{2}\mathfrak{h}}+Lg^{(1)}\sin^2\chi_1\big|_{L=\infty}\right]$$
$$+\sum_{K=1}^{\infty}(-1)^K\frac{B_K}{(2K)!}\mathfrak{h}^{2K-1}$$
$$\times\left.\left[\frac{d^{2K-1}Lg^{(1)}\sin^2\chi_1}{dL^{2K-1}}\bigg|_{L=\frac{1}{2}\mathfrak{h}}-\frac{d^{2K-1}Lg^{(1)}\sin^2\chi_1}{dL^{2K-1}}\bigg|_{L=\infty}\right]\right\}. \quad (34)$$

In the treatment of $Q^{(1)}$ it is convenient to write the integral in the Euler–MacLaurin expansion as the sum of two terms

$$\frac{4\pi}{E}\int_{\frac{1}{2}\mathfrak{h}}^{\infty}Lg^{(1)}\sin^2\chi_1 dL$$
$$=\frac{4\pi}{E}\left[\int_0^{\infty}Lg^{(1)}\sin^2\chi_1 dL-\int_0^{\frac{1}{2}\mathfrak{h}}Lg^{(1)}\sin^2\chi_1 dL\right]. \quad (35)$$

With the series expressions given by Eqs. (20) and (25), the first integral on the right above becomes

$$\frac{2\pi}{E}\int_0^{\infty}dL\left[2Ls_0^{(1)}+\mathfrak{h}(s_0^{(1)}+2Ls_1^{(1)})+\mathfrak{h}^2(s_1^{(1)}+2Ls_2^{(1)})\right.$$
$$\left.+\mathfrak{h}^3(s_2^{(1)}+2Ls_3^{(1)})+\mathfrak{h}^4(s_3^{(1)}+2Ls_4^{(1)})+\cdots\right].$$

By integration by parts the terms in $\mathfrak{h}$ and $\mathfrak{h}^3$ can be shown to be zero. Further, the terms in $\mathfrak{h}^2$ and $\mathfrak{h}^4$ can be integrated by parts so as to reduce the orders of the derivatives. Thus, the last expression becomes

$$\frac{4\pi}{E}\int_0^{\infty}L\sin^2\chi_{10}dL$$
$$+\mathfrak{h}^2\left[\frac{4\pi}{E}\int_0^{\infty}dL\left[-\tfrac{1}{12}L(\chi_{10}')^2\cos 2\chi_{10}\right.\right.$$
$$\left.\left.+(L\psi_{10}+\tfrac{1}{12}\chi_{10}')\sin 2\chi_{10}\right]\right]$$
$$+\mathfrak{h}^4\left[\frac{4\pi}{E}\int_0^{\infty}dL\Big(\left[\tfrac{1}{360}L(\chi_{10}'')^2+\tfrac{1}{6}L\chi_{10}''\psi_{10}\right.\right.$$
$$\left.+L\psi_{10}^2+\tfrac{1}{720}L(\chi_{10}')^4+\tfrac{1}{6}\chi_{10}'\psi_{10}\right]\cos 2\chi_{10}$$
$$+\left[\tfrac{1}{360}(\chi_{10}')^3+L\varphi_{10}-\tfrac{1}{6}L(\chi_{10}')^2\psi_{10}\right]\sin 2\chi_{10}\Big)$$
$$\left.+(4\pi/E)\{\tfrac{1}{60}[\chi_{10}'(0)]^2\}\right]+\cdots. \quad (36)$$

In the evaluation of the second integral of Eq. (35) and the Euler–MacLaurin correction terms, it is convenient to make use of the Taylor series expansion of the functions $s_n(L)$. In terms of the coefficients $g_K^{(1)}$ and $s_{nm}^{(1)}$, defined by Eqs. (25) and (28), it is readily shown that

$$Lg^{(1)}\sin^2\chi_1=\sum_{Knm}L^{m+1-K}\mathfrak{h}^{n+K}g_K^{(1)}s_{nm}^{(1)}.$$

It then follows that the second integral of Eq. (35) is

$$-\frac{4\pi}{E}\int_0^{\frac{1}{2}\mathfrak{h}}Lg^{(1)}\sin^2\chi_1 dL=-\frac{2\pi}{E}\sum_{Knm}\frac{\mathfrak{h}^{n+m+2}}{2^{m+2-K}}g_K^{(1)}s_{nm}^{(1)}$$
$$=-(3\pi/2E)\mathfrak{h}^2+(15\pi/16E)\mathfrak{h}^4$$
$$\times(\chi_{10}'(0))^2+\cdots. \quad (37)$$

The first Euler–MacLaurin correction term is

$$(2\pi/E)\mathfrak{h}Lg^{(1)}\sin^2\chi_1\big|_{L=\frac{1}{2}\mathfrak{h}} \quad (38)$$

or in terms of the expansions

$$(2\pi/E)\sum_{Knm}L^{m+1-K}\mathfrak{h}^{n+K+1}g_K^{(1)}s_{nm}^{(1)}\big|_{L=\frac{1}{2}\mathfrak{h}}$$
$$=\frac{2\pi}{E}\sum_{Knm}\frac{\mathfrak{h}^{n+m+2}}{2^{m+1-K}}g_K^{(1)}s_{nm}^{(1)}.$$

Then using the explicit expression for the $s_{nm}^{(1)}$ this term becomes

$$(2\pi/E)\mathfrak{h}^2-(2\pi/E)\mathfrak{h}^4(\chi_{10}'(0))^2+\cdots. \quad (39)$$

The second Euler–MacLaurin correction term (and all others evaluated at $L=\infty$) gives no contribution to $Q^{(1)}$.

The third Euler–MacLaurin correction term is

$$-\frac{\pi}{3E}\mathfrak{h}^2\frac{d}{dL}Lg^{(1)}\sin^2\chi_1\big|_{L=\frac{1}{2}\mathfrak{h}} \quad (40)$$

or in terms of the expansions

$$-\frac{\pi}{3E}\frac{d}{dL}\sum_{Knm}L^{m+1-K}\mathfrak{h}^{n+K+2}g_K^{(1)}s_{nm}^{(1)}\big|_{L=\frac{1}{2}\mathfrak{h}}$$
$$=-\frac{\pi}{3E}\sum_{Knm}(m+1-K)\frac{\mathfrak{h}^{n+m+2}}{2^{m-K}}g_K^{(1)}s_{nm}^{(1)}.$$

Then using the explicit expressions for the $s_{nm}^{(1)}$ this term becomes

$$-(\pi/3E)\mathfrak{h}^2+(\pi/E)(\chi_{10}'(0))^2\mathfrak{h}^4+\cdots. \quad (41)$$

The fifth Euler–MacLaurin correction term is

$$(\pi/180)\mathfrak{h}^4(d^3/dL^3)Lg^{(1)}\sin^2\chi_1\big|_{L=\frac{1}{2}\mathfrak{h}} \quad (42)$$

or in terms of the expansions

$$\frac{\pi}{180}\frac{d^3}{dL^3}\sum_{Knm}L^{m+1-K}\mathfrak{h}^{n+m+2}g_K^{(1)}s_{nm}^{(1)}\big|_{L=\frac{1}{2}\mathfrak{h}}$$
$$=\frac{\pi}{180}\sum_{Knm}'(m+1-K)(m-K)(m-1-K)\frac{\mathfrak{h}^{n+m+2}}{2^{m-2-K}}s_{nm}^{(1)}.$$

Then again using the explicit expressions for the $s_{nm}^{(1)}$ this term becomes

$$-(\pi/30E)\mathfrak{h}^4(\chi_{10}'(0))^2+\cdots. \tag{43}$$

Higher terms in the Euler–MacLaurin series involve powers of $\mathfrak{h}$ greater than 4.

In summary, the complete expansion for $Q^{(1)}$ through terms of order $\mathfrak{h}^4$ is

$$\begin{aligned}Q^{(1)}=&\frac{4\pi}{E}\int_0^\infty L\sin^2\chi_{10}dL\\&+\frac{4\pi}{E}\mathfrak{h}^2\Big[\int_0^\infty dL[-\tfrac{1}{12}L(\chi_{10}')^2\cos2\chi_{10}\\&+(L\psi+\tfrac{1}{12}\chi_{10}')\sin2\chi_{10})]+\tfrac{1}{24}\Big]\\&+\frac{4\pi}{E}\mathfrak{h}^4\Big[\int_0^\infty dL\{[\tfrac{1}{360}(\chi_{10}'')^2+\tfrac{1}{6}L\chi_{10}''\psi_{10}\\&+L\psi_{10}^2+\tfrac{1}{720}L(\chi_{10}')^4+\tfrac{1}{6}\chi_{10}'\psi_{10}]\cos2\chi_{10}\\&+[\tfrac{1}{360}(\chi_{10}')^3+L\varphi_{10}-\tfrac{1}{6}(\chi_{10}')^2\psi_{10}]\sin2\chi_{10}\}\\&-\tfrac{7}{960}[\chi_{10}'(0)]^2\Big].\end{aligned} \tag{44}$$

Since $Q^{(1)}$ is expressed as a power series in $\mathfrak{h}^2$, this form of $Q^{(1)}$ is useful in those cases where the quantum effects begin to play a small but significant role in the collisions.

4. EXPANSION OF THE CROSS SECTION $Q^{(2)}$

The treatment of $Q^{(2)}$ is more complicated than that of $Q^{(1)}$ since the series expansion of $g^{(2)}$ is valid only for $l>\frac{1}{2}$. To avoid this difficulty, the first term in the sum of Eq. (15) is treated explicitly and the sum of the remaining terms carried out by the Euler–MacLaurin approximation. After the transformation from l to L, the expression for $Q^{(2)}$ becomes

$$\begin{aligned}Q^{(2)}=&\frac{8\pi}{3E}\mathfrak{h}^2\sin^2\chi_2|_{L=\frac{1}{2}\mathfrak{h}}+\frac{2\pi}{E}\int_{\frac{3}{2}\mathfrak{h}}^\infty Lg^{(2)}\sin^2\chi_2dL\\&+(2\pi\mathfrak{h}/E)\Big(\tfrac{1}{2}[Lg^{(2)}\sin^2\chi_2|_{L=\frac{3}{2}\mathfrak{h}}+Lg^{(2)}\sin^2\chi_2|_{L=\infty}]\\&+\sum_{K=1}^\infty(-1)^K\frac{B_K}{(2K)!}\mathfrak{h}^{2K-1}[(d^{2K-1}/dL^{2K-1})Lg^{(2)}\sin^2\chi_2|_{L=\frac{3}{2}\mathfrak{h}}\\&-(d^{2K-1}/dL^{2K-1})Lg^{(2)}\sin^2\chi_2|_{L=\infty}]\Big).\end{aligned} \tag{45}$$

The first term in the last equation, the $l=0$ term in the original sum, may be handled in a manner quite similar to that used in the discussion of the correction terms in the preceding section. From the series expansions of $\sin^2\chi_2$ Eq. (20) and (28) it follows that

$$\begin{aligned}(8\pi/3E)\mathfrak{h}^2\sin^2\chi_2|_{L=\frac{1}{2}\mathfrak{h}}&=(8\pi/3E)\sum_{nm}L^m\mathfrak{h}^{n+2}s_{nm}^{(2)}|_{L=\frac{1}{2}\mathfrak{h}},\\&=(8\pi/3E)\sum_{nm}(\mathfrak{h}^{n+m+2}/2^m)s_{nm}^{(2)},\\&=(6\pi/E)(\chi_{20}'(0))^2\mathfrak{h}^4+\cdots.\end{aligned} \tag{46}$$

In treating the integral of Eq. (45) it is again convenient to write the integral as the sum of two integrals:

$$\begin{aligned}&\frac{2\pi}{E}\int_{\frac{3}{2}\mathfrak{h}}^\infty Lg^{(2)}\sin^2\chi_2dL\\&=\frac{2\pi}{E}\Big[\int_\lambda^\infty Lg^{(2)}\sin^2\chi_2dL-\int_\lambda^{\frac{3}{2}\mathfrak{h}}Lg^{(2)}\sin^2\chi_2dL\Big],\end{aligned} \tag{47}$$

where λ is an arbitrary constant. In order to make use of the series form of $g^{(2)}$ this constant λ is taken to be greater than $\frac{3}{2}\mathfrak{h}$.

From the series expansions of $g^{(2)}$ and $\sin^2\chi_2$, Eqs. (20) and (25), it is readily seen that the first integral on the right of the last equation is

$$\frac{2\pi}{E}\int_\lambda^\infty Lg^{(2)}\sin^2\chi_2dL=\frac{2\pi}{E}\sum_{nK}\mathfrak{h}^{n+K}g_K^{(2)}\int_\lambda^\infty L^{1-K}s_n^{(2)}dL. \tag{48}$$

Let us consider next the correction term in Eq. (47). From the series expansion of $g^{(2)}$, $\sin^2\chi_2$, and $s_n^{(2)}$, Eqs. (20), (25), and (28), it is found that

$$\begin{aligned}&-\frac{2\pi}{E}\int_\lambda^{\frac{3}{2}\mathfrak{h}}Lg^{(2)}\sin^2\chi_2dL\\&=-\frac{2\pi}{E}\sum_{nmK}\mathfrak{h}^{n+K}g_K^{(2)}s_{nm}^{(2)}\int_\lambda^{\frac{3}{2}\mathfrak{h}}L^{m-K+1}dL,\\&=-\frac{2\pi}{E}\ln\frac{3\mathfrak{h}}{2\lambda}\sum_{nm}\mathfrak{h}^{n+m+2}g_{m+2}^{(2)}s_{nm}^{(2)}\\&\quad-\frac{2\pi}{E}\sum_{nm}\sum_{K\neq m+2}\frac{\mathfrak{h}^{n+K}g_K^{(2)}s_{nm}^{(2)}}{(m-K+2)}\\&\quad\times[(\tfrac{3}{2}\mathfrak{h})^{m-K+2}-\lambda^{m-K+2}].\end{aligned} \tag{49}$$

Combining the last two results, one finds that

$$\frac{2\pi}{E}\int_{\frac{3}{2}\mathfrak{h}}^\infty Lg^{(2)}\sin^2\chi_2dL=\frac{2\pi}{E}\sum_{nK}\mathfrak{h}^{n+K}g_K^{(2)}S_{nK}+T, \tag{50}$$

where

$$\begin{aligned}S_{nK}=&\int_\lambda^\infty L^{1-K}s_n^{(2)}dL+s_{n,K-2}^{(2)}\ln\lambda\\&+\sum_{m\neq K-2}\frac{s_{nm}^{(2)}}{m-K+2}\lambda^{m-K+2},\end{aligned} \tag{51}$$

and T is the correction term

$$T=-\frac{2\pi}{E}(\ln\tfrac{3}{2}\mathfrak{h})\sum_{nm}\mathfrak{h}^{n+m+2}g_{m+2}{}^{(2)}s_{nm}{}^{(2)}$$

$$-\frac{2\pi}{E}\sum_{nm}\sum_{K\neq m+2}(\tfrac{3}{2})^{m-K+2}\mathfrak{h}^{n+m+2}\frac{g_K{}^{(2)}s_{nm}{}^{(2)}}{m-K+2}. \quad (52)$$

It is easily shown that the S_{nK} are independent of the parameter λ. Hence in evaluating these coefficients we consider the limit $\lambda\to 0$. It is clear that the terms in negative powers of λ are just those necessary to remove divergences which arise in extending the integral of the first term to zero. In this limit the terms in the sum with positive powers of λ are zero. From the explicit form of the s_{nm} Eq. (33), it is readily seen that terms involving negative powers of λ and that involving $\ln\lambda$ do not contribute to the sum on the right of Eq. (51) to terms of order $\mathfrak{h}^4$ or lower (in fact, $\mathfrak{h}^5$ or lower). Thus, restricting the consideration to these terms

$$S_{nK}=\int_0^\infty L^{1-K}s_n{}^{(2)}dL; \qquad n+K\leq 4. \quad (53)$$

Again the terms in $\mathfrak{h}$ and $\mathfrak{h}^3$ can be shown to be zero and the terms in $\mathfrak{h}^2$ and $\mathfrak{h}^4$ can be simplified by integration by parts. The resulting expression for the first term on the right of Eq. (50) is thus found to be

$$\frac{2\pi}{E}\int_0^\infty L\sin^2\chi_{20}dL$$

$$+\frac{2\pi}{E}\mathfrak{h}^2\int_0^\infty dL[L\psi_{20}\sin 2\chi_{20}$$

$$-\tfrac{1}{3}L(\chi_{20}')^2\cos 2\chi_{20}-(4L)^{-1}\sin^2\chi_{20}]$$

$$+\frac{2\pi}{E}\mathfrak{h}^4\bigg[\int_0^\infty dL\{[\tfrac{2}{45}L(\chi_{20}'')^2-\tfrac{1}{45}L(\chi_{20}')^4+\tfrac{2}{3}L\chi_{20}''\psi_{20}$$

$$+\tfrac{2}{3}\chi_{20}'\psi_{20}+L\psi_{20}{}^2]\cos 2\chi_{20}$$

$$+[-\tfrac{2}{45}(\chi_{20}')^3-\tfrac{2}{3}L(\chi_{20}')^2\psi_{20}+L\varphi_{20}$$

$$-(24L)^{-1}\chi_{20}''-(4L)^{-1}\psi_{20}]\sin 2\chi_{20}\}$$

$$+\frac{1}{60}(\chi_{20}'(0))^2\bigg]+\cdots. \quad (54)$$

The first series in the correction term T, Eq. (52) is unusual in that it involves $\ln\frac{3}{2}\mathfrak{h}$ as a factor. The series multiplying this factor does not contain any terms of order $\mathfrak{h}^6$ or lower and will not be considered further here. The second series, however, does give a term of order $\mathfrak{h}^4$ (but not $\mathfrak{h}^2$, since $s_{00}{}^{(2)}=0$). Thus neglecting the terms in $\ln\frac{3}{2}\mathfrak{h}$

$$T=-(567\pi/32E)(\chi_{20}'(0))^2\mathfrak{h}^4+\cdots. \quad (55)$$

The Euler–MacLaurin correction terms in Eq. (45) are evaluated in a manner similar to that used in the previous section. Since in this case $g^{(2)}$ is an infinite series in $\mathfrak{h}/L$ it would appear that there would be an infinite number of correction terms. It is shown, however, there are only three. In terms of the coefficients $g_K{}^{(2)}$ and $s_{nm}{}^{(2)}$, defined by Eqs. (25) and (28), it is readily shown that the first Euler–MacLaurin correction term is

$$(\pi/E)\mathfrak{h}Lg^{(2)}\sin^2\chi_2$$

$$=(\pi/E)\sum_{nmK}L^{m+1-K}\mathfrak{h}^{n+K+1}g^{(2)}s_{nm}{}^{(2)}\big|_{L=\frac{3}{2}\mathfrak{h}}$$

$$=(\pi/E)\sum_{nmK}(\tfrac{3}{2})^{m+1-K}\mathfrak{h}^{n+K+1}g_K{}^{(2)}s_{nm}{}^{(2)}\big|_{L=\frac{3}{2}\mathfrak{h}}$$

$$=(15\pi/E)(\chi_{20}'(0))^2\mathfrak{h}^4+\cdots. \quad (56)$$

The other Euler–MacLaurin terms are found from the first term of the sum in Eq. (45). If the derivative of the product $Lg^{(2)}\sin^2\chi_2$ is considered explicitly the result is

$$\frac{\pi}{E}\sum_{j=1}^{\infty}\sum_{p=0}^{2j-1}\frac{(-1)^jB_j\mathfrak{h}^{2j+1}}{jp!(2j-p-1)!}\left[\frac{d^{2j-p-1}}{dL^{2j-p-1}}\frac{L}{\mathfrak{h}}g^{(2)}\right]$$

$$\times\left[\frac{d^p}{dL^p}\sin^2\chi_2\right]_{L=\frac{3}{2}\mathfrak{h}}. \quad (57)$$

In terms of the expansion of $\sin^2\chi_2$ Eqs. (20) and (28) this expression becomes

$$\frac{\pi}{E}\sum_{j=1}^{\infty}\sum_{p,n,m}\frac{(-1)^jm!B_j(\frac{3}{2})^{m-p}}{jp!(2j-p-1)!(m-p)!}\mathfrak{h}^{2j+n+m-p+1}$$

$$\times s_{nm}{}^{(2)}\left[\frac{d^{2j-p-1}}{dL^{2j-p-1}}\frac{L}{\mathfrak{h}}g^{(2)}\right]. \quad (58)$$

According to Eq. (14), $g^{(2)}$ is a function of the ratio $\mathfrak{h}/L$, only. Thus,

$$\frac{d^{2j-p-1}}{dL^{2j-p-1}}\left(\frac{L}{\mathfrak{h}}g^{(2)}\right)\bigg|_{L=\frac{3}{2}\mathfrak{h}}=\mathfrak{h}^{p-2j+1}A_{2j-p-1}, \quad (59)$$

where

$$A_K=\frac{d^K}{dx^K}\left(\frac{x^2+2x+\frac{3}{4}}{x+1}\right)\bigg|_{x=\frac{3}{2}} \quad (60)$$

and the expression given in Eq. (58) becomes

$$\frac{\pi}{E}\sum_{j=1}^{\infty}\sum_{p,n,m}\frac{(-1)^jm!B_j}{jp!(2j-p-1)!(m-p)!}\left(\frac{3}{2}\right)^{m-p}$$

$$\times A_{2j-p-1}\mathfrak{h}^{n+m+2}s_{nm}{}^{(2)}. \quad (61)$$

The sum over n, m, and p may be carried out explicitly. We find from Eq. (33) that the term becomes

$$\frac{2\pi}{E}\mathfrak{h}^4(\chi_{20}'(0))^2\sum_{j=1}^{\infty}(-1)^j\frac{Bj}{(2j)!}$$

$$\times[\tfrac{25}{4}A_{2j-1}+5(2j-1)A_{2j-2}+(2j-1)(2j-2)A_{2j-3}]$$

$$+\cdots. \quad (62)$$

From the definition of $g^{(2)}$, Eq. (14), and definition of the A_K, Eq. (60), it is found that

$$A_0=\tfrac{12}{5},$$

$$A_1=\tfrac{26}{25},$$

$$A_K=(-1)^{K+1}K!(2^{K-1}/5^{K+1}) \qquad K\geq 2. \tag{63}$$

With these expressions it can be shown that only the first two terms (that is, $j=1$ and 2) contribute to the sum in Eq. (62), and that the explicit result is

$$-\tfrac{46}{15}(\pi/E)(\chi_{20}'(0))^2\hbar^4+\cdots. \tag{64}$$

In summary, the complete expression for $Q^{(2)}$ through terms of order $\hbar^4$ is

$$\begin{aligned} Q^{(2)}=&\frac{2\pi}{E}\int_0^\infty L\sin^2\chi_{20}dL \\ &+\frac{2\pi}{E}\hbar^2\int_0^\infty dL[L\psi_{20}\sin^2\chi_{20} \\ &-\tfrac{1}{3}L(\chi_{20}')^2\cos 2\chi_{20}-(1/4L)\sin^2\chi_{20}] \\ &+\frac{2\pi}{E}\hbar^4\bigg[\int_0^\infty dL\{[\tfrac{2}{45}L(\chi_{20}'')^2+\tfrac{1}{45}L(\chi_{20}')^4+L\psi_{20}^2 \\ &+\tfrac{2}{3}\chi_{20}'\psi_{20}+\tfrac{2}{3}L\chi_{20}''\psi_{20}]\cos 2\chi_{20} \\ &+[\tfrac{2}{45}(\chi_{20}')^3-\tfrac{2}{3}L(\chi_{20}')^2\psi_{20}+L\varphi_{20}-(1/24L)\chi_{20}'' \\ &-(1/4L)\psi_{20}]\sin 2\chi_{20}\}+\tfrac{119}{960}(\chi_{20}'(0))^2\bigg]+\cdots. \end{aligned} \tag{65}$$

It is interesting to note that in $Q^{(2)}$ all correction terms arising from the Euler–MacLaurin series and the integral from 0 to $\frac{3}{2}\hbar$ are of order $\hbar^6$ or higher.

The expression for the cross section $Q^{(2)}$ for collisions between identical molecules is modified by the effects of statistics. The correct expression for $Q^{(2)}$ in this case is similar to that given by Eq. (9) for collisions between unlike molecules and is simply modified by the replacement of the sum by twice the sum over only even or only odd l, depending on the statistics of the molecules. The explicit evaluation of these sums has been carried out in a manner similar to that discussed in this section. The result is that the series expression for $Q^{(2)}$ is not modified by the statistics, at least through terms of order $\hbar^4$.

5. DISCUSSION

In this paper we have obtained the first and second quantum corrections to the cross sections $Q^{(1)}$ and $Q^{(2)}$ for collisions involving spherically symmetric potentials. The first quantum corrections to $Q^{(1)}$ and $Q^{(2)}$ have been developed previously by de Boer and Bird[5] based upon expressions for the phase shifts developed by Kahn.[6] The purpose of the present development is twofold. First, the present expressions are not restricted (as the earlier results are) to monotonic potentials. Second, in the present development explicit expressions are obtained for the first two quantum corrections.

The present paper is based on expressions for the phase shifts obtained by Curtiss and Powers.[1] These expressions are not restricted to monotonic (repulsive) potentials (as were Kahn's earlier results). The expressions differ from those of Kahn, however, because of the use of a different boundary condition. In the Curtiss–Powers solution of the radial wave equation the boundary condition at the origin is considered explicitly. Kahn's solution is essentially a solution on the full infinite interval. De Boer[7] has pointed out that at least through the first correction term the two approaches give identical results in that the differences are of higher order in $\hbar$ (for a fixed value of $l\hbar$, not a fixed value of l). This is probably true if the series are truncated after any finite number of terms. Thus the two series expressions for the phase shifts probably give identical series expressions for the cross sections.

The first correction term to $Q^{(1)}$ (but not $Q^{(2)}$) obtained in the present paper differs, however, from that obtained by de Boer and Bird in that it is larger by $\frac{2}{3}\pi$. The origin of this difference lies in the neglect by de Boer and Bird of the Euler–MacLaurin correction terms.

The use of the expressions for $Q^{(1)}$ and $Q^{(2)}$ in the evaluation of the quantum corrections to the transport properties will be discussed in later papers.

ACKNOWLEDGMENTS

The authors wish to thank Professor R. B. Bird for his help with the first quantum corrections through various discussions and considerable correspondence. The authors also wish to thank Professor J. de Boer for his correspondence and in particular for pointing out the equivalence of the two series expressions for the phase shifts.

[5] J. de Boer and R. B. Bird, Physica 20, 185 (1954).
[6] B. Kahn, dissertation, Utrecht, 1938.
[7] J. de Boer (personal communication).

APPENDIX II. The Quantum Mechanical Expression for $Q^{(\ell)}$

The quantum mechanical expressions for $Q^{(1)}$ and $Q^{(2)}$ in the convenient forms of Eqns. (2.1-1) and (2.1-2) were first derived by Kramers.[35] The expression for $Q^{(3)}$ was first published by Mason, Smith, and Munn.[11] In this appendix a general expression for $Q^{(\ell)}$ is presented.

In general, $Q^{(N)}$ is[22]

$$Q^{(N)} = 2\pi \int_0^{\pi} (1-\cos^N \chi)\, \sigma(E,\chi) \sin\chi \, d\chi \tag{2A-1}$$

where

$$\sigma = \frac{\hbar^2}{4E} \left| \sum_{\ell=0}^{\infty} (2\ell+1)(e^{2i\eta_\ell}-1) P_\ell(\cos\chi) \right|^2 \tag{2A-2}$$

so that

$$Q^{(N)} = \frac{\hbar^2 \pi}{2E} \sum_{\ell,\ell'=0}^{\infty} (2\ell+1)(2\ell'+1)(e^{-2i\eta_\ell}-1)(e^{2i\eta_{\ell'}}-1) \times$$

$$\times \int_0^{\pi} (1-\cos^N\chi) \sin\chi \, P_\ell(\cos\chi)\, P_{\ell'}(\cos\chi)\, d\chi \tag{2A-3}$$

With $x = \cos\chi$ we define

$$\mathcal{S}_{\ell\ell'}^{(N)} = \int_{-1}^{1} (1-x^N)\, P_\ell(x) P_{\ell'}(x)\, dx \tag{2A-4}$$

which is

$$\mathcal{S}_{\ell\ell'}^{(N)} = \frac{2}{2\ell+1}\,\delta_{\ell\ell'} - \int_{-1}^{1} x^{n}\, P_{\ell}(x)\, P_{\ell'}(x)\, dx \qquad \text{(2A-5)}$$

The quantity x^{N} can be written as

$$x^{N} = \sum_{k} c_{k}\, P_{k}(x) \qquad \text{(2A-6)}$$

where

$$c_{k} = \frac{2k+1}{2^{k}}\,\frac{N!}{(N-k)!} \sum_{r=0}^{k} \frac{(-1)^{k+r}}{r!\,(\ell-r)!\,(N+k-2r+1)} \qquad \text{(2A-7)}$$

For even N, $c_k = 0$ for odd k and vice-versa. In terms of this coefficient $\mathcal{S}_{\ell\ell'}^{(N)}$ is

$$\mathcal{S}_{\ell\ell'}^{(N)} = \frac{2}{2\ell+1}\,\delta_{\ell\ell'} - \sum_{k} \frac{(2k+1)\,N!}{2^{k}(N-k)!} \sum_{r=0}^{k} \frac{(-1)^{k+r}}{r!\,(\ell-r)!\,(N+k+1-2r)} \times$$

$$\times \int_{-1}^{1} P_{\ell}(x)\, P_{\ell'}(x)\, P_{k}(x)\, dx \qquad \text{(2A-8)}$$

The integral has the value[36]

$$2\,\frac{(p!)^{2}\,(\ell'+k-\ell)!\,(\ell+k-\ell')!\,(\ell'+\ell-k)!}{(2p+1)!\left[(p-\ell)!\,(p-\ell')!\,(p-k)!\right]^{2}} \qquad \text{(2A-9)}$$

where

$$2p = \ell' + \ell + k \tag{2A-10}$$

and ℓ, ℓ', and k are subject to the triangle inequality

$$\ell + k \geq \ell' \geq |\ell - k| \quad , \quad \ell + \ell' \geq k \tag{2A-11}$$

Thus, $S_{\ell\ell'}^{(N)}$ is

$$S_{\ell\ell'}^{(N)} = \frac{2}{2\ell+1}\delta_{\ell\ell'} - T_{\ell\ell'}^{(N)} \tag{2A-12}$$

where

$$T_{\ell\ell'}^{(N)} = \sum_{k=0}^{N} c_k \frac{(p!)^2(\ell'+k-\ell)!\,(\ell+k-\ell')!\,(\ell+\ell'-k)!}{(2p+1)!\left[(p-\ell)!\,(p-\ell')!\,(p-k)!\right]^2}$$

(2A-13)

Because of the alternating nature of the c_k, it is convenient to consider even and odd N separately. The rest of the treatment will be for odd N. For odd N let $k = 2i+1$ and sum over i. Further, from the limits on ℓ', Eqn. (2A-11), $\ell' = 2j+1+\ell$ where the sum over j is from $-(i+1)$ to i. Then $T_{\ell\ell'}^{(N)}$ is

$$T^{(N)}_{\ell\ell'} = \sum_{i=0}^{\frac{N-1}{2}} \sum_{j=-(i+1)}^{i} \frac{[(\ell+i+j+1)!]^2(2\ell+2j-2i)!(2i+2j+2)!(2i-2j)!}{(2\ell+2i+2j+3)![(\ell+j-i)!(j+i+1)!(i-j)!]^2} \times$$

$$\times\ \delta_{\ell',\ell+2j+1} \tag{2A-14}$$

The sum from $j = -(i+1)$ to i can be replaced by the sum from $j = 0$ to i if $Q^{(N)}$ is rewritten as

$$Q^{(N)} = \frac{\pi\hbar^2}{E}\sum_{\ell=0}^{\infty}\Bigg[(2\ell+1)\left(2-e^{2i\eta_\ell}-e^{-2i\eta_\ell}\right) - \sum_{i=0}^{\frac{N-1}{2}}\sum_{j=0}^{i} C_{2i+1}\frac{[(\ell+i+j+1)!]^2}{(2\ell+2i+2j+3)!} \times \frac{(2\ell+2j-2i)!(2i+2j+2)!(2i-2j)!}{[(\ell+j-1)!(j+i+1)!(i-j)!]^2} \times (2\ell+1)(2\ell+4j+3) \times \Big[2-e^{2i\eta_\ell}-e^{-2i\eta_\ell}-e^{2i\eta_{\ell+2j+1}} - e^{-2i\eta_{\ell+2j+1}} - e^{2i(\eta_{\ell+2j+1}-\eta_\ell)} - e^{-2i(\eta_{\ell+2j+1}-\eta_\ell)}\Big]\Bigg] \tag{2A-15}$$

With the explicit expression for C_{2i+1} it is possible to rewrite this as

$$Q^{(N)} = \frac{4\pi\hbar^2}{E} \sum_{\ell=0}^{\infty} \sum_{j=0}^{\frac{N-1}{2}} \sum_{i=j}^{\frac{N-1}{2}} \sum_{\tau=0}^{2i+1} \frac{(4i+3)\, N!\, (-1)^{\tau+1}}{2^{4i+2}(N-2i-1)!\,\tau!\,(2i+1-\tau)!\,(N+2i+2-2\tau)} \times$$

$$\times (2\ell+1)(2\ell+4j+3)\frac{(\ell+j-i+1)\cdots(\ell+j+i+1)}{(2\ell+2j-2i+1)(2\ell+2j-2i+3)\cdots(2\ell+2j+2i+3)} \times$$

$$\times \frac{(2j+2i+2)!\,(2i-2j)!}{\left[(i+j+1)!\,(i-j)!\right]^2} \sin^2(\eta_{\ell+2j+1} - \eta_\ell)$$

(2A-16)

For even N

$$Q^{(N)} = \frac{4\pi\hbar^2}{E} \sum_{\ell=0}^{\infty} \sum_{j=0}^{\frac{N}{2}} \sum_{i=j}^{\frac{N}{2}} \sum_{\tau=0}^{2i} \frac{(4i+1)!\; N!\; (-1)^{\tau}}{2^{4i}(N-2i)!\,\tau!\,(2i-\tau)!\,(N+2i-2\tau+1)} \times$$

$$\times (2\ell+1)(2\ell+4j+1)\frac{(\ell+j-i+1)\cdots(\ell+j+i)}{(2\ell+2j-2i+1)(2\ell+2j-2i+3)\cdots(2\ell+2j+2i+1)} \times$$

$$\times \frac{(2i+2j)!\,(2i-2j)!}{\left[(i+j)!\,(i-j)!\right]^2} \sin^2(\eta_{\ell+2j} - \eta_\ell)$$

(2A-17)

These formulae appear difficult to use, but actually they are not. The sums over i and j extend to only $\frac{1}{2}N$, and the factorials cancel to a great extent.

APPENDIX III. The Computer Program

Three sets of computer programs were used in the numerical evaluation of the expressions obtained in this thesis, one set for each potential. These programs are written in Fortran 63 and were run on the CDC 1604 computer at the University of Wisconsin Computing Center. This appendix contains a listing of these programs and information as to how they are used.

1. Square Well Potential - Program SQWELLP

This program is written in double prevision. In order to use this program four quantities must be specified: (1) the value of E^* (called GEESQD in the program), (2) the value of Λ^* (called ELAMST in the program), (3) the maximum value of ℓ (called LEL in the program. Note that LEL is an integer. This quantity is found from Eqn. (5.2-1)), and (4) the correct dimensions for the subscripted quantities. The dimension for the quantity PHASE is equal to ℓ . The dimension for A, B, C, and T is $2\ell + 10$.

The program prints out each ℓ followed by the phase shift for that value of ℓ . This is followed on the next line by a print out of ℓ and the partial sums of $Q_{qu}^{(1)*}$ and $Q_{qu}^{(2)*}$. The process then repeats. The final print out is E^* , Λ^* , $Q_{qu}^{(1)*}$, and $Q_{qu}^{(2)*}$.

2. The Perturbation Expansion - Programs MONOTON, FIRST, and SECOND.

These programs calculate the quantities associated with the monotonic potential given by Eqn. (4.2-18).

Program MONOTON calculates and prints out the quantities χ_{20} (called CHI in the program), χ'_{20} (CHIP), χ''_{20} (CHIDP), ψ_{20} (PSI), φ_{20} (PHI), $A_0^{(a)}$ (A1 and A2), $B_0^{(a)}$ (B1 and B2), and $C_0^{(a)}$ (C1 and C2) given by Eqns. (2.1-7), (2.1-8), (2.1-9), (2.1-10), (2.1-11), (4.2-20), (4.2-21), and (4.2-22) respectively. This program is not restricted to the r^{-12} potential, as are programs FIRST and SECOND. The absolute value of the exponent must be put into the program as the quantity L, an integer, and EL, a floating point number. The quantities pointed out are all labelled.

Program FIRST calculates and prints out the quantities $\frac{\partial \chi_{20}}{\partial \lambda}$ (called CHIL in the program), $\frac{\partial \chi'_{20}}{\partial \lambda}$ (CHIPL) , $\frac{\partial \psi_{20}}{\partial \lambda}$ (PSIL), $A_1^{(a)}$ (AL1 and AL2), and $B_1^{(a)}$ (BL1 and BL2) given by Eqns. (4.2-14), (4.2-16), (4.2-17), (4.2-23), and (4.2-24) respectively. The program is designed to include the second quantum correction if $\frac{\partial \varphi_{20}}{\partial \lambda}$ is derived. The quantities printed out are all labelled.

Program SECOND calculates and prints out the quantities $\frac{\partial^2 \chi_{20}}{\partial \lambda^2}$ (CHIDL) and $A_2^{(a)}$ (A12 and B12, which is misnamed) given by Eqns. (4.2-15) and (4.2-25). The quantities printed out are all labeled.

Programs FIRST and SECOND are made to be calculated only once, since the potential is fixed in this derivation of the quantities. Their listings are included in case they are extended to higher terms in the series. Program MONOTON is not restricted, but works for any repulsive potential which falls off faster than $\frac{1}{r}$

3. The Lennard-Jones Potential-Programs TRYBNTEG and OMEGA.

These programs calculate the quantities associated with the Lennard-Jones (12-6) potential given by Eqn. (5.4-1).

Program TRYBNTEG calculates and prints out the turning points (RONE, RTWO, and RTHREE) for the particular combination of b^* and E^* used, the values of the maximum (RGREATER) and minimum (RLESSER) of the effective potential (if they exist), b (BEE), the five functions χ_{20} (CHI), χ_{20}' (CHIP), χ_{20}'' (CHIDP), ψ_{20} (PSI), and φ_{20} (PHI) corresponding to Eqns. (2.2-3) through (2.2-7), and $Q_{CL}^{(1)*}$ (QONECL), $Q_{CL}^{(2)*}$ (QTWOCL), $Q_{II}^{(1)*}$ (QONEI), $Q_{II}^{(2)*}$ (QTWOI), $Q_{IV}^{(1)*}$ (QONEII), and $Q_{IV}^{(2)*}$ (QTWOII) corresponding to Eqns. (2.1-14) and (2.1-15). The program also prints out the "type" of collision as classified in Figs. 5.4a, b, c, and d. Cases I, II, and III are regarded by the program as SECTION C, D, and A respectively.

The data is provided on punched cards placed at the end of the program. The first data card, under a format of 4I2, specifies the number of points in the integration over b^*, and for sections A, C, and D respectively. The Gauss-Legendre points and weights for the number of points specified in the b^* integration must also be placed in the body of the program, subscripted from minus to plus (as an example, the set of 32 Gauss-Legendre points and weights are included in the program listing. This number of points was used in the numerical integration). The number of points in the integration for SECTION A was 96, for SECTION C , 64, and for SECTION D, 96. It is also necessary to set the DIMENSION statement so that the dimensions of the subscripted quantities are greater than those read in.

The rest of the data cards give the values of the reduced energies for which the calculations are to be performed. Each card contains, under a format of F12.0, the logarithm to the base ten of the energy. The last data card must be 1001. This provides a means of stopping the program when all the data has been processed.

The program OMEGA calculates the $\Omega^{(\ell,s)*}$ of Eqn. (2.3-4) using the $Q^{(\ell)*}$ as the input data. The suffixes CL, OI, IO, 00, and II represent the classical limit and the first, second, third, and fourth quantum corrections respectively. The $Q^{(\ell)*}_{cl}$ are called QONECL, the $Q^{(\ell)*}_{I}$ are called QONEOI, etc., for both ℓ = 1 and 2 .

The data is placed at the end of the program in the following order: (1) the values of s and ℓ on the same card (with a format of 2F10.0), (2) the lowest value of the reduced temperature (with a format of F10.0), (3) the increment of the reduced temperature (with a format of F10.0), (4) the highest reduced temperature (with a format of F10.0), and (5) the $Q^{(l)*}$. The data cards for the $Q^{(l)*}$ are punched as described by statements 2 and 14 in the program. Note that two cards are necessary to read in all of the values at a particular energy. The cards are read by pairs, in groups of five pairs. The last pair of one group must be identical with the first pair of the next group of five pairs. The last card must be -1001.

```
      PROGRAM TRYBNTEG
      DIMENSION AY(128),CY(99),DY(128),       GY(64),GCOEF(64)
      COMMON MEHLERA,MEHLERC,MEHLERD,        NGAUSS,GCOEF, AY,CY,DY,GY
      COMMON GEE,BEE,GSQ,BSQ,RONE,PLESSER
      COMMON S,T,U,V,DHIDP,DSI,DHILO
      READ 12,        NGAUSS,        MEHLERA,MEHLERC,MEHLERD
   12 FORMAT (4I2)
      PRINT 2,        NGAUSS,        MEHLERA,MEHLERC,MEHLERD
    2 FORMAT(    33HINO. GAUSS PTS. FOR D INTEGRATIONI5,4X/1X,
     131HNO. MEHLER PTS. FOR K,SECTION AI5,10H,SECTION CI5,10H,SECTION D
     2I5)
      FA=MEHLERA
      FC=MEHLERC
      FD=MEHLERD
      DO 7 I=1, MEHLERA
      FI=I
    7 AY(I)=COSF(((2.*FI-1.)/(2.*FA))*3.141592654)
      DO 8 J=1,MEHLERC
      FJ=J
    8 CY(J)=COSF(((2.*FJ-1.)/(2.*FC))*3.141592654)
      DO 9 K=1,MEHLERD
      FK=K
    9 DY(K)=COSF(((2.*FK-1.)/(2.*FD))*3.141592654)
      GY(01)=-.9972638618
      GY(02)=-.9856115115
      GY(03)=-.9647622556
      GY(04)=-.9349060759
      GY(05)=-.8963211558
      GY(06)=-.8493676137
      GY(07)=-.7944837960
      GY(08)=-.7321821187
      GY(09)=-.6630442669
      GY(10)=-.5877157572
      GY(11)=-.5068999089
      GY(12)=-.4213512761
      GY(13)=-.3318686023
      GY(14)=-.2392873623
      GY(15)=-.1444719616
      GY(16)=-.0483076657
      GY(17)= .0483076657
      GY(18)= .1444719616
      GY(19)= .2392873623
      GY(20)= .3318686023
      GY(21)= .4213512761
      GY(22)= .5068999089
      GY(23)= .5877157572
      GY(24)= .6630442669
      GY(25)= .7321821187
```

```
      GY(26)= .7944837960
      GY(27)= .8493676137
      GY(28)= .8963211558
      GY(29)= .9349060759
      GY(30)= .9647622556
      GY(31)= .9856115115
      GY(32)= .9972638618
      GCOEF(01)=.007018610
      GCOEF(02)=.0162743947
      GCOEF(03)=.0253920653
      GCOEF(04)=.0342738629
      GCOEF(05)=.0428358980
      GCOEF(06)=.0509980593
      GCOEF(07)=.0586840935
      GCOEF(08)=.0658222228
      GCOEF(09)=.0723457941
      GCOEF(10)=.0781938957
      GCOEF(11)=.0833119242
      GCOEF(12)=.0876520930
      GCOEF(13)=.0911738787
      GCOEF(14)=.0938443991
      GCOEF(15)=.0956387201
      GCOEF(16)=.0965400885
      GCOEF(17)=.0965400885
      GCOEF(18)=.0956387201
      GCOEF(19)=.0938443991
      GCOEF(20)=.0911738787
      GCOEF(21)=.0876520930
      GCOEF(22)=.0833119242
      GCOEF(23)=.0781938957
      GCOEF(24)=.0723457941
      GCOEF(25)=.0658222228
      GCOEF(26)=.0586840935
      GCOEF(27)=.0509980593
      GCOEF(28)=.0428358980
      GCOEF(29)=.0342738629
      GCOEF(30)=.0253920653
      GCOEF(31)=.0162743947
      GCOEF(32)=.007018610
    6 READ 1, GSQ
    1 FORMAT (F12.0)
      IF(1000-GSQ) 3,3,4
    3 STOP
    4 PRINT 14, GSQ
   14 FORMAT (     11H1LOG10 GSQ=E20.10/)
      GSQ=10.**GSQ
      S=T=U=V=DHIDP=DSI=DHILO=0.
      NGAUSS=32
```

```
      RONE=(2.*(-1.-SQRTF(1.-GSQ))/GSQ)**.166666667
      BLESSER=1.12246
C     B INTEGRALS
      SUMT=0.
      SUMU=0.
      SUMV=0.
      SUMW=0.
      SUMX=0.
      SUMY=0.
      IF(GSQ-2.) 15,15,16
   15 IF(GSQ-.8) 17,17,16
   18 BPRIME=1.8
      GO TO 19
   17 RI=(4./GSQ*(1.+SQRTF(1.-1.25*GSQ)))**.166666667
      BPRIME=RI*SQRTF(1.-F(0,RI)/GSQ)
   19 DO 22 J=1, NGAUSS
      BEE=(1.+GY(J))*BPRIME/2.
      DBEE=BPRIME/2.
      BSQ=BEE*BEE
      CALL KINTEG(CHI,CHIP,CHIDP,PSI,PHILO)
      CHISQ=CHI*CHI
      CHIPSQ=CHIP*CHIP
      CHIPPSI=CHIP*PSI
      SINEA=SINF(.5*CHI)
      COSINE=COSF(CHI)
      SUMT=SUMT+GCOEF(J)*BEE*SINEA*SINEA*DBEE
      SINEB= SINF(CHI)
      FOURB=.25/BEE
      BCHIDP=BEE*CHIDP
      SUMU=SUMU+DBEE*GCOEF(J)*(-.0208333333*BEE*CHIPSQ*COSINE+(.5*BEE
     1*PSI+.0416666667*CHIP)*SINEB)
      SUMV=SUMV+DBEE*GCOEF(J)*(COSINE*( .000694444*CHIDP*CHIDP*BEE+
     1.041666667*PSI*BEE*CHIDP+.00364583333*CHIP*CHIDP
     2        +.25*BEE*PSI*PSI+.868055555E-04*BEE*CHIPSQ*CHIPSQ+.0416666
     3667*CHIPPSI)+(.000347222*CHIP*CHIPSQ+.5*BEE*PHILO-.0208333333
     4*BEE*CHIPSQ*PSI-.00364583333*CHIPSQ*CHIP)*SINEB)
      SUMW=SUMW+GCOEF(J)*DBEE*SINEB*SINEB*BEE
      CHID=2.*CHI
      SINED=SINF(CHID)
      COSINEB=COSF(CHID)
      SUMX=SUMX+GCOEF(J)*DBEE*(BEE*(PSI*SINED-.333333333*CHIPSQ*COSINED
     1)-FOURB*SINEB*SINEB)
      SUMY=SUMY+GCOEF(J)*DBEE*(( -.247916667*CHIDP*CHIP+
     1  (.0444444444*CHIDP*CHIDP+.0222222222*CHIPSQ*CHIPSQ)*BEE
     2+BEE*PSI*PSI+.0666666667*(CHIPPSI+BCHIDP*PSI))*COSINEB+(.04444444
     3444*CHIPSQ*CHIP-.0666666667*BEE*CHIPSQ*PSI+BEE*PHILO-.0416666667/
     4BEE*CHIDP-FOURB*PSI+.247916667*CHIPSQ*CHIP)*SINED)
   22 CONTINUE
```

```
      IF(GSQ-.8) 23,23,24
   23 RI=(4./GSQ*(1.-SQRTF(1.-1.25*GSQ)))**.1666666667
      BPROME=RI*SQRTF(1.-F(O,RI)/GSQ)
      DO 25 J=1, NGAUSS
      BEE=(BPROME+BPRIME+(BPROME-BPRIME)*GY(J))/2.
      DBEE=(BPROME-BPRIME)/2.
      BSQ=BEE*BEE
      CALL RINTEG(CHI,CHIP,CHIDP,PSI,PHILO)
      CHISQ=CHI*CHI
      CHIPSQ=CHIP*CHIP
      CHIPPSI=CHIP*PSI
      SINEA=SINF(.5*CHI)
      COSINE=COSF(CHI)
      SUMT=SUMT+GCOEF(J)*BEE*SINEA*SINEA*DBEE
      SINEB= SINF(CHI)
      FOURB=.25/BEE
      BCHIDP=BEE*CHIDP
      SUMU=SUMU+DBEE*GCOEF(J)*(-.0208333333*BEE*CHIPSQ*COSINE+(.5*BEE
     1*PSI+.0416666667*CHIP)*SINEB)
      SUMV=SUMV+DBEE*GCOEF(J)*(COSINE*( .0006944444*CHIDP*CHIDP*BEE+
     1.0416666667*PSI*BEE*CHIDP+.00364583333*CHIP*CHIDP
     2        +.25*BEE*PSI*PSI+.8680555555E-04*BEE*CHIPSQ*CHIPSQ+.0416666
     3667*CHIPPSI)+(.0003472222*CHIP*CHIPSQ+.5*BEE*PHILO-.0208333333
     4*BEE*CHIPSQ*PSI-.0036458333*CHIPSQ*CHIP)*SINEB)
      SUMW=SUMW+GCOEF(J)*DBEE*SINEB*SINEB*BEE
      CHID=2.*CHI
      SINED=SINF(CHID)
      COSINEB=COSF(CHID)
      SUMX=SUMX+GCOEF(J)*DBEE*(BEE*(PSI*SINED-.3333333333*CHIPSQ*COSINEB
     1)-FOURB*SINEB*SINEB)
      SUMY=SUMY+GCOEF(J)*DBEE*(( -.2479166667*CHIDP*CHIP+
     1  (.0444444444*CHIDP*CHIDP+.0222222222*CHIPSQ*CHIPSQ)*BEE
     2+BEE*PSI*PSI+.6666666667*(CHIPPSI+BCHIDP*PSI))*COSINEB+(.044444444
     3444*CHIPSQ*CHIP-.6666666667*BEE*CHIPSQ*PSI+BEE*PHILO-.0416666667/
     4BEE*CHIDP-FOURB*PSI+.2479166667*CHIPSQ*CHIP)*SINED)
   25 CONTINUE
      BPRIME=BPROME
   24 NGAUSS=24
      DO 21 J=1, NGAUSS
      BEE=2.*BPRIME/(1.-GY(J))
      DBEE=2.*BPRIME/((1.-GY(J ))*(1.-GY(J)))
      BSQ=BEE*BEE
      CALL RINTEG(CHI,CHIP,CHIDP,PSI,PHILO)
      CHISQ=CHI*CHI
      CHIPSQ=CHIP*CHIP
      CHIPPSI=CHIP*PSI
      SINEA=SINF(.5*CHI)
      COSINE=COSF(CHI)
```

```
      SUMT=SUMT+GCOEF(J)*BEE*SINEA*SINEA*DBEE
      SINEB= SINF(CHI)
      FOURB=.25/BEE
      BCHIDP=BEE*CHIDP
      SUMU=SUMU+DBEE*GCOEF(J)*(-.0208333333*BEE*CHIPSQ*COSINE+(.5*BEE
     1*PSI+.0416666667*CHIP)*SINEB)
      SUMV=SUMV+DBEE*GCOEF(J)*(COSINE*( .0006944444*CHIDP*CHIDP*BEE+
     1.0416666667*PSI*BEE*CHIDP+.0036458333333*CHIP*CHIDP
     2        +.25*BEE*PSI*PSI+.86805555555E-04*BEE*CHIPSQ*CHIPSQ+.0416666
     3667*CHIPPSI)+(.0003472222*CHIP*CHIPSQ+.5*BEE*PHILO-.020833333333
     4*BEE*CHIPSQ*PSI-.003645833333*CHIPSQ*CHIP)*SINEB)
      SUMW=SUMW+GCOEF(J)*DBEE*SINEB*SINEB*BEE
      CHID=2.*CHI
      SINED=SINF(CHID)
      COSINEB=COSF(CHID)
      SUMX=SUMX+GCOEF(J)*DBEE*(BEE*(PSI*SINED-.3333333333*CHIPSQ*COSINEB
     1)-FOURB*SINEB*SINEB)
      SUMY=SUMY+GCOEF(J)*DBEE*(( -.2479166667*CHIDP*CHIP+
     1  (.0444444444*CHIDP*CHIDP+.0222222222*CHIPSQ*CHIPSQ)*BEE
     2+BEE*PSI*PSI+.6666666667*(CHIPPSI+BCHIDP*PSI))*COSINEB+(.044444444
     3444*CHIPSQ*CHIP-.6666666667*BEE*CHIPSQ*PSI+BEE*PHILO-.0416666667/
     4BEE*CHIDP-FOURB*PSI+.2479166667*CHIPSQ*CHIP)*SINED)
   21 CONTINUE
      GO TO 20
   16 DO 10 J=1,NGAUSS
      BPRUME=3.
      BEE=(1.+GY(J))*BPRUME/2.
      DBEE=BPRUME/2.
      BSQ=BEE*BEE
      CALL RINTEG(CHI,CHIP,CHIDP,PSI,PHILO)
      CHISQ=CHI*CHI
      CHIPSQ=CHIP*CHIP
      CHIPPSI=CHIP*PSI
      SINEA=SINF(.5*CHI)
      COSINE=COSF(CHI)
      SUMT=SUMT+GCOEF(J)*BEE*SINEA*SINEA*DBEE
      SINEB= SINF(CHI)
      FOURB=.25/BEE
      BCHIDP=BEE*CHIDP
      SUMU=SUMU+DBEE*GCOEF(J)*(-.0208333333*BEE*CHIPSQ*COSINE+(.5*BEE
     1*PSI+.0416666667*CHIP)*SINEB)
      SUMV=SUMV+DBEE*GCOEF(J)*(COSINE*( .0006944444*CHIDP*CHIDP*BEE+
     1.0416666667*PSI*BEE*CHIDP+.0036458333333*CHIP*CHIDP
     2        +.25*BEE*PSI*PSI+.86805555555E-04*BEE*CHIPSQ*CHIPSQ+.0416666
     3667*CHIPPSI)+(.0003472222*CHIP*CHIPSQ+.5*BEE*PHILO-.020833333333
     4*BEE*CHIPSQ*PSI-.003645833333*CHIPSQ*CHIP)*SINEB)
      SUMW=SUMW+GCOEF(J)*DBEE*SINEB*SINEB*BEE
      CHID=2.*CHI
```

```
      SINED=SINF(CHID)
      COSINEB=COSF(CHID)
      SUMX=SUMX+GCOEF(J)*DBEE*(BEE*(PSI*SINED-.333333333*CHIPSQ*COSINEB
     1)-FOURB*SINEB*SINED)
      SUMY=SUMY+GCOEF(J)*DBEE*((  -.247916667*CHIDP*CHIP+
     1   (.044444444*CHIDP*CHIDP+.022222222*CHIPSQ*CHIPSQ)*BEE
     2+BEE*PSI*PSI+.666666667*(CHIPPSI+BCHIDP*PSI))*COSINEB+(.044444444
     3444*CHIPSQ*CHIP-.666666667*BEE*CHIPSQ*PSI+BEE*PHILO-.0416666667/
     4BEE*CHIDP-FOURB*PSI+.247916667*CHIPSQ*CHIP)*SINED)
   10 CONTINUE
   20 QONECL=4.*SUMT
      QONEI=.1013212 /GSQ*(SUMU+.0416666667)
      QONEII=.025664956/(GSQ*GSQ)* SUMV
      QTWOCL=3.*SUMW
      QTWOI=.075990887/GSQ*SUMX
      QTWOII = .0019246723 / (GSQ*GSQ)* SUMY
      PRINT 11,QONECL,QONEI,QONEII,QTWOCL,QTWOI,QTWOII
   11 FORMAT (1X,7HQ(1)CL=E20.10,3X,6HQ(1)I=E20.10,3X,7HQ(1)II=E20.10/
     1          1X,7HQ(2)CL=E20.10,3X,6HQ(2)I=E20.10,3X,7HQ(2)II=E20.10)
      GO TO 6
      END



      SUBROUTINE RINTEG(CHI,CHIP,CHIDP,PSI,PHILO)
      DIMENSION AY(128),CY(99),DY(128),        GY(64),GCOEF(64)
      COMMON MEHLERA,MEHLERC,MEHLERD,          NGAUSS,GCOEF, AY,CY,DY,GY
      COMMON GEE,BEE,GSQ,BSQ,RONE,RLESSER
      COMMON S,T,U,V,DHIDP,DSI,DHILO
      VAR=1.                 $  VARI=1.12
      RTWO=0.
      RTHREE=0.
      GSQBSQ=GSQ*BSQ
      IF(GSQBSQ-2.462365368)2,2,1
    2 IF( GSQ-0.6) 3,3,5
    1 JUMP=1
      R=RONE
      GO TO 16
    3 RI=(4./GSQ*(1.+SQRTF(1.-1.25*GSQ    )))**.1666666667
      BPRIME=RI*SQRTF(1.-F(0,RI)/GSQ)
      IF(BEE-BPRIME)5,4,4
    5 SW=1.
      SET=1.
      GO TO 6
    4 RI=(4./GSQ*(1.-SQRTF(1.-1.25*GSQ)))**.1666666667
      BPROME=RI*SQRTF(1.-F(0,RI)/GSQ)
```

```
      IF(BEE-BPROME) 12,14,14
   12 SW=0.
      SET=0.
    6 CONTINUE
      R=RLESSER
    7 VALU=PHIHI(1,R)
      SAVE=R-VALU/PHIHI(2,R)
      IF(ABSF(SAVE-R)-1.E-08)8,9,9
    9 R=ABSF(SAVE)
      GO TO 7
    8 IF(SW-1.)11,10,11
   10 RLESSER=SAVE
      SW=0.
  700 R=RLESSER*VARI
      GO TO 7
   11 IF(SET-1.)15,13,13
   13 RGREATR=SAVE
      IF(RGREATR-RLESSER) 620,620,403
  403 IF(ABSF(RGREATR-RLESSER)-1.E-10) 620,620,402
  402 JUMP=3
      R=RONE
      GO TO 16
   14 JUMP=1
      R=RI*SQRTF(1.+4./(GSQ*(RI**6)))
      GO TO 16
   15 RLESSER=SAVE
      JUMP=4
      R=RONE
   16 CONTINUE
      SW=0.
   19 SAVE=R-((1.-PHIHI(0,R))/(-PHIHI(1,R)))
      IF(SW - 2.) 37, 32, 32
   32 IF(ABSF(SAVE) - RTWO) 606, 606, 34
   34 IF(ABSF(SAVE) - 100.) 37, 606, 606
   37 IF(ABSF(SAVE-R)-1.E-09)18,17,17
   17 R=ABSF(SAVE)
      GO TO 19
   18 GO TO (20,20,21,22),JUMP
   20 RONE=SAVE
      GO TO 23
   21 RONE=SAVE
      GO TO 24
   22 IF(SW-1.)26,27,28
   26 RONE=SAVE
      R=2.*RLESSER-RONE
      SW=1.
      GO TO 19
   27 RTWO=SAVE
```

```
 36 R=(RTWO+RONE)*VAR
    SW=2.
    GO TO 19
 28 RTHREE=SAVE
599 IF(RONE-RTWO          ) 600,606,606
600 IF(ABSF(RONE-RTWO)-5.E-10) 606,606,601
601 IF(RONE-RTHREE          ) 602,606,606
602 IF(ABSF(RONE-RTHREE)-5.E-10) 606,606,603
603 IF(RTWO-RTHREE          ) 604,606,606
604 IF(ABSF(RTWO-RTHREE)-5.E-10) 606,606,605
605 PRINT 406, VAR
406 FORMAT(4HVAR=,E20.10)
    GO TO 25
620 VARI=VARI+.02
    IF (VARI-2.)700,700,609
606 VAR=VAR+.05
    IF(VAR-2.)   35, 35,609
 35 GO TO 36
609 PRINT 610
610 FORMAT(31HRANGE          HAS BEEN EXCEEDED)
    STOP
 23 CONTINUE
C   INTEGRATION SECTIONA
    PRINT 60
 60 FORMAT (10H SECTION A)
    PRINT 38, RONE
 38 FORMAT (1X,5HRONE=E20.10)
    SUMJ=0.
    SUMK=0.
    SUML=0.
    SUMM=0.
    SUMN=0.
    DO 29 N=1,MEHLERA
    DIV=1.-AY(N)
    RB=2.*RONE/DIV
    DRB=RB/DIV
    CALL ABCD(RB,A,B,C,D,0.)
    SAME=DRB*SQRTF((1.-AY(N)*AY(N))/(1.-PHIHI(0,RB)))
    SUMJ=SUMJ+SAME/(RB*RB)
    SUMK=SUMK+SAME*A
    SUML=SUML+SAME*B
    SUMM=SUMM+SAME*C
    SUMN=SUMN+SAME*D
 29 CONTINUE
    SAVE=    BEE
    CONST=3.141592654/FLOATF(MEHLERA)
    CHI=3.141592654-2.*BEE*CONST*SUMJ
    CHIP=2.    *CONST*SUMK
```

```
      CHIDP=-2.*SAVE*CONST*SUML
      PSI=.1666666667*SAVE*CONST*SUMM
      PHILO=2.*CONST*SAVE*SUMN
      PRINT 503,BEE,CHI,CHIP,CHIDP,PSI,PHILO
  503 FORMAT (1X,4HBEE=E20.10,2X,4HCHI=E20.10,2X,5HCHIP=E20.10/1X,6HCHI
     1P=E20.10,2X,4HPSI=E20.10,2X,4HPHI=E20.10/)
      RETURN
  .24 CONTINUE
C     INTEGRATION SECTION C
      PRINT 61
   61 FORMAT (10H SECTION C)
      PRINT 39, RONE, RLESSER, RGREATR
   39 FORMAT (1X,5HRONE=E20.10,2X,8HRLESSER=E20.10,2X,9HRGREATER=E20.10
      RV=(RONE+RLESSER)*.5
      RQ=RGREATR +1.
      SUMA=0.
      SUMB=0.
      SUMC=0.
      SUMD=0.
      SUME=0.
      SUMF=0.
      SUMG=0.
      SUMH=0.
      SUMI=0.
      SUMJ=0.
      SUMK=0.
      SUML=0.
      SUMM=0.
      DRBCDE=(RV-RONE)*.5
      DRJKLM=(RQ-RV)*.5
      DO 30 N=1,MEHLERC
      DIV=1.-CY(N)
      RA=2.*RONE/DIV
      DRA=RA/DIV
      CULT=CY(N)-1.
      RBCDE=RV+DRBCDE*CULT
      RJKLM=RQ+DRJKLM*CULT
      CFACT=SQRTF(1.-CY(N)*CY(N))
      SUMA=SUMA+DRA/(RA*RA*SQRTF(1.-PHIHI(0,RA)))*CFACT
      CALL ABCD(RBCDE,A,B,C,D,0.)
      SAME=DRBCDE/SQRTF(1.-PHIHI(0,RBCDE))*CFACT
      SUMB=SUMB+SAME*A
      SUMC=SUMC+SAME*B
      SUMD=SUMD+SAME*C
      SUME=SUME+SAME*D
      CALL ABCD(RJKLM,A,B,C,D,0.)
      SAME=1.-PHIHI(0,RJKLM)
      SAMERT=SQRTF(SAME)
```

```
      SAMECU=SAME*SAMERT
      SAMEFIV=SAMECU*SAME
      RSQ=RJKLM*RJKLM
      PTWO=PHIHI(2,RJKLM)
      RFOR=RSQ*RSQ
      RSIX=RFOR*RSQ
      TERM=DRJKLM*CFACT
      SUMJ=SUMJ+TERM*(1./(RSQ*SAMERT)+BSQ/(RFOR*SAMECU))
      SUMK=SUMK+3.*TERM*(1./(RFOR*SAMECU)+BSQ/(RSIX*SAMEFIV))
      SUML=SUML+TERM*(PTWO/(RSQ*SAMEFIV)+6./(RFOR*SAMECU))
      SUMM=SUMM+TERM*((-804.    /RSIX-(228.   *PTWO/RSQ+10.       *PHIHI(
     14,RJKLM))/(RSQ*SAME)-49.        *PTWO*PTWO/(RSQ*SAME*SAME))/SAMEFIV
     2) /1536.
      RFGHI=2.*RQ/DIV
      DRFGHI=RFGHI/DIV
      CALL ABCD(RFGHI,A,B,C,D,0.)
      SAME=DRFGHI/SQRTF(1.-PHIHI(0,RFGHI))*CFACT
      SUMF=SUMF+SAME*A
      SUMG=SUMG+SAME*B
      SUMH=SUMH+SAME*C
      SUMI=SUMI+SAME*D
   30 CONTINUE
      CONST=3.141592654/FLOATF(NEHLERC)
      CALL ABCD(RQ,HOLDA,HOLDB,HOLDC,HOLDD,1.)
      CALL ABCD(RV,ANSA,ANSB,ANSC,ANSD,1.)
      SAVE=    BEE
      CHI=3.141592654-2.*BEE*CONST*SUMA
      CHIP=2.     *(CONST*(SUMB+SUMF-SUMJ)+HOLDA-ANSA)
      IF(S) 41, 41,42
   41 S=1.
      CHIDP=-2.*SAVE*(CONST*(SUMC+SUMG+SUMK)-HOLDB+ANSB)
      PSI=.1666666667*SAVE*(CONST*(SUMD+SUMH+.75*SUML)-HOLDC+ANSC)
      PHILO=2.*SAVE    *(CONST*(SUME+SUMI+SUMM)+HOLDD-ANSD)
      DHIDP=CHIDP
      DSI=PSI
      DHILO=PHILO
      CHIDP=0.
      PSI=0.
      PHILO=0.
      GO TO 43
   42 CHIDP=-2.*SAVE*(CONST*(SUMC+SUMG+SUMK)-HOLDB+ANSB)
      IF(CHIDP-DHIDP) 49,49,47
   47 DHIDP=CHIDP
      CHIDP=0.
   49 PSI=.1666666667*SAVE*(CONST*(SUMD+SUMH+.75*SUML)-HOLDC+ANSC)
      IF(PSI-DSI) 54,54,52
   52 DSI=PSI
      PSI=0.
```

```
   54 PHILO=2.*SAVE     *(CONST*(SUME+SUMI+SUMM)+HOLDD-ANSD)
      IF(PHILO-DHILO) 43, 43,57
   57 DHILO=PHILO
      PHILO=0.
   43 PRINT 504,BEE,CHI,CHIP,CHIDP,PSI,PHILO
  504 FORMAT (1X,4HBEE=E20.10,2X,4HCHI=E20.10,2X,5HCHIP=E20.10/1X,6HCHID
     1P=E20.10,2X,4HPSI=E20.10,2X,4HPHI=E20.10/)
      RETURN
   25 CONTINUE
C     INTEGRATION SECTION D
      PRINT 62
   62 FORMAT (10H SECTION D)
      PRINT 40, RONE, RTWO, RTHREE, RLESSER
   40 FORMAT (1X,5HRONE=E20.10,2X,5HRTWO=E20.10,2X,7HRTHREE=E20.10,2X,
     18HRLESSER=E20.10)
      RV=(RONE+RLESSER)*.5
      RQ=(RLESSER+RTWO)*.5
      SUMA=0.
      SUMB=0.
      SUMC=0.
      SUMD=0.
      SUME=0.
      SUMF=0.
      SUMG=0.
      SUMH=0.
      SUMI=0.
      SUMJ=0.
      SUMK=0.
      SUML=0.
      SUMM=0.
      SUMN=0.
      SUMO=0.
      SUMP=0.
      SUMQ=0.
      SUMR=0.
      DRA=(RTWO-RONE)*.5
      DRBCDE=(RV-RONE)*.5
      DRKLMN=(RTWO-RQ)*.5
      DROPQR=(RQ-RV)*.5
      DO 31 N=1,MEHLERD
      CULT=DY(N)-1.
      DIV=1.-DY(N)
      RA=RTWO+DRA*CULT
      RBCDE=RV+DRBCDE*CULT
      RKLMN=RTWO+DRKLMN*CULT
      ROPQR=RQ+DROPQR*CULT
       RFGHIJ=2.*RTHREE/DIV
      DRFGHIJ=RFGHIJ/DIV
```

```
      CFACT=SQRTF(1.-DY(N)*DY(N))
      SUMA=SUMA+DRA/(RA*RA*SQRTF(1.-PHIHI(0,RA)))*CFACT
      CALL ABCD(RBCDE,A,B,C,D,0.)
      SAME=DRBCDE/SQRTF(1.-PHIHI(0,RBCDE))*CFACT
      SUMB=SUMB+SAME*A
      SUMC=SUMC+SAME*B
      SUMD=SUMD+SAME*C
      SUME=SUME+SAME*D
      CALL ABCD(RFGHIJ,A,B,C,D,0.)
      SAME=DRFGHIJ/SQRTF(1.-PHIHI(0,RFGHIJ))*CFACT
      SUMF=SUMF+SAME/(RFGHIJ*RFGHIJ)
      SUMG=SUMG+SAME*A
      SUMH=SUMH+SAME*B
      SUMI=SUMI+SAME*C
      SUMJ=SUMJ+SAME*D
      CALL ABCD(RKLMN,A,B,C,D,0.)
      SAME=DRKLMN/SQRTF(1.-PHIHI(0,RKLMN))*CFACT
      SUMK=SUMK+SAME*A
      SUML=SUML+SAME*B
      SUMM=SUMM+SAME*C
      SUMN=SUMN+SAME*D
      SAVE=1.-PHIHI(0,ROPQR)
      SAVERT=SQRTF(SAVE)
      SAVECU=SAVE*SAVERT
      RSQ=ROPQR*ROPQR
      SAVEFIV=SAVECU*SAVE
      PTWO=PHIHI(2,ROPQR)
      RFOR=RSQ*RSQ
      RSIX=RFOR*RSQ
      TERM=DROPQR*CFACT
      SUMO=SUMO+TERM*(1./(RSQ*SAVERT)+BSQ/(RFOR*SAVECU))
      SUMP=SUMP+TERM*(3./(RFOR*SAVECU)+3.*BSQ/(RSIX*SAVEFIV))
      SUMQ=SUMQ+TERM*(PTWO/(RSQ*SAVEFIV)+6./(RFOR*SAVECU))
      SUMR=SUMR+TERM*((-804.     /RSIX-(226.   *PTWO/RSQ+10.        *PHIHI(
     14,ROPQR))/(RSQ*SAME)-49.        *PTWO*PTWO/(RSQ*SAME*SAME))/SAMEFIV
     2) /1536.
   31 CONTINUE
      CONST=3.141592654/FLOATF(MEHLERD)
      CALL ABCD(RQ,HOLDA,HOLDB,HOLDC,HOLDD,1.)
      CALL ABCD(RV,ANSA,ANSB,ANSC,ANSD,1.)
      CHI=3.141592654-2.*BEE*(CONST*(SUMA+SUMF))
      CHIP=2.*(CONST*(SUMG+SUMB+SUMK-SUMO)+HOLDA-ANSA)
      CHIDP=-2.*BEE*(CONST*(SUMH+SUMC+SUML+SUMP)-HOLDB+ANSB)
      PSI=.1666666667*BEE*(CONST*(SUMI+SUMD+SUMM+.75*SUMQ)-HOLDC+ANSC)
      PHILO=2.*BEE*(CONST*(SUMJ+SUME+SUMN+SUMR)+HOLDD-ANSD)
      PRINT 505,BEE,CHI,CHIP,CHIDP,PSI,PHILO
  505 FORMAT (1X,4HBEE=E20.10,2X,4HCHI=E20.10,2X,5HCHIP=E20.10/1X,6HCHID
     1P=E20.10,2X,4HPSI=E20.10,2X,4HPHI=E20.10/)
```

```
      RETURN
      END



      FUNCTION F(K,X)
      FACTFI=NFACT(5+K)
      F=(-1.)**K*4.*(GACT(K)/(X**(12+K))-FACTFI/(120.*X**(6+K)))
      END



      FUNCTION GACT(K)
      GACT=1.
      DO 1 J=1,K
    1 GACT=GACT*(J+11)
      END



      FUNCTION NFACT(K)
      NFACT=1
      DO 2 J=1,K
    2 NFACT=NFACT*J
      END



      FUNCTION PHIHI(M,X)
      DIMENSION AY(128),CY(99),DY(128),        GY(64),GCOEF(64)
      COMMON MEHLERA,MEHLERC,MEHLERD,         NGAUSS,GCOEF, AY,CY,DY,GY
      COMMON GEE,BEE,GSQ,BSQ,RONE,RLESSER
      COMMON S,T,U,V,DHIDP,DSI,DHILO
      FACTM=NFACT(M+1)
      PHIHI= F(M,X)/GSQ+(-1.)**M*FACTM*BSQ/X**(M+2)
      END
```

```
      SUBROUTINE ABCD(X,[illegible]D,COUNT)
      DIMENSION AY(128),CY(99),DY(128),       GY(64),GCOEF(64)
      COMMON MEHLERA,MEHLERC,MEHLERD,         NGAUSS,GCOEF, AY,CY,DY,GY
      COMMON GEE,BEE,GSQ,BSQ,RONE,RLESSER
      COMMON S,T,U,V,DHIDP,DSI,DHILO
      ONE=PHIHI(1,X)
      TWO=PHIHI(2,X)
      THREE=PHIHI(3,X)
      FOUR =PHIHI(4,X)
      FIVE =PHIHI(5,X)
      ONESQ=ONE*ONE
      ONECUB=ONESQ*ONE
      ONEFOR=ONECUB*ONE
      ONEFIV=ONEFOR*ONE
      ONESIX=ONEFIV*ONE
      ONESEV=ONESIX*ONE
      ONEEIGH=ONESEV*ONE
      TWOSQ=TWO*TWO
      TWOCU=TWOSQ*TWO
      TWOFOR=TWOCU*TWO
      TWOFIV=TWOFOR*TWO
      THREESQ=THREE*THREE
      XSQ=X* X
      XCU=XSQ*X
      XFOR=XCU*X
      XFIV=XFOR*X
      XSIX=XFIV*X
      XSEV=XSIX*X
      IF(COUNT)2,1,2
    1 FONE=TWO/(XFOR*ONESQ)
      FTWO=1./(XSEV*ONESQ*X)
      FTHREE=1./(XFOR*ONEFOR)
      FFOUR=1./(XSQ*ONEFIV)
      FFIVE=1./(XSQ*ONESEV)
      FSIX=1./(XSQ*ONESIX)
      FSEVEN=1./(XSQ*ONEFOR)
      FEIGH=1./(XCU*ONESEV)
      FNIN=1./(XCU*ONESIX)
      FTEN=1./(XCU*ONEFIV)
      FELEV=1./(XCU*ONEFOR)
      FTWEL=1./(XCU*ONECUB)
      FTHIR=1./(XSQ*ONEEIGH)
      A=-1./XSQ-8.*BSQ/(XFIV*ONE)-2.*BSQ*FONE
      B=24./(XFIV*ONE)+6.*FONE+168.*BSQ*FTWO+72.*BSQ*TWO/(XSEV*ONECUB)+
     112.*BSQ*TWOSQ/(XSIX*ONEFOR)-4.*BSQ*THREE/(XSIX*ONECUB)
      C=36./(XFIV*ONE)+15.*FONE+6.*TWOSQ/(XCU*ONECUB)-4.*(THREE/(XCU
     1*ONESQ)+TWO*THREE/(XSQ*ONECUB))+3.*TWOCU/(XSQ*ONEFOR)+FOUR/(XSQ*
     2ONESQ)
```

```
      D=-42210. *FTWO-31770. *TWO/(XSEV*ONECUB)+7845.      *THREE/(XSIX*
     1ONECUB)-17535.      *TWOSQ/(XSIX*ONEFOR)-8520.      *TWOCU/(XFIV*
     2ONEFIV)+8640.*TWO*THREE/(XFIV*ONEFOR)-1488.*FOUR/(XFIV*ONECUB)
     3-3600.*TWOFOR/(XFOR*ONESIX)-960.      *THREESQ*FTHREE+5790.      *
     4TWOSQ*THREE/(XFOR*ONEFIV)-1482.      *TWO*FOUR*FTHREE+204.
     5*FIVE/(XFOR*ONECUB)-1470.      *TWOFOR*TWO*FEIGH+3360.   *
     6TWOCU*THREE*FNIN-1400.      *TWO*THREESQ*FTEN   -1060.      *TWOSQ
     7*FOUR*FTEN+   2205.*      TWOFOR*THREE*FFIVE-1540.      *TWOSQ
     8*THREESQ*FSIX-810. *TWOCU*FOUR*FSIX+222.      *TWOSQ*FIVE*FFOUR+
     9680.      *TWO*THREE*FOUR*FFOUR-76.      *THREE*FIVE*FSEVEN
      D=D-44.      *TWO*PHIHI(6,X)*FSEVEN-47.      *FOUR**2*FSEVEN+
     1140.      *THREESQ*THREE*FFOUR+5.      *PHIHI(7,X)/(XSQ*
     2ONECUB)   +376.      *THREE*FOUR*FELEV   +232.      *TWO*FIVE*FEL
     3EV   -30.      *PHIHI(6,X)*FTWEL      -735.      *TWOFIV*TWO*FTH
     4IR
      D=D/1440.
      RETURN
C     Q OR V PORTION OF SUBROUTINE
    2 FSIX=1./(XFOR*ONE)
      FONE=1./(XCU*ONEFOR)
      FTWO=1./(XSQ*ONEFOR)
      FTHREE=1./(XSQ*ONEFIV)
      FFOUR=1./(XCU*ONECUB)
      FFIVE=1./(XSQ*ONECUB)
      FSEV=1./(XCU*ONESQ)
      FEIGHT=1./(XFOR*ONEFOR)
      FNINE=1./(XSQ*ONESQ)
      FTEN=1./(XFIV*ONEFOR)
      E=48240./(XSIX*X*ONESQ)+26280. *TWO/(XSIX*ONECUB)+ 12288.      *TWO
     1SQ*FTEN  -7296.      *THREE/(XFIV*ONECUB)+4752.*TWOCU/(XFOR*ONEFIV
     2)-5664.      *TWO*THREE*FEIGHT+1152.*FOUR/(XFOR*ONECUB)+1680.
     3*TWOFOR/(XCU*ONESIX)-3136.      *TWOSQ*THREE/(XCU*ONEFIV)+
     4 672.      *THREESQ*FONE+912.      *TWO*FOUR*FONE- 160.*
     5FIVE*FFOUR-  232.      *TWO*FIVE*FTWO+40.      *PHIHI(6,X)*FFIV
     5E-
     6376.*      THREE*FOUR*FTWO +848.      *TWOSQ*FOUR*FTHREE+1120.
     7*TWO*THREESQ*FTHREE-2240.*      TWOCU*THREE/(XSQ*ONESIX)+840.
     8*TWOFIV/(XSQ*ONESIX*ONE)
      F=4020.      /(XSIX*ONE)+1824.      *TWO/(XFIV*ONESQ)+624.
     1*TWOSQ/(XFOR*ONECUB)-456.      *THREE/(XFOR*ONESQ)+168.*
     2TWOCU*FONE+40.      *FOUR*FSEV-224.*      TWO*THREE*FFOUR+
     384.      *TWOFOR/(XSQ*ONEFIV)+56.      *THREESQ*FFIVE-
     4196.      *TWOSQ*THREE/(XSQ*ONEFOR)+76.      *TWO*FOUR*FFIVE-
     520.      *FIVE*FNINE
      G=684.  *TWO*FSIX+84.      *TWOSQ*FSEV+42.      *TWOCU*FFIVE+
     130.      *FOUR/(XSQ*ONE)-84.      *TWO*THREE*FNINE
      COEF=2.*BSQ
      CKEEP=1.-PHIHI(0,X)
```

```
 CKEEPRT=SQRTF(CKEEP)
 A=COEF*FSIX/CKEEPRT
 B=COEF/(XSIX*ONE*CKEEPRT*CKEEP)+(6.*FSIX+24.*BSQ/(XSIX*X*ONESQ )+
1+.*BSQ*TWO/(XSIX*ONECUB))/CKEEPRT
 C=(9.*FSIX+2.*TWO*FSEV+TWOSQ*FFIVE-THREE*FNINE)/CKEEPRT+.5*TWO/(XS
1Q*ONE*CKEEP*CKEEPRT)
 D=(E+(F+(G+105.        *TWOSQ/(XSQ*ONE*CKEEP))/CKEEP)/CKEEP)/CKEEPRT
 D=D/11520.
 END
 END



 FUNCTION NFACT(K)
 NFACT=1
 DO 1 J=1,K
1 NFACT=NFACT*J
 END
 END
```

```
      PROGRAM OMEGA
      DIMENSION Z(100),QONECL(100),QONEIO(100),QONEII(100),F(100)
     1QONEOI(100),QONEOO(100)
      READ 9, S,EL
    9 FORMAT (2F10.0)
      PRINT 10, S,EL
   10 FORMAT (    3H1S=E20.10,3X,2HL=E20.10//)
      READ 11, T
   11 FORMAT (F10.0)
      READ 12, DELTAT
   12 FORMAT(F10.0)
      READ 13, TEND
   13 FORMAT(F10.0)
      JIN=1
    4 JON=JIN+4
      DO 1 K=JIN,JON
      READ 2, Z(K),QONECL(K),QONEIO(K),QONEII(K)
    2 FORMAT (E9.0,11X,E11.0,9X,E11.0,9X,E11.0)
      READ 14, QONEOI(K),QONEOO(K)
   14 FORMAT (E11.0,9X,E11.0)
      IF(Z(K)+1000.)3,3,8
    8 Z(K)=2.30258509*Z(K)
    1 F(K)=(S+2.)*Z(K)
      JIN=JON+1
      GO TO 4
    3 ACL=0.
      AOI=0.
      AIO=0.
      AOO=0.
      AII=0.
      N= JIN-1
      DO 5 J=1,N,5
       ACL=ACL+(14.*QONECL(J)*EXPF(F(J)-EXPF(Z(J))/T)
     1+81.*QONECL(J+1)*EXPF(F(J+1)-EXPF(  Z(J+1))/T)
     2+110.*QONECL(J+2)*EXPF(F(J+2)-EXPF(  Z(J+2))/T)
     3+81.*QONECL(J+3)*EXPF(F(J+3)-EXPF(  Z(J+3))/T)+
     414.*QONECL(J+4)*EXPF(F(J+4)-EXPF(  Z(J+4))/T))*(Z(J+4)-Z(J))/2.
       AOI=AOI+(14.*QONEOI(J)*EXPF(F(J)-EXPF(Z(J))/T)
     1+81.*QONEOI(J+1)*EXPF(F(J+1)-EXPF(  Z(J+1))/T)
     2+110.*QONEOI(J+2)*EXPF(F(J+2)-EXPF(  Z(J+2))/T)
     3+81.*QONEOI(J+3)*EXPF(F(J+3)-EXPF(  Z(J+3))/T)+
     414.*QONEOI(J+4)*EXPF(F(J+4)-EXPF(  Z(J+4))/T))*(Z(J+4)-Z(J))/2.
       AIO=AIO+(14.*QONEIO(J)*EXPF(F(J)-EXPF(Z(J))/T)
     1+81.*QONEIO(J+1)*EXPF(F(J+1)-EXPF(  Z(J+1))/T)
     2+110.*QONEIO(J+2)*EXPF(F(J+2)-EXPF(  Z(J+2))/T)
     3+81.*QONEIO(J+3)*EXPF(F(J+3)-EXPF(  Z(J+3))/T)+
     414.*QONEIO(J+4)*EXPF(F(J+4)-EXPF(  Z(J+4))/T))*(Z(J+4)-Z(J))/2.
       AOO=AOO+(14.*QONEOO(J)*EXPF(F(J)-EXPF(Z(J))/T)
```

```
 1+81.*QONECO(J+1)*EXPF(F(J+1)-EXPF( Z(J+1))/T)
 2+110.*QONECO(J+2)*EXPF(F(J+2)-EXPF( Z(J+2))/T)
 3+81.*QONECO(J+3)*EXPF(F(J+3)-EXPF( Z(J+3))/T)+
 414.*QONECO(J+4)*EXPF(F(J+4)-EXPF( Z(J+4))/T))*(Z(J+4)-Z(J))/2.
5  AII=AII+(14.*QONEII(J)*EXPF(F(J)-EXPF(Z(J))/T)
 1+81.*QONEII(J+1)*EXPF(F(J+1)-EXPF( Z(J+1))/T)
 2+110.*QONEII(J+2)*EXPF(F(J+2)-EXPF( Z(J+2))/T)
 3+81.*QONEII(J+3)*EXPF(F(J+3)-EXPF( Z(J+3))/T)+
 414.*QONEII(J+4)*EXPF(F(J+4)-EXPF( Z(J+4))/T))*(Z(J+4)-Z(J))/2.
  ACL=ACL/150.
  AOI=AOI/150.
  AIO=AIO/150.
  AOO=AOO/150.
  AII=AII/150.
  M=S
  SFACT=NFACT(M+1)
  OMEGACL=ACL/(SFACT*(T**(S+2.)))
  OMEGAOI=AOI/(SFACT*(T**(S+2.)))
  OMEGAIO=AIO/(SFACT*(T**(S+2.)))
  OMEGAOO=AOO/(SFACT*(T**(S+2.)))
  OMEGAII=AII/(SFACT*(T**(S+2.)))
  PRINT 7, T,OMEGACL,OMEGAOI,OMEGAIO,OMEGAOO,OMEGAII
7 FORMAT (1X,2HT=E9.2,2X,8HOMEGACL=E11.4,2X,7HOMEGAI=E11.4,2X,8HOMEG
 1AII=E11.4,2X,9HOMEGAIII=E11.4,2X,8HOMEGAIV=E11.4/)
  T=T-DELTAT
  IF(T-TEND) 6,6,3
6 STOP
  END


  FUNCTION NFACT(K)
  NFACT=1
  DO 1 J=1,K
1 NFACT=NFACT*J
  END
  END
```

```
      PROGRAM SOWELLP
      TYPE DOUBLE QONE,QTWO,PHASE,A,B,C,T,ARGU,ARGUP,G,GP,RESULT,FR,X,F
      DIMENSION PHASE(105),A(300),B(300),C(300),T(300)
      GEESQD=1.66
      ELAMST=.1
      LEL=105
      ARGU=2.*3.141592653589793238462643*DSQRT(GEESQD)/ELAMST
      ARGUP=2.*3.141592653589793238462643*DSQRT(GEESQD+1.)/ELAMST
      D = 1.
      G=DSQRT(3.141592653589793238462643/(2.*ARGU))
      GP=DSQRT(3.141592653589793238462643/(2.*ARGUP))
      EL = 0.
      CALL SPHEBE(LEL ,ARGU,A,RESULT)
      DO 23  J=1,LEL
   23 A(J)=A(J)/G
      CALL SPHEBE(LEL ,ARGUP,B,RESULT)
      DO 24 K=1,LEL
   24 B(K)=B(K)/GP
      CALL SPHEBE(-LEL ,ARGU,C,RESULT)
      DO 25 L=1,LEL
   25 C(L)=C(L+1)/G
      DO 26 L=1,LEL
      FR=((ARGU*B(L)*A(L+1)-ARGUP*A(L)*B(L+1))/(ARGUP*C(L)*B(L+1)+
     1ARGU*B(L)*C(L+1)))*D
      D=-1.*D
      PHASE(L+1)=DATAN(FR)
      PRINT 20, EL, PHASE(L + 1)
   20 FORMAT (E20.0,D45.25)
      IF(EL - 1.) 7, 8, 17
    8 QONE      = 4.*EL* DSIN(PHASE( L + 1 )- PHASE( L))*DSIN(PHASE(L + 1
     1) - PHASE(L))/(ARGU*ARGU)
      QTWO    =0.
    7 EL = EL + 1.
      GO TO 26
   17 QTWO      = QTWO              + 3.*(EL - 1.)*EL* DSIN(PHASE( L + 1 ) -
     1PHASE(L-1))*DSIN(PHASE(L+1)-PHASE(L-1))/((EL-.5)*ARGU*ARGU)
      QONE      = QONE              + 4.*EL* DSIN(PHASE( L + 1 ) - PHASE( L))
     1*DSIN(PHASE(L+1)-PHASE(L))/(ARGU*ARGU)
      PRINT 102, EL, QONE     , QTWO
  102 FORMAT (E20.0,2D45.25)
      GO TO 7
   26 CONTINUE
      PRINT 13, GEESQD, ELAMST, QONE    , QTWO
   13 FORMAT (2E20.10,2D45.25)
      END
```

```
      SUBROUTINE SPHEBE(LEL,X,T,RESULT)
      TYPE DOUBLE QONE,QTWO,PHASE,A,B,C,T,ARGU,ARGUP,G,GP,RESULT,FR,X,F
      DIMENSION PHASE(105),A(300),B(300),C(300),T(300)
    1 IF(X) 18, 12, 18
   12 IF(LEL) 16, 13, 14
   13 RESULT=1.0
      RETURN
   14 RESULT=0.0
      RETURN
   16 RESULT=.9999999999E199
      RETURN
   18 IF(LEL) 55, 51, 19
   19 MO=LEL
      JO=2*XFIXF(X)
      IF(MO-JO) 2, 21, 21
    2 MO=JO
   21 MO=MO+11
   22 T(MO)=0.
      T(MO-1)=1.0E-300
      LO=MO-2
   23 F=2*(MO-1)
  231 MO=MO-3
      I2=MO
  232 F=F-2.0
      T(I2+1)=(F+1.)/X*T(I2+2)-T(I2+3)
      IF(I2) 4,3,4
    4 I2=I2-1
      GO TO 232
    3 F=DSIN(X)/X/T(1)
      DO 5 J=1,MO
    5 T(J)=F*T(J)
      RESULT=T(LEL+1)
      RETURN
   51 RESULT=DSIN(X)/X
      RETURN
   55 LO=-LEL+1
      T(1)=DSIN(X)/X
      T(2)=DCOS(X)/X
      DO 6 J=3,LO
    6 T(J )=(-2.*FLOATF(J-2)+1.)/X*T(J-1 )-T(J-2)
      RESULT=T(LO)
      RETURN
      END
      END
```

```
      PROGRAM MONOTON
      DIMENSION AY(128),OY(64),GCOEF(64),GY(64)
      COMMON MEHLERA,MEHLERO,NGAUSS,AY,OY,GY,GCOEF,GEE,GSQ,YO,YONE,L
      NGAUSS=32
      MEHLERA=64
      L=12
      PRINT 3, L
    3 FORMAT (3H1L=I2//)
      EL=12.
      G=.0005
      FA=MEHLERA
      DO 7 I=1, MEHLERA
      FI=I
    7 AY(I)=COSF(((2.*FI-1.)/(2.*FA))*3.141592654)
C     32 GAUSS-LEGENDRE WEIGHTS AND POINTS - TO +
      GY(01)=-.9972638618
      GY(02)=-.9856115115
      GY(03)=-.9647622556
      GY(04)=-.9349060759
      GY(05)=-.8963211558
      GY(06)=-.8493676137
      GY(07)=-.7944837960
      GY(08)=-.7321821187
      GY(09)=-.6630442669
      GY(10)=-.5877157572
      GY(11)=-.5068999089
      GY(12)=-.4213512761
      GY(13)=-.3318686023
      GY(14)=-.2392873623
      GY(15)=-.1444719616
      GY(16)=-.0483076657
      GY(17)= .0483076657
      GY(18)= .1444719616
      GY(19)= .2392873623
      GY(20)= .3318686023
      GY(21)= .4213512761
      GY(22)= .5068999089
      GY(23)= .5877157572
      GY(24)= .6630442669
      GY(25)= .7321821187
      GY(26)= .7944837960
      GY(27)= .8493676137
      GY(28)= .8963211558
      GY(29)= .9349060759
      GY(30)= .9647622556
      GY(31)= .9856115115
      GY(32)= .9972638618
      GCOEF(01)=.007018610
```

```
      GCOEF(02)=.0162743947
      GCOEF(03)=.0253920653
      GCOEF(04)=.0342738629
      GCOEF(05)=.0428358980
      GCOEF(06)=.0509980593
      GCOEF(07)=.0586840935
      GCOEF(08)=.0658222228
      GCOEF(09)=.0723457941
      GCOEF(10)=.0781938957
      GCOEF(11)=.0833119242
      GCOEF(12)=.0876520930
      GCOEF(13)=.0911738787
      GCOEF(14)=.0938443991
      GCOEF(15)=.0956387201
      GCOEF(16)=.0965400885
      GCOEF(17)=.0965400885
      GCOEF(18)=.0956387201
      GCOEF(19)=.0938443991
      GCOEF(20)=.0911738787
      GCOEF(21)=.0876520930
      GCOEF(22)=.0833119242
      GCOEF(23)=.0781938957
      GCOEF(24)=.0723457941
      GCOEF(25)=.0658222228
      GCOEF(26)=.0586840935
      GCOEF(27)=.0509980593
      GCOEF(28)=.0428358980
      GCOEF(29)=.0342738629
      GCOEF(30)=.0253920653
      GCOEF(31)=.0162743947
      GCOEF(32)=.007018610
C     Q INTEGRALS
      SUMT=0.
      SUMU=0.
      SUMV=0.
      SUMW=0.
      SUMX=0.
      SUMY=0.
      DIV=1.-GY(1)
      YO=(GY(1)+1.)/DIV
      YONE=YO*(EL**(1./L))
      ALPHA=((1.-EL*G)/(2.*G))**(1./L)
      DO 10 J=1,NGAUSS
      YO=ALPHA*(1.+GY(J))/2.
      DYO=ALPHA/2.
      CALL RINTEG(CHI,CHIP,CHIDP,PSI,PHILO)
      COSINE=COSF(CHI)
      SINEB= SINF(CHI)
```

```
      CHID=2.*CHI
      SINED=SINF(CHID)
      COSINEB=COSF(CHID)
      CHISQ=CHI*CHI
      CHIPPSI=CHIP*PSI
      CHIPSQ=CHIP*CHIP
      SINEA=SINF(.5*CHI)
      SUMT=SUMT+GCOEF(J)*YO *SINEA*SINEA*DYO
      SUMU=SUMU+DYO *GCOEF(J)*(                   -YO *CHIPSQ*COSINE+(24.*YO
     1*PSI+2.         *CHIP)*SINEB)/48.
      SUMV=SUMV+DYO *GCOEF(J)*(COSINE*( 8.          *CHIDP*CHIDP*YO +
     1480.        *PSI*YO*CHIDP+42.*CHIP*CHIDP
     2+PSI*PSI*2880.* YO     +                   YO *CHIPSQ*CHIPSQ+480.
     3    *CHIPPSI          )+(4.*CHIP*CHIPSQ+5760.*PHILO* YO     -42.*CHIPS
     4Q*CHIP-240.   *CHIPSQ*PSI*YO)*SINEB)/11520.
      SUMW=SUMW+GCOEF(J)*DYO *SINEB*SINEB*YO
      SUMX=SUMX+GCOEF(J)*DYO*(12.*PSI*YO*SINED-4.      *YO*CHIPSQ*COSINEB
     1 -3./YO*SINEB*SINEB)/12.
      SUMY=SUMY+GCOEF(J)*DYO *
     1(((-89.25*CHIP*CHIDP+36.*CHIDP*CHIDP+5.*CHIPSQ*CHIPSQ)*YO+360.*PSI
     2*PSI* YO      +240. *YO*(CHIPPSI/YO+ CHIDP*PSI))*COSINEB+(16.
     3    *CHIPSQ*CHIP-240. YO*CHIPSQ*PSI+360.*PHILO* YO      -15.
     4/YO*CHIDP-90.*PSI/(YO    )+89.25*CHIPSQ*CHIP)*SINED)/360.
   10 CONTINUE
      QONECL=4.*SUMT
      QONEI=.101321184    *(SUMU+1./24.)
      QONEII=.0025664955б*SUMV
      QTWOCL=3.*SUMW
      QTWOI=.075990887      *SUMX
      QTWOII = .0019248717*SUMY
      PRINT 11,QONECL,QONEI,QONEII,QTWOCL,QTWOI,QTWOII
   11 FORMAT (1X,3HA1=,E20.10,3X,3HB1=,E20.10,3X,3HC1=,E20.10/
     11X,3HA2=,E20.10,3X,3HB2=E20.10,3X,3HC2=E20.10)
      END
```

```
      SUBROUTINE RINTEG(CHI,CHIP,CHIDP,PSI,PHILO)
      DIMENSION AY(128),OY(64),GCOEF(64),GY(64)
      COMMON KEHLERA,KEHLERO,NGAUSS,AY,OY,GY,GCOEF,GEE,GSQ,YO,YONE,L
      R=YONE
   19 SAVE=R-((1.-PHIHI(0,R))/(-(R**(L-1))/(YO**L)-2.*(R**1)))
      IF(ABSF(ABSF(SAVE/R)-1.)-1.E-03)18,17,17
   17 R=ABSF(SAVE)
      GO TO 19
   18 YONE=SAVE
```

```
      PRINT 38, YONE
   38 FORMAT (1X,5HYONE=E20.10)
      SUMJ=0.
      SUMK=0.
      SUML=0.
      SUMM=0.
      SUMN=0.
      DO 29 N=1,MEHLERA
      RB=YONE*(1.+AY(N))/2.
      DRB=YONE/2.
      SAME=DRB*SQRTF((1.-AY(N)*AY(N))/(1.-PHIHI(0,RB)))
      CALL ABCD(RB,A,B,C,D)
      SUMJ=SUMJ+SAME
      SUMK=SUMK+SAME*A
      SUML=SUML+SAME*B
      SUMM=SUMM+SAME*C
      SUMN=SUMN+SAME*D
   29 CONTINUE
      CONST=3.141592654/FLOATF(MEHLERA)
      CHI=3.141592654-2.     *CONST*SUMJ
      CHIP=2.     *CONST*SUMK/YO
      CHIDP=-2.      *CONST*SUML/(YO*YO)
      PSI=.1666666667       *CONST*SUMM/(YO*YO)
      PHILO=2.*CONST        *SUMN/(YO**4)
      PRINT 503,YO ,CHI,CHIP,CHIDP,PSI,PHILO
  503 FORMAT (1X,4HYO =E20.10,2X,4HCHI=E20.10,2X,5HCHIP=E20.10/1X,6HCHID
     1P=E20.10,2X,4HPSI=E20.10,2X,4HPHI=E20.10/)
      RETURN
      END


      SUBROUTINE ABCD(X,A,B,C,D)
      DIMENSION AY(128),OY(64),GCOEF(64),GY(64)
      COMMON MEHLERA,MEHLERO,NGAUSS,AY,OY,GY,GCOEF,GEE,GSQ,YO,YONE,L
      ONE=PHIHI(1,X)
      TWO=PHIHI(2,X)
      THREE=PHIHI(3,X)
      FOUR =PHIHI(4,X)
      FIVE =PHIHI(5,X)
      ONESQ=ONE*ONE
      ONECUB=ONESQ*ONE
      ONEFOR=ONECUB*ONE
      ONEFIV=ONEFOR*ONE
      ONESIX=ONEFIV*ONE
      ONESEV=ONESIX*ONE
```

```
 ONEEIGH=ONESEV*ONE
 TWOSQ=TWO*TWO
 TWOCU=TWOSQ*TWO
 TWOFOR=TWOCU*TWO
 TWOFIV=TWOFOR*TWO
 THREESQ=THREE*THREE
 XSQ=1./(X*X)
 XCU=XSQ/X
 XFOR=XCU/X
 XFIV=XFOR/X
 XSIX=XFIV/X
 XSEV=XSIX/X
 FONE=TWO/(XFOR*ONESQ)
 FTWO=1./(XSEV*ONESQ/X)
 FTHREE=1./(XFOR*ONEFOR)
 FFOUR=1./(XSQ*ONEFIV)
 FFIVE=1./(XSQ*ONESEV)
 FSIX=1./(XSQ*ONESIX)
 FSEVEN=1./(XSQ*ONEFOR)
 FEIGH=1./(XCU*ONESEV)
 FNIN=1./(XCU*ONESIX)
 FTEN=1./(XCU*ONEFIV)
 FELEV=1./(XCU*ONEFOR)
 FTWEL=1./(XCU*ONECUB)
 FTHIR=1./(XSQ*ONEEIGH)
 A=-1./XSQ-6.     /(XFIV*ONE)-2.     *FONE
 B=24./(XFIV*ONE)+6.*FONE+168.     *FTWO+72.     *TWO/(XSEV*ONECUB)+
112.     *TWOSQ/(XSIX*ONEFOR)-4.     *THREE/(XSIX*ONECUB)
 C=36./(XFIV*ONE)+15.*FONE+6.*TWOSQ/(XCU*ONECUB)-4.*(THREE/(XCU
1*ONESQ)+TWO*THREE/(XSQ*ONECUB))+3.*TWOCU/(XSQ*ONEFOR)+FOUR/(XSQ*
2ONESQ)
 D=-42210. *FTWO-31770. *TWO/(XSEV*ONECUB)+7845.        *THREE/(XSIX*
1ONECUB)-17535.        *TWOSQ/(XSIX*ONEFOR)-8520.        *TWOCU/(XFIV*
2ONEFIV)+8640.*TWO*THREE/(XFIV*ONEFOR)-1488.*FOUR/(XFIV*ONECUB)
3-3600.*TWOFOR/(XFOR*ONESIX)-960.       *THREESQ*FTHREE+5790.       *
4TWOSQ*THREE/(XFOR*ONEFIV)-[illegible]       *TWO*FOUR*FTHREE+204.
5*FIVE/(XFOR*ONECUB)-1470.        *TWOFOR*TWO*FEIGH+5360.    *
6TWOCU*THREE*FNIN-1400.       *TWO*THREESQ*FTEN    -1060.       *TWOSQ
7*FOUR*FTEN+    2205.*      TWOFOR*THREE*FFIVE-1340.        *TWOSQ
8*THREESQ*FSIX-810. *TWOCU*FOUR*FSIX+222.        *TWOSQ*FIVE*FFOUR+
9680.       *TWO*THREE*FOUR*FFOUR-76.        *THREE*FIVE*FSEVEN
 D=D-44.        *TWO*PHIHI(6,X)*FSEVEN-47.        *FOUR**2*FSEVEN+
1140.       *THREESQ*THREE*FFOUR+5.         *PHIHI(7,X)/(XSQ*
2ONECUB)    +376.      *THREE*FOUR*FELEV    +232.       *TWO*FIVE*FEL
3EV    -30.       *PHIHI(5,X)*FTWEL          -735.       *TWOFIV*TWO*FTH
4IR
 D=D/1440.
 A=A*XSQ
```

```
      B=B*XSQ
      C=C*XSQ
      D=D*XSQ
      RETURN
      END



      FUNCTION F(K,X)
      DIMENSION AY(128),OY(64),GCOEF(64),GY(64)
      COMMON MEHLERA,MEHLERO,NGAUSS,AY,OY,GY,GCOEF,GEE,GSQ,YO,YONE,L
      F=((-1.)**K)*GACT(K)*(X**(L+K))/(YO**L)
      END



      FUNCTION GACT(K)
      DIMENSION AY(128),OY(64),GCOEF(64),GY(64)
      COMMON MEHLERA,MEHLERO,NGAUSS,AY,OY,GY,GCOEF,GEE,GSQ,YO,YONE,L
      GACT=1./L
      DO 1 J=1,K
    1 GACT=GACT*(J+L-1)
      END



      FUNCTION NFACT(K)
      NFACT=1
      DO 2 J=1,K
    2 NFACT=NFACT*J
      END



      FUNCTION PHIHI(M,X)
      DIMENSION AY(128),OY(64),GCOEF(64),GY(64)
      COMMON MEHLERA,MEHLERO,NGAUSS,AY,OY,GY,GCOEF,GEE,GSQ,YO,YONE,L
      PHIHI=F(M,X)+((-1.)**M)*NFACT(M+1)*(X**(M+2))
      END
      END
```

```
      PROGRAM FIRST
      DIMENSION AY(128),CY(64),GCOEF(64),GY(64)
      COMMON MEHLERA,MEHLERB,NGAUSS,AY,CY,GY,GCOEF,GEE,GSQ,YO,YONE,L
      NGAUSS=32
      MEHLERA=64
      L=12
      PRINT 3, L
    3 FORMAT (3H1L=I2//)
      FL=12.
      G=.0005
      FA=MEHLERA
      DO 7 I=1, MEHLERA
      FI=I
    7 AY(I)=COSF(((2.*FI-1.)/(2.*FA))*3.141592654)
C     32 GAUSS-LEGENDRE WEIGHTS AND POINTS - TO +
      GY(01)=-.9972638618
      GY(02)=-.9856115115
      GY(03)=-.9647622556
      GY(04)=-.9349060759
      GY(05)=-.8963211558
      GY(06)=-.8493676137
      GY(07)=-.7944837960
      GY(08)=-.7321821187
      GY(09)=-.6630442669
      GY(10)=-.5877157572
      GY(11)=-.5068999089
      GY(12)=-.4213512761
      GY(13)=-.3318686023
      GY(14)=-.2392873623
      GY(15)=-.1444719616
      GY(16)=-.0483076657
      GY(17)= .0483076657
      GY(18)= .1444719616
      GY(19)= .2392873623
      GY(20)= .3318686023
      GY(21)= .4213512761
      GY(22)= .5068999089
      GY(23)= .5877157572
      GY(24)= .6630442669
      GY(25)= .7321821187
      GY(26)= .7944837960
      GY(27)= .8493676137
      GY(28)= .8963211558
      GY(29)= .9349060759
      GY(30)= .9647622556
      GY(31)= .9856115115
      GY(32)= .9972638618
      GCOEF(01)=.007018610
```

```
      GCOEF(02)=.0162743947
      GCOEF(03)=.0253920653
      GCOEF(04)=.0342738629
      GCOEF(05)=.0428358980
      GCOEF(06)=.0509980593
      GCOEF(07)=.0586840935
      GCOEF(08)=.0658222228
      GCOEF(09)=.0723457941
      GCOEF(10)=.0781938957
      GCOEF(11)=.0833119242
      GCOEF(12)=.0876520930
      GCOEF(13)=.0911738787
      GCOEF(14)=.0938443991
      GCOEF(15)=.0956387201
      GCOEF(16)=.0965400885
      GCOEF(17)=.0965400885
      GCOEF(18)=.0956387[illegible]
      GCOEF(19)=.093844[illegible]
      GCOEF(20)=.09117387[illegible]
      GCOEF(21)=.0876520[illegible]
      GCOEF(22)=.08331[illegible]
      GCOEF(23)=.07819[illegible]
      GCOEF(24)=.0723457[illegible]
      GCOEF(25)=.06582[illegible]
      GCOEF(26)=.058684[illegible]
      GCOEF(27)=.0509980[illegible]
      GCOEF(28)=.042835[illegible]
      GCOEF(29)=.034273862[illegible]
      GCOEF(30)=.025392065[illegible]
      GCOEF(31)=.0162743947
      GCOEF(32)=.0070186610
C     Q INTEGRALS
      SUMT=0.
      SUMU=0.
      SUMV=0.
      SUMW=0.
      SUMX=0.
      SUMY=0.
      DIV=1.-GY(1)
      YO=(GY(1)+1.)/DIV
      YONE=YO*(EL**(1./L))
      ALPHA=((1.-EL*G)/(2.*[illegible]))**(1./L)
      DO 10 J=1,NGAUSS
      YO=ALPHA*(1.+GY(J))/2.
      DYO=ALPHA/2.
      CALL RINTEG(CHI,CHIP,CHIDP,PSI,PHILO,CHIL,CHIPL,CHIDPL,PSIL,PHIL
     1)
      CHIPSQ=CHIP*CHIP
```

```
      COSINE=COSF(CHI)
      SINEB= SINF(CHI)
      CHID=2.*CHI
      SINED=SINF(CHID)
      COSINEB=COSF(CHID)
      SUMT=SUMT+GCOEF(J)*YO*CHIL*SINEB*DYO/2.
      BO=-2.
      SUMU=SUMU+DYO*GCOEF(J)*((BO*YO*CHIP*CHIPL+24.*YO*PSI*CHIL+2.*CHIP*
     1CHIL)*COSINE+(24.*YO*PSIL+2.*CHIPL+YO*CHIPSQ*CHIL)*SINEB)/48.
      SUMV=0.
      SUMW=SUMW+GCOEF(J)*YO*CHIL*SINED*DYO
      SUMX=SUMX+GCOEF(J)*DYO*((12.*YO*PSIL+8.*YO*CHIPSQ*CHIL-3.*CHIL/YO)
     1*SINED+(24.*YO*PSI*CHIL-8.*YO    *CHIP*CHIPL)*COSINEB)/12.
      SUMY=0.
   10 CONTINUE
      QONECL=4.*SUMT
      QONEI=.101321184    * SUMU
      QONEII=.00256649556*SUMV
      QTWOCL=3.*SUMW
      QTWOI=.075990887     *SUMX
      QTWOII = .0019248717*SUMY
      PRINT 11,QONECL,QONEI,QONEII,QTWOCL,QTWOI,QTWOII
   11 FORMAT (1X,4HAL1=E20.10,3X,4HBL1=E20.10,3X,4HCL1=E20.10/1X,4HAL2=E
     120.10,3X,4HBL2=E20.10,3X,4HCL2=E20.10)
      END



      SUBROUTINE RINTEG(CHI,CHIP,CHIDP,PSI,PHILO,CHIL,CHIPL,CHIDPL,PSIL,
     1PHILOL)
      DIMENSION AY(128),OY(64),GCOEF(64),GY(64)
      COMMON MEHLERA,MEHLERO,GAUSS,AY,OY,GY,GCOEF,GEE,GSQ,YO,YONE,L
      R=YONE
   19 SAVE=R-((1.-PHIHI(0,R))/(-(R**(L-1))/(YO**L)-2.*(R**1)))
      IF(ABSF(ABSF(SAVE/R)-1.)-1.E-07)18,17,17
   17 R=ABSF(SAVE)
      GO TO 19
   18 YONE=SAVE
      PRINT 38, YONE
   38 FORMAT (1X,5HYONE=E20.10)
      SUMJ=0.
      SUMK=0.
      SUML=0.
      SUMM=0.
      SUMN=0.
      SUMO=0.
```

```
      SUMP=0.
      SUMR=0.
      DO 29 N=1,MEHLERA
      RB=YONE*(1.+AY(N))/2.
      DRB=YONE/2.
      SAME=DRB*SQRTF((1.-AY(N)*AY(N))/(1.-PHIHI(0,RB)))
      CALL ABCD(RB,A,B,C,D,E,F,G,H,O)
      SUMJ=SUMJ+SAME
      SUMK=SUMK+SAME*A
      SUML=SUML+SAME*B
      SUMM=SUMM+SAME*C
      SUMN=SUMN+SAME*D
      SUMO=SUMO+SAME*E
      SUMP=SUMP+SAME*F
      SUMR=SUMR+SAME*H
   29 CONTINUE
      CONST=3.141592654/FLOATF(MEHLERA)
      CHI=3.141592654-2.     *CONST*SUMJ
      CHIP=2.     *CONST*SUMK/YO
      CHIDP=-2.      *CONST*SUML/(YO*YO)
      PSI=.1666666667      *CONST*SUMM/(YO*YO)
      PHILO=2.*CONST      *SUMN/(YO**4)
      CHIL=8.*CONST*SUMO/(YO**6)
      CHIPL=8.*CONST*SUMP/(YO**7)
      CHIDPL=0.
      PSIL=.3333333333*CONST*SUMP/(YO**8)
      PHILOL=0.
      PRINT 1, CHIL,CHIPL,CHIDPL,PSIL,PHILOL
    1 FORMAT (1X,5HCHIL=E20.10,2X,6HCHIPL=E20.10,2X,7HCHIDPL=E20.10/1X,
     15HPSIL=E20.10,2X,7HPHILOL=E20.10/)
      RETURN
      END


      SUBROUTINE ABCD(X,A,B,C,D,E,F,G,H,O)
      DIMENSION AY(128),OY(64),GCOEF(64),GY(64)
      COMMON MEHLERA,MEHLERO,NGAUSS,AY,OY,GY,GCOEF,GEE,GSQ,YO,YONE,L
      ONE=PHIHI(1,X)
      TWO=PHIHI(2,X)
      THREE=PHIHI(3,X)
      FOUR =PHIHI(4,X)
      FIVE =PHIHI(5,X)
      ONESQ=ONE*ONE
      ONECUB=ONESQ*ONE
      ONEFOR=ONECUB*ONE
```

```
ONEFIV=ONEFOR*ONE
ONESIX=ONEFIV*ONE
ONESEV=ONESIX*ONE
ONEEIGH=ONESEV*ONE
TWOSQ=TWO*TWO
TWOCU=TWOSQ*TWO
TWOFOR=TWOCU*TWO
TWOFIV=TWOFOR*TWO
THREESQ=THREE*THREE
XSQ=1./(X*X)
XCU=XSQ/X
XFOR=XCU/X
XFIV=XFOR/X
XSIX=XFIV/X
XSEV=XSIX/X
XEIGH=XSEV/X
XNIN=XEIGH/X
XTEN=XNIN/X
XELEV=XTEN/X
XTWEL=XELEV/X
FONE=TWO/(XFOR*ONESQ)
FTWO=1./(XSEV*ONESQ/X)
FTHREE=1./(XFOR*ONEFOR)
FFOUR=1./(XSQ*ONEFIV)
FFIVE=1./(XSQ*ONESEV)
FSIX=1./(XSQ*ONESIX)
FSEVEN=1./(XSQ*ONEFOR)
FEIGH=1./(XCU*ONESEV)
FNIN=1./(XCU*ONESIX)
FTEN=1./(XCU*ONEFIV)
FELEV=1./(XCU*ONEFOR)
FTWEL=1./(XCU*ONECUB)
FTHIR=1./(XSQ*ONEEIGH)
FFOURT=1./(XEIGH*ONESQ)
FFIVT=1./(XNIN*ONE  )
FSIXT=1./(XTWEL*ONESQ)
FSEVT=1./(XELEV*ONECUB)
FEIGHT=1./(XTEN*ONECUB)
FNINT=1./(XTEN*ONEFOR)
FTWT=1./(XNIN*ONEFIV)
FTWTON=1./(XNIN*ONEFOR)
FTWTTW=1./(XEIGH*ONEFIV)
FTWTTH=1./(XEIGH*ONEFOR)
FTWTFO=1./(XNIN*ONECUB)
FTWTFI=1./(XEIGH*ONESIX)
FTWTSI=1./(XEIGH*ONECUB)
A=-1./XSQ-8.     /(XFIV*ONE)-2.     *FONE
B=0.
```

```
 C=36./(XFIV*ONE)+15.*FONE+8.*TWOSQ/(XCU*ONECUB)-4.*(THREE/(XCU
1*ONESQ)+TWO*THREE/(XSQ*ONECUB))+3.*TWOCU/(XSQ*ONEFOR)+FOUR/(XSQ*
2ONESQ)
 D=0.
 D=D/1440.
 E=8.*FFIVT+TWO*FFOURT
 F=8.*FFIVT+TWO*FFOURT+220.*FSIXT+60.*TWO*FSEVT-2.*THREE*FEIGHT+6.*
1TWOSQ*FNINT
 G=0.
 SAM=-5610.
 H=SAM   *FSIXT-2250.*TWO*FSEVT-585.*TWOSQ*FNINT-120.*TWOCU*FTWT+267
1.*THREE*FEIGHT+128.*TWO*THREE*FTWTON+25.*TWOSQ*THREE*FTWTTW-7.*TWO
2*FOUR*FTWTTH-4.*THREESQ*FTWTTH-24.*FOUR*FTWTFO-15.*TWOFOR*FTWTFI+
3FIVE*FTWTSI
 A=A*XSQ
 B=B*XSQ
 C=C*XSQ
 D=D*XSQ
 E=E*XSQ
 F=F*XSQ
 G=G*XSQ
 H=H*XSQ
 O=O*XSQ
 RETURN
 END
```

```
 FUNCTION F(K,X)
 DIMENSION AY(128),OY(64),GCOEF(64),GY(64)
 COMMON MEHLERA,MEHLERO,NGAUSS,AY,OY,GY,GCOEF,GEE,GSQ,YO,YONE,L
 F=((-1.)**K)*GACT(K)*(X**(L+K))/(YO**L)
 END
```

```
 FUNCTION GACT(K)
 DIMENSION AY(128),OY(64),GCOEF(64),GY(64)
 COMMON MEHLERA,MEHLERO,NGAUSS,AY,OY,GY,GCOEF,GEE,GSQ,YO,YONE,L
 GACT=1./L
 DO 1 J=1,K
1 GACT=GACT*(J+L-1)
 END
```

```
      FUNCTION NFACT(K)
      NFACT=1
      DO 2 J=1,K
    2 NFACT=NFACT*J
      END
```

```
      FUNCTION PHIHI(M,X)
      DIMENSION AY(128),OY(64),GCOEF(64),GY(64)
      COMMON MEHLERA,MEHLERO,NGAUSS,AY,OY,GY,GCOEF,GEE,GSQ,YO,YONE,L
      PHIHI=F(M,X)+((-1.)**M)*NFACT(M+1)*(X**(M+2))
      END
      END
```

```
      PROGRAM SECOND
      DIMENSION AY(128),OY(64),GCOEF(64),GY(64)
      COMMON MEHLERA,MEHLERO,NGAUSS,AY,OY,GY,GCOEF,GEE,GSQ,YO,YONE,L
      NGAUSS=32
      MEHLERA=64
      L=12
      PRINT 3, L
    3 FORMAT (3H1L=I2//)
      EL=12.
      G=.0005
      FA=MEHLERA
      DO 7 I=1, MEHLERA
      FI=I
    7 AY(I)=COSF(((2.*FI-1.)/(2.*FA))*3.141592654)
C     32 GAUSS-LEGENDRE WEIGHTS AND POINTS - TO +
      GY(01)=-.9972638618
      GY(02)=-.9856115115
      GY(03)=-.9647622556
      GY(04)=-.9349060759
      GY(05)=-.8963211558
      GY(06)=-.8493676137
      GY(07)=-.7944837960
      GY(08)=-.7321821187
      GY(09)=-.6630442669
      GY(10)=-.5877157572
      GY(11)=-.5068999089
      GY(12)=-.4213512761
      GY(13)=-.3318686023
      GY(14)=-.2392873623
      GY(15)=-.1444719616
      GY(16)=-.0483076657
      GY(17)= .0483076657
      GY(18)= .1444719616
      GY(19)= .2392873623
      GY(20)= .3318686023
      GY(21)= .4213512761
      GY(22)= .5068999089
      GY(23)= .5877157572
      GY(24)= .6630442669
      GY(25)= .7321821187
      GY(26)= .7944837960
      GY(27)= .8493676137
      GY(28)= .8963211558
      GY(29)= .9349060759
      GY(30)= .9647622556
      GY(31)= .9856115115
      GY(32)= .9972638618
      GCOEF(01)=.007018610
```

```
      GCOEF(02)=.0162743947
      GCOEF(03)=.0253920653
      GCOEF(04)=.0342738629
      GCOEF(05)=.0428358980
      GCOEF(06)=.0509980593
      GCOEF(07)=.0586840935
      GCOEF(08)=.0658222228
      GCOEF(09)=.0723457941
      GCOEF(10)=.0781938957
      GCOEF(11)=.0833119242
      GCOEF(12)=.0876520930
      GCOEF(13)=.0911738787
      GCOEF(14)=.0938443991
      GCOEF(15)=.0956387201
      GCOEF(16)=.0965400885
      GCOEF(17)=.0965400885
      GCOEF(18)=.0956387201
      GCOEF(19)=.0938443991
      GCOEF(20)=.0911738787
      GCOEF(21)=.0876520930
      GCOEF(22)=.0833119242
      GCOEF(23)=.0781938957
      GCOEF(24)=.0723457941
      GCOEF(25)=.0658222228
      GCOEF(26)=.0586840935
      GCOEF(27)=.0509980593
      GCOEF(28)=.0428358980
      GCOEF(29)=.0342738629
      GCOEF(30)=.0253920653
      GCOEF(31)=.0162743947
      GCOEF(32)=.007018610
C     Q INTEGRALS
      SUMT=0.
      SUMW=0.
      DIV=1.-GY(1)
      YO=(GY(I)+1.)/DIV
      YONE=YO*(EL**(1./L))
      ALPHA=((1.-EL*G)/(2.*G))**(1./L)
      DO 10 J=1,NGAUSS
      YO=ALPHA*(1.+GY(J))/2.
      DYO=ALPHA/2.
      CALL RINTEG(CHI,CHIL,CHIDL)
      COSINE=COSF(CHI)
      SINEB= SINF(CHI)
      CHID=2.*CHI
      SINED=SINF(CHID)
      COSINEB=COSF(CHID)
      SUMT=SUMT+GCOEF(J)*DYO*YO*(CHIDL*SINEB+    CHIL*CHIL*COSINE)/2.
```

```
      SUMW=SUMW+GCOEF(J)*DYO*YO*(CHIDL*SINED+2.*CHIL*CHIL*COSINEB)
   10 CONTINUE
      QONECL=4.*SUMT
      QTWOCL=3.*SUMW
      PRINT 11,QONECL,QTWOCL
   11 FORMAT(1X,4HAL2=E20.10,3X,4HBL2=E20.10)
      END




      SUBROUTINE RINTEG(CHI,CHIL,CHIDL)
      DIMENSION AY(128),OY(64),GCOEF(64),GY(64)
      COMMON MEHLERA,MEHLERO,NGAUSS,AY,OY,GY,GCOEF,GEE,GSQ,YO,YONE,L
      R=YONE
   19 SAVE=R-((1.-PHIHI(0,R))/(-(R**(L-1))/(YO**L)-2.*(R**1)))
      IF(ABSF(ABSF(SAVE/R)-1.)-1.E-09)18,17,17
   17 R=ABSF(SAVE)
      GO TO 19
   18 YONE=SAVE
      PRINT 38, YONE
   38 FORMAT (1X,5HYONE=E20.10)
      SUMJ=0.
      SUMO=0.
      SUMT=0.
      DO 29 N=1,MEHLERA
      RB=YONE*(1.+AY(N))/2.
      DRB=YONE/2.
      SAME=DRB*SQRTF((1.-AY(N)*AY(N))/(1.-PHIHI(0,RB)))
      CALL ABCD(RB,E,P)
      SUMJ=SUMJ+SAME
      SUMO=SUMO+SAME*E
      SUMT=SUMT+SAME*P
   29 CONTINUE
      CONST=3.141592654/FLOATF(MEHLERA)
      CHI=3.141592654-2.     *CONST*SUMJ
      CHIL=8.*CONST*SUMO/(YO**6)
      CHIDL= 8.*CONST*SUMT/(YO**12)
      PRINT 503, YO,CHIDL
  503 FORMAT(1X,3HYO=E20.10,2X,6HCHIDL=E20.10/)
      RETURN
      END
```

```
SUBROUTINE ABCD(X,E,P)
DIMENSION AY(128),OY(64),GCOEF(64),GY(64)
COMMON MEHLERA,MEHLERO,NGAUSS,AY,OY,GY,GCOEF,GEE,GSQ,YO,YONE,L
ONE=PHIHI(1,X)
TWO=PHIHI(2,X)
THREE=PHIHI(3,X)
ONESQ=ONE*ONE
ONECUB=ONESQ*ONE
ONEFOR=ONECUB*ONE
TWOSQ=TWO*TWO
XSQ=1./(X*X)
XCU=XSQ/X
XFOR=XCU/X
XFIV=XFOR/X
XSIX=XFIV/X
XSEV=XSIX/X
XEIGH=XSEV/X
XNIN=XEIGH/X
XTEN=XNIN/X
XELEV=XTEN/X
XTWEL=XELEV/X
XTHIR=XTWEL/X
XFORT=XTHIR/X
XFIVT=XFORT/X
XSIXT=XFIVT/X
FFOURT=1./(XEIGH*ONESQ)
FFIVT=1./(XNIN*ONE )
FTWTSE=1./(XSIXT*ONESQ)
FTWTEI=1./(XFIVT*ONECUB)
FTWTNI=1./(XFORT*ONECUB)
FTHTON=1./(XFORT*ONEFOR)
E=8.*FFIVT+TWO*FFOURT
P=-840.*FTWTSE-168.*TWO*FTWTEI+4.*THREE*FTWTNI-12.*TWOSQ*FTHTON
E=E*XSQ
P=P*XSQ
RETURN
END
```

```
FUNCTION F(K,X)
DIMENSION AY(128),OY(64),GCOEF(64),GY(64)
COMMON MEHLERA,MEHLERO,NGAUSS,AY,OY,GY,GCOEF,GEE,GSQ,YO,YONE,L
F=((-1.)**K)*GACT(K)*(X**(L+K))/(YO**L)
END
```

```
      FUNCTION GACT(K)
      DIMENSION AY(128),OY(64),GCOEF(64),GY(64)
      COMMON MEHLERA,MEHLERO,NGAUSS,AY,OY,GY,GCOEF,GEE,GSQ,YO,YONE,L
      GACT=1./L
      DO 1 J=1,K
    1 GACT=GACT*(J+L-1)
      END
```

```
      FUNCTION NFACT(K)
      NFACT=I
      DO 2 J=1,K
    2 NFACT=NFACT*J
      END
```

```
      FUNCTION PHIHI(M,X)
      DIMENSION AY(128),OY(64),GCOEF(64),GY(64)
      COMMON MEHLERA,MEHLERO,NGAUSS,AY,OY,GY,GCOEF,GEE,GSQ,YO,YONE,L
      PHIHI=F(M,X)+((-1.)**M)*NFACT(M+1)*(X**(M+2))
      END
      END
```

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