Programs in Mathematica relevant to Phase Integral Approximation for coupled ODEs of the Schrödinger type

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Three programs in Mathematica are presented, which produce expressions for the lowest order and the higher order corrections of the Phase Integral Approximation. First program is pertinent to one ordinary differential equation of the Schrödinger type. The remaining two refer to a set of two such equations.

I. INTRODUCTION

In this paper we present three programs in Mathematica related to the Phase Integral Approximation (PIA) [1]. They produce expressions for the lowest order approximation and the higher order corrections. The first program generates the higher order corrections $Y_{2n}(x)$ pertinent to one ordinary differential equation of the Schrödinger type. The second program gives the vectors $b_m(x)$ and the third one the corrections $Y_m(x)$ and the vectors $s_m(x)$. These quantities are pertinent to a set of two ordinary differential equations of the Schrödinger type. The programs will be referred to as $Y_{2n}$, $b_m$ and $Y_m s_m$, respectively. They should be saved in file.mat (file equal to $Y_{2n}$, $b_m$ or $Y_m s_m$) and run by using the standard Mathematica input command $<<$ file.mat. The user supplied input data should be saved in file.dat. If file.dat is an empty file, the default input data contained in each program will be used in computation.

Each program opens a dialog in Mathematica session in which the user is asked to specify the form of output from Mathematica (OutputForm, TeXForm or FortranForm), give the number of terms to be determined and answer a few questions specific to each program. The results produced by Mathematica will be saved as file.res, file.resTeX or file.resFor. All equation and section numbers given in what follows refer to [1].

One should answer $y$ to the dialog question Expand[ , Trig -> True ], $y/n$?, if the user supplied data file contains some trig functions, and $n$ otherwise.

The factor $g(x)$ after the dialog question Factor g[x] in eigenvector = ? in the program $Y_m s_m$, can be chosen either to be equal to one, or to the denominator in the just printed expression for $s_02/s_01$ (=$s_{02}(x)/s_{01}(x)$), see Eq. (124). In the last case, the implied factors should also be included, e.g., $\sin x$ coming from $\tan x$ etc.

All three programs deal with multiple sums, see Eqs. (40) and (54). These sums are programmed in the simplest possible way, e.g., the sum

$$ \sum_{\alpha+\beta+\gamma+\delta+\sigma=m, \sigma \geq 1} Y_\alpha Y_\beta Y_\gamma Y_\delta s_\sigma $$

present in Eq. (54), where $0 \leq \alpha, \beta, \gamma, \delta, \sigma \leq m - 1$, is programmed as

```mathematica
sum2 = 0;
Do[ sum2 += If[ a + b + g + d + s == m, (*then*)
    Y[a] Y[b] Y[g] Y[d] sv[s], (*else*) 0 ],
    {a, 0, m - 1}, {b, 0, m - 1}, {g, 0, m - 1}, {d, 0, m - 1}, {s, 1, m - 1} ];
```

etc. This makes the programs as close as possible to mathematical formulas thereby eliminating programming errors. For the same reasons, the integral which defines the coordinate $(e, s_m)$, see Eq. (105), was not simplified by using Eqs. (106)–(108) which would make the computation faster. However, this would make programming a bit more complicated and error-prone. In our computations, this type of optimizations was not necessary. Our aim was to produce correct results in a reasonable time (seconds or minutes rather than hours). A strong test for the correctness of programming was the vanishing of the odd order corrections, $Y_{2n-1}(x) \equiv 0$ (which required cancellation of many terms), see Sec. VIIIA. Another check was the fact that in hermitian cases, the same results were produced in the simplified hermitian and non-hermitian theory, see Secs. VIII–VIIIIC and VIEE.

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II. PROGRAM TO DETERMINE THE CORRECTIONS $Y_{2n}$ FROM THE RECURRENCE RELATION (40)

File Y2n.mat:

(*-----------------------------------------------------------------------------------------------*

Calculation of the phase integral corrections $Y_{2n}$ from recurrence relations, Eq. (40) in [1], for a scalar case, i.e. for one ODE of the Schroedinger type:

$$u''(x) + R(x) u(x) = 0.$$ 

[1] A. A. Skorupski, "Phase Integral Approximation for coupled ODEs of the Schroedinger type", arXiv: 0710.5868, Sec. II.

********************************************************************************
***************** Define type of output from Mathematica ********************
*)
outpform = InputString["Output, TeX or Fortran form of results, o/t/f? "];
sc = If[ outpform == "o", OpenWrite["Y2n.res", FormatType -> OutputForm],
If[ outpform == "t", OpenWrite["Y2n.resTeX", FormatType -> TeXForm],
OpenWrite["Y2n.resFor", FormatType -> FortranForm ] ] ];
(**)
outpYm = InputString["Simple fractions or Common denominator or in Y_{2n}, s/c?"];
(**)
WriteString[sc, "\n Formulas for corrections $Y_{2n}$ as functions of x or z
(= zeta variable). \n"];
(*
****************** Define maximum value of n in $Y_{2n}$ ********************
*)
nmax = Input["nmax = ? "];
WriteString[sc, "\n nmax = "]; Write[ sc, nmax ];
(*
***************** Define type of input to Mathematica ********************
*)
inptform = InputString["Input of $R(x)$ and $a(x)$ or General $Y_{2n}$, i/g? "];
(**)
t0 = TimeUsed[];
(**)
If [ inptform == "i", 
(*then*)
(*
*********************** Define default input data ****************************
*)
(** Parabolic Model  ***)
af = 0;
R = coef (x^2 - x1^2);
(*
*************** Read new input data from file Y2n.dat ****************************
*)
<< Y2n.dat;
WriteString[sc, "\n Y2n[x] for \n"];
(*
*************** Write input data ****************************
*)
WriteString[sc, "\n R[x] = \n"]; Write[sc, R];
WriteString[sc, "\n Auxiliary function a[x] = \n"]; Write[sc, af];
\[ Q_{sq} = R - af; \quad dQ_{sq} = D[Q_{sq}, x]; \]

\[ Q_{sq01} = Q_{sq}; \]

\[ \epsilon_0 = \frac{(5/16) (dQ_{sq}/Q_{sq})^2 - (1/4) D[dQ_{sq}, x]/Q_{sq} + af}{Q_{sq}}; \]

\[ \text{aux} = \text{Simplify}[\epsilon_0]; \]

\[ \text{aux1} = \text{Together}[\text{aux}]; \]

WriteString[sc, "\n \epsilon_0[x] = \\
"]; Write[sc, aux1], (*else*)

(********** Prepare quantities for general calculations  **********)

\[ \epsilon_0 = \epsilon_0[x]; \quad Q_{sq} = Q_{sq}[x]; \]

\[ x_{or z} = \text{InputString}["x or zeta variable, x/z? ";] \]

If[ xorz == "x", (*then*) WriteString[sc, "\n Y2n[x] as functions of \epsilon_0[x], Q_{sq}[x] = Q^2[x] and derivatives \n"],

\[ Q_{sq01} = Q_{sq}; (*else*) \]

\[ Q_{sq01} = 1; x = z; \text{WriteString}[sc, "\n Y2n[z] as functions of \epsilon_0[z] and derivatives \n"]; ]

(***)

\[ Qm2 = 1/Q_{sq01}; \]

\[ Y[0] = 1; (* \]

(************ Start iterations for \[ Y[2 \, n] \] ************)

\[ \]

For[\[n = 1, n \leq n_{max}, n++\],

\[ \text{sum1} = 0; \text{sum2} = 0; \text{sum3} = 0; \]

\[ m = 2 \, n; \]

Do[ sum1 += If[ a + b == m, (*then*) Y[a] Y[b], (*else*) 0 ],

\{a, 0, m - 2, 2\}, \{b, 0, m - 2, 2\} ];

Do[ sum2 += If[ a + b + g + d == m, (*then*)

\[ Y[a] Y[b] Y[g] Y[d], (*else*) 0 \],

\{a, 0, m - 2, 2\}, \{b, 0, m - 2, 2\}, \{g, 0, m - 2, 2\}, \{d, 0, m - 2, 2\} ];

Do[ sum3 += If[ a + b == m - 2, (*then*)

\[ \epsilon_0 \, Y[a] Y[b] + (3/4) \, Qm2 \, D[Y[a], x] \, D[Y[b], x] -

(1/2) \, Y[a] \, Qm2 \, D[Y[b], x], \{d, 0, m - 2, 2\} ]

(*else*) 0 ],

\{a, 0, m - 2, 2\}, \{b, 0, m - 2, 2\} ];

(***)

\[ Y[m] = (1/2) \, (\text{sum1 - sum2 + sum3}); \]

(***)

\]

\[ t = \text{TimeUsed[]}; \]

WriteString[sc, "\n CPU time used for computation (seconds) = "]; Write[sc, t - t0]; (*

(********** Simplify and write results  **********)

\]

For[\[n = 1, n \leq n_{max}, n++\],

\[ m = 2 \, n; \]

WriteString[sc, "\n n = "]; Write[sc, n];

\[ \text{aux} = \text{Simplify}[Y[m]]; \]

\[ \text{aux1} = \text{If}[\text{outpYm} == "c", \text{Together}[\text{aux}], \text{Apart}[\text{aux}, x]]; \]

WriteString[sc, "\n Y2n = "]; Write[sc, aux1 ]

\]

\[ t = \text{TimeUsed[]}; \]

WriteString[sc, "\n CPU time used for computation & simplification (seconds) = "]; Write[sc, t - t0];
The file that follows is an example of the data file for the program Y2n. As it stands it is an empty file containing only comments. By uncommenting the definition of the functions \( a(x) \) and \( R(x) \): \((\ast \rightarrow (**))\) and \((\ast) \rightarrow (**))\), one activates the input data.

File Y2n.dat:

\[
\begin{align*}
&\text{(* Data pertinent to } R[x] \text{ in the differential equation } u''[x] + R[x] \ u[x] = 0. \\
&\text{By default the auxiliary function } af[x] = 0. \text{ For other choice} \\
&\text{include the data command: } af = \text{your}\_\text{function}[x]; \\
&\ast)
\end{align*}
\]

\[
\begin{align*}
&\text{******************** Budden's Model: ********************} \\
&\ast) \\
&af = 0; \\
&R = \text{coef } x/(x - p); \\
&\ast)
\end{align*}
\]

End of file Y2n.dat.

III. PROGRAM TO DETERMINE \( b_m \) FROM THE RECURRENCE RELATION (54)

File bvm.mat:

\[
\begin{align*}
&\text{*******************************************************************************} \\
&\text{Calculation of } bv[m] \text{ from the recurrence relation, Eq. (54) in [1]} \\
&\text{*******************************************************************************}
\end{align*}
\]

[1] A. A. Skorupski, "Phase Integral Approximation for coupled ODEs of the Schroedinger type", arXiv: 0710.5868, Sec. III.

\[
\begin{align*}
&\text{*******************************************************************************} \\
&\ast) \\
bvm = \text{OpenWrite}["bvm.res", \text{FormatType} \rightarrow \text{OutputForm}]; \\
&\text{(***)} \\
&\text{WriteString[bvm, "\n Formulas for vectors } bv[m] \text{ as functions of } x \text{ or } z \\
&\text{ (= zeta variable). } \n"]; \\
t0 = \text{TimeUsed[]} \\
&\text{Unprotect[Sqrt, Power];} \\
&Sqrt[x_\^2] := x; \\
i^n_ := (-1)^((n-1)/2) /; OddQ[n]; \\
i^n_ := i (-1)^((n-1)/2) /; EvenQ[n]; \\
&\text{re}[x_] := \text{Coefficient}[x, i, 0]; \\
&\text{im}[x_] := \text{Coefficient}[x, i, 1]; \\
&\text{cc}[x_] := \text{re}[x] - i \ \text{im}[x]; \\
&\text{Protect [Sqrt, Power];} \\
&\ast) \\
&\text{******************** Define maximum value of } m \text{ in } bv[m] ******************** \\
&\ast)
\end{align*}
\]

\[
\begin{align*}
&\text{mmax = Input["\n mmax = ? "];} \\
&\text{(***)} \\
&\text{xorz = InputString["\n x or zeta variable, } x/z \text{ ? "];} \\
&\text{If[ xorz == "z", (*then*) Q[x_] := 1; } x = z; \\
&Qm1 = Q[x]^(-1); Qm2 = Qm1^2; dQ = D[ Q[x], x ];} \\
&\text{(***)} \\
&Y[x, 0] = 1; \\
bv[1] = i Qm1 D[sv[x, 0], x]; \\
Y1eq0Q = \text{InputString["\n } Y[x, 1] = 0, \ y/n? "];
\end{align*}
\]
If[ Y1eq0Q == "y", (*then*) Y[x, 1] = 0 ];
(*
************************************************************************ Start iterations for bv[m] ************************************************************************
*)
For[ m = 2, m <= mmax + 1, m++,
(**)
  sum1 = 0; sum2 = 0; sum3 = 0; sum4 = 0; sum5 = 0; sum6 = 0;
Do[ sum1 += If[ a + b + s == m, (*then*)
    Y[x, a] Y[x, b] ( sv[x, s] + 2 (Y[x, s] sv[x, 0] - bv[s]) ), (*else*)
    0 ], {a, 0, m - 1}, {b, 0, m - 1}, {s, 1, m - 1} ];
Do[ sum2 += If[ a + b + g + d + s == m, (*then*)
    Y[x, a] Y[x, b] Y[x, g] Y[x, d] sv[x, s], (*else*) 0 ],
    {a, 0, m - 1}, {b, 0, m - 1}, {g, 0, m - 1}, {d, 0, m - 1}, {s, 1, m - 1} ];
Do[ sum3 += If[ a + b == m, (*then*) Y[x, a] Y[x, b], (*else*) 0 ],
    {a, 1, m - 1}, {b, 1, m - 1} ];
Do[ sum4 += If[ a + b + g + d == m, (*then*)
    Y[x, a] Y[x, b] Y[x, g] Y[x, d], (*else*) 0 ],
    {a, 0, m - 1}, {b, 0, m - 1}, {g, 0, m - 1}, {d, 0, m - 1} ];
Do[ sum5 += If[ a + b + g + s == m - 1, (*then*)
    Y[x, a] Y[x, b] Y[x, g] Qm1 D[sv[x, s], x], (*else*) 0 ],
    {a, 0, m - 1}, {b, 0, m - 1}, {g, 0, m - 1}, {s, 0, m - 1} ];
Do[ sum6 += If[ a + b + s == m - 2, (*then*)
    Y[x, a] ( Y[x, b] ( Qm2 ( D[sv[x, s], {x, 2}] - Qm1 dQ D[sv[x, s], x ] ) +
      eps[x] sv[x, s]) - Qm2 dQ D[sv[x, s], x] D[sv[x, s], x] -
    (1/2) Qm2 ( D[Y[x, b], {x, 2}] - Qm1 dQ D[Y[x, b], x] ) sv[x, s] ) +
    (3/4) Qm2 D[ Y[x, a], x] D[Y[x, b], x] sv[x, s], (*else*) 0 ],
    {a, 0, m - 2}, {b, 0, m - 2}, {s, 0, m - 2} ];
(**) bv[m] = (1/2) (sum1 - sum2 + ( sum3 - sum4 ) sv[x, 0] + i 2 sum5 + sum6);
(**)
  ];
  t = TimeUsed[];
  WriteString[bvm, "\n CPU time used (seconds) = "]; Write[bvm, t - t0];
(**)
(*
************************************************************************ Simplify and write results ************************************************************************
*)
For[ m = 1, m <= mmax, m++,
  WriteString[bvm, "\n m = "]; Write[bvm, m];
  aux = Simplify[ bv[m] ];
  aux1 = Together[aux];
  WriteString[bvm, "\n bv[m] = \n"]; Write[ bvm, aux1 ];
(**)
  ];
End of file bvm.mat.

IV. PROGRAM TO DETERMINE $Y_m$ AND $s_m$ FROM RECURRENCE RELATIONS FOR 2 ODES WITH EITHER HERMITIAN OR NON-HERMITIAN MATRIX, SEE [1], SEC. VI

File Ymsvm.mat:

************************************************************************** Calculation of $Y[m]$ and $sv[m]$ from recurrence relations for 2 ODEs with either hermitian or non-hermitian matrix [1].**************************************************************************

[1] A. A. Skorupski, "Phase Integral Approximation for coupled ODEs of the
Schroedinger type", arXiv: 0710.5868, Sec. VI.

******************************************************************************
outpform = InputString["Output, TeX or Fortran form of results, o/t/f? "];
vc = If[ outpform == "o", (*then*) OpenWrite["Ymsvm.res", 
FormatType -> OutputForm], 
(*else*) If[ outpform == "t", (*then*) OpenWrite["Ymsvm.resTeX", 
FormatType -> TeXForm], (*else*) OpenWrite["Ymsvm.resFor", 
FormatType -> FortranForm] ] ];
t0 = TimeUsed[];
Unprotect[Sqrt, Power];
Sqrt[x_^2] := x;
i^n_ := (-1)^((n/2) /; EvenQ[n]);
i^n_ := i (-1)^((n-1)/2) /; OddQ[n];
re[x_] := Coefficient[x, i, 0];
im[x_] := Coefficient[x, i, 1];
ce[x_] := re[x] - i im[x];
Protect [Sqrt, Power];

(*
************************** Define maximum value of m in Y[m] and sv[m] ****************************
*)
mmax = Input["mmax = ? "];
WriteString[vc, "\mmax = "]; Write[vc, mmax];
mmxp1 = mmax + 1;

******************************************************************************
Define default input data ******************************************************************************

One must define the auxiliary function a(x, p) -> af and the matrix elements 
Rjk(x, p) -> Rjk, where p represents parameter(s). By default, the variable 
automatic = True. In that case, one must define a list of meaningful numerical 
replacements: parrepls = { x -> x0, p -> p0 } which is necessary to calculate 
automatically the variables: Delta given by Eq. (121), sqrtDel (= Sqrt[Delta]) 
and signQsq (= sign of Qsq given by Eq. (121)). If one puts automatic = False 
in the data file Ymsvm.dat, the definitions of Delta, sqrtDel and signQsq must 
be given in the file Ymsvm.dat.

(*** Example A ***)
af = 0;
R11 = x Cos[x]^2 + Sin[x]^2;
R12 = (x - 1) Cos[x] Sin[x];
R21 = (x - 1) Cos[x] Sin[x];
R22 = x Sin[x]^2 + Cos[x]^2;
parrepls = { x -> 2 };
automatic = True;

******************************************************************************
Read new input data from file Ymsvm.dat ******************************************************************************

<< Ymsvm.dat;

******************************************************************************
Write input data ******************************************************************************

WriteString[vc, "\n R11 = \n"]]; Write[vc, R11];
WriteString[vc, "\n R12 = \n"]]; Write[vc, R12];
WriteString[vc, "\n R21 = \n"]]; Write[vc, R21];
WriteString[vc, "\n R22 = \n"]]; Write[vc, R22];
WriteString[vc, "\n af = \n"]]; Write[vc, af];
If[ automatic, (*then*)}
WriteString[vc, "\n paramter replacement list = \n"]; Write[vc, parrepls], (*else*)
WriteString[vc, "\n *** Non-automatic calculation *** \n"]
];
(**)
G11 = R11 - af; G12 = R12; G21 = R21; G22 = R22 - af;
(**)
exptrig = InputString["Expand[ , Trig -> True ], y/n? "];
QsqmQ = InputString["Qsqr with minus or plus Sqrt[ Delta ], m/p? "];
WriteString[vc, "\n Qsqr with "];
If[ QsqmQ == "m", WriteString[vc, "minus "], WriteString[vc, "plus "] ];
WriteString[vc, "Sqrt[ Delta ] "];
(**)
(* ************ Find eigenvalues and eigenvectors of the G matrix ************** *)
If[ automatic, (*then*) Delta = (G11 - G22)^2 + 4 G12 G21 ];
If[ exptrig == "y", Delta = Expand[ Delta, Trig -> True ] ];
Delta = Factor[ Delta ];
WriteString[vc, "\n Delta = \n"]; Write[vc, Delta];
If[ automatic, (*then*) sqrtDel = Sqrt[ Delta ] ];
(**)
Qsq = (1/2) (G11 + G22 + If[ QsqmQ == "m", (*then*) -sqrtDel, (*else*) sqrtDel ]);
Qsq = Simplify[ Qsq ];
If[ exptrig == "y", Qsq = Expand[ Qsq, Trig -> True ] ];
(**)
If[ automatic, (*then*) signQsq = If[ ( Qsq /. parrepls ) < 0, (*then*) -1, (*else*) 1,
(*and if neither True or False then*) 1 ] ];
WriteString[vc, "\n signQsq = "]; Write[vc, signQsq];
WriteString[vc, "\n Qsq = \n"]; Write[vc, Qsq];
(**)
eps0 = Simplify[ (Qsq^(1/4) D[Qsq^(-1/4), {x, 2}] + af)/Qsq ];
eps0 = Together[ Simplify[ ( (5/16) ( D[Qsq, x]/Qsq)^2 -
(1/4) D[Qsq, {x, 2}]/Qsq + af )/Qsq ] ];
WriteString[vc, "\n eps0 = \n"]; Write[vc, eps0];
(* << eps0.mat; *)
(**)
Q = If[ signQsq < 0, (*then*) - i (- Qsq)^(-1/2), (*else*) Qsq^(-1/2) ];
WriteString[vc, "\n Q = \n"]; Write[vc, Q];
(**)
Qm1 = Q^(-1); Qm2 = Qm1^2; dQ = D[ Q, x ];
(**)
s02os01 = ( Qsq - G11 )/G12;
If[ exptrig == "y", s02os01 = Expand[ s02os01, Trig -> True ] ];
s02os01 = Simplify[ s02os01 ];
WriteString[vc, "\n s02/s01 = \n"]; Write[vc, s02os01];
Print[ "s02/s01 = ", s02os01 ];
(**)
fact = Input["Factor g[x] in eigenvector = ? "];
WriteString[vc, "\n Factor g[x] = \n"]; Write[vc, fact];
s0v1 = fact; s0v2 = fact s02os01;
(**)
asqr = s0v1 cc[s0v1] + s0v2 cc[s0v2];
If[ exptrig == "y", asqr = Expand[ asqr, Trig -> True ] ];
(**)
normeigv = InputString["Normalized eigenvector, y/n? "];

If[ normeigv == "y", (*then*)
ms0v = Sqrt[ Simplify[ asqr ] ];
s0v1 = s0v1/ms0v; s0v2 = s0v2/ms0v;
asqr = 1;
Print[ "\n(s0v(x), s0v'(x)) = " ];
intg = cc[s0v1] D[ s0v1, x ] + cc[s0v2] D[ s0v2, x ];
If[ exprtrig == "y", intg = Expand[ intg, Trig -> True ] ];
intg = Simplify[intg];
(** Print["intg = ", intg]; **) 
If[ intg =!= 0, (*then*) (* Print[ "No, (s0v, s0v'(x)) = " ]; *) Print[ intg ]
theta = InputString[
"Integrate (s0v(x), s0v'(x)) dx to calculate theta, y/n? ";
If[ theta == "y", (*then*)
theta = i Integrate[ intg, x ];
Print["\ntheta = "];
Write[vc, theta];
phasf = Cos[theta] + i Sin[theta];
s0v1 = s0v1 phasf; s0v2 = s0v2 phasf
], (*else*) Print[0]
];
s0v1 = Simplify[ s0v1 ]; s0v2 = Simplify[ s0v2 ];
s0v = { s0v1, s0v2 }
spv = { - cc[s0v2], cc[s0v1] }
(**)
WriteString[vc, "\n s0v = "; Write[vc, s0v]
WriteString[vc, "\n spv = "]; Write[vc, spv]
WriteString[vc, "\n *** sv_m = cp_m spv + c_m s0v, m = 1, 2, ..., mmax *** \n"]
(**) s0v1ms = s0v1 cc[s0v1]; s0v2ms = s0v2 cc[s0v2];
den = s0v1ms (G22 - Qsq) + s0v2ms (G11 - Qsq) -
cc[s0v1] s0v2 G12 - s0v1 cc[s0v2] G21;
If[ exprtrig == "y", den = Expand[ den, Trig -> True ] ];
den = Apart[ Simplify[ den ] ];
WriteString[vc, "\n D = "]; Write[vc, den]
(**) coef = - 2 Qsq/den;
(**) Y[0] = 1; sv[0] = s0v
(**) bv[1] = i Qm1 D[sv[0], x];
hrmthQ = InputString["Hermitian or Non-hermitian theory, h/n? "]; WriteString[vc,
If[ hrmthQ == "h", " *** Hermitian ", " *** Non-hermitian " ];
WriteString[vc, "theory *** \n"];
simthQ = If[ hrmthQ == "h", (*then*) InputString[ 
"Simplified, Fulling or Wronskian conserving theory, s/f/w? "],
(*else*) "s" ];
wresQ = InputString["Write results, y/n? "];
sresQ = InputString["Simplify results, y/n? "];
If[ wresQ == "y", (*then*)
outpYm = InputString[ 
"Simple fractions, Common denominator or NO output spec. in Ym, s/c/n? "];
outpsv = InputString[ 
"Simple fractions, Common denominator or NO output spec. in svm, s/c/n? "] ];
aprog = InputString["Append program, y/n? "]; (*
*************** Start iterations for Y[m] and sv[m] ***************

For[ m = 2, m <= mmxp1, m++,
  m1 = m - 1;
(**)
  cpf[m1] = coef { -s0v2, s0v1 } . bv[m1];
  If[ exprtrig == "y", cpf[m1] = Expand[ cpf[m1], Trig -> True ] ];
  Print[ " m = ", m1 ];
  intgnt[m1] = If[ simthQ == "s", 0, If[ OddQ[m1] && simthQ == "w",
    2 re[ cpf[m1] { cc[D[s0v1, x]], cc[D[s0v2, x]] } . spv ],
    2 im[ cpf[m1] { cc[D[s0v1, x]], cc[D[s0v2, x]] } . spv ] ];
  If[ exprtrig == "y", intgnt[m1] = Expand[ intgnt[m1], Trig -> True ] ];
(**)
  If[ m1 > 1, (*then*)
    For[ alpha = 1, alpha <= m1-1, alpha++,
      intgnt[m1] -= If[ simthQ == "s", 0, If[ OddQ[alpha] && simthQ == "w",
                      -1, 1 ] {cc[sv[alpha][1]], cc[sv[alpha][2]], D[sv[m1 - alpha],
                      x ] ] ];
    ];
  If[ exprtrig == "y", intgnt[m1] = Expand[ intgnt[m1], Trig -> True ] ];
  intgnt[m1] = Simplify[ intgnt[m1] ];
(* WriteString[vc, "\n m = "] Write[vc, m1];
 WriteString[vc, "\n integrant[m] = "] Write[vc, intgnt[m1]]; *)
(**)
  cf[m1] = If[ simthQ == "s", 0, Integrate[ intgnt[m1], x ] ];
  sv[m1] = cpf[m1] spv + cf[m1] s0v;
  If[ exprtrig == "y", sv[m1] = Expand[ sv[m1], Trig -> True ] ];
  (***) sv[m1] = Simplify[ sv[m1] ]; (***)
(***)
  Y[m1] = If[ hrmthQ == "h",
    (*then*) ( { cc[s0v1], cc[s0v2] } . bv[m1])asqr,
    (*else*) ( Qm2 cpf[m1] G12 asqr/(2 s0v1) +
    bv[m1][[1]])/s0v1 ];
  If[ exprtrig == "y", Y[m1] = Expand[ Y[m1], Trig -> True ] ];
(* WriteString[vc, "\n Y[m] = "] Write[vc, Y[m1]]; *)
  (***) Y[m1] = Simplify[ Y[m1] ]; (***)
(***)
  If[ m < mmxp1, (*then*)
    sum1 = 0; sum2 = 0; sum3 = 0; sum4 = 0; sum5 = 0; sum6 = 0;
    Do[ sum1 += If[ a + b + s == m, ( *then*)
      Y[a] Y[b] ( sv[s] + 2 ( Y[s] sv[0] - bv[s] ) ) ],
      (*else*)
      0 ], {a, 0, m - 1}, {b, 0, m - 1}, {s, 1, m - 1} ];
    Do[ sum2 += If[ a + b + g + d + s == m, ( *then*)
      Y[a] Y[b] Y[g] Y[d] sv[s],
      (*else*) 0 ],
      {a, 0, m - 1}, {b, 0, m - 1}, {g, 0, m - 1}, {d, 0, m - 1}, {s, 1, m - 1} ];
    Do[ sum3 += If[ a + b == m, ( *then*) Y[a] Y[b],
      (*else*) 0 ],
      {a, 1, m - 1}, {b, 1, m - 1} ];
    Do[ sum4 += If[ a + b + g + d == m, ( *then*)
      Y[a] Y[b] Y[g] Y[d],
      (*else*) 0 ],
      {a, 0, m - 1}, {b, 0, m - 1}, {g, 0, m - 1}, {d, 0, m - 1} ];
    Do[ sum5 += If[ a + b + g + s == m - 1, ( *then*)
      Y[a] Y[b] Y[g] Qm1 D[sv[s], x],
      (*else*) 0 ],
      {a, 0, m - 1}, {b, 0, m - 1}, {g, 0, m - 1}, {s, 0, m - 1} ];
    Do[ sum6 += If[ a + b + s == m - 2, ( *then*)
      Y[a] ( Y[b] ( Qm2 ( D[sv[s], x], 2) - Qm1 dQ D[sv[s], x] ) +
eps0 sv[s] ) - Qm2 D[Y[b], x] D[sv[s], x] -
(1/2) Qm2 ( D[Y[b], {x, 2}] - Qm1 dQ D[Y[b], x ] ) sv[s] ) +
(3/4) Qm2 D[Y[a], x] D[Y[b], x] sv[s], (*else*) 0 ];
{a, 0, m - 2}, {b, 0, m - 2}, {s, 0, m - 2} ];

(**)

bv[m] = (1/2) (sum1 - sum2 + ( sum3 - sum4 ) sv[0] + i 2 sum5 + sum6));

(**)

t = TimeUsed[];

(*)

If[ wresQ == "y", (*then*)
(*
*************** Simplify and/or write results  ***********************
*)

For[m = 1, m <= mmax, m++,

WriteString[vc, "\n m = "]]; Write[vc, m];
aux1 = If[ sresQ == "y", (*then*) Simplify[ Y[m] ], (*else*) Y[m] ];
aux = If[ outpYm == "c", Together[aux1], If[ outpYm == "s", Apart[aux1],

WriteString[vc, "\n Y_m = 
"]]; Write[ vc, aux1 ];

(**)
aux = cpf[m];
aux1 = If[ exprtrig == "y", Expand[aux, Trig -> True], aux ];
aux2 = If[ sresQ == "y", (*then*) Simplify[aux1], (*else*) aux1 ];
aux3 = If[ outpsv == "c", Together[aux2], If[ outpsv == "s", Apart[aux2],

WriteString[vc, "\n cp_m = 
"]]; Write[ vc, aux3 ];

(**)
aux = cf[m];
aux1 = If[ exprtrig == "y", Expand[aux, Trig -> True], aux ];
aux2 = If[ sresQ == "y", (*then*) Simplify[aux1], (*else*) aux1 ];
aux3 = If[ outpsv == "c", Together[aux2], If[ outpsv == "s", Apart[aux2],

WriteString[vc, "\n c_m = 
"]]; Write[ vc, aux3 ]
]
];

(**)

If[ aprog == "y", (*then*) << ap.mat ];
t = TimeUsed[];
WriteString[vc, "\n CPU time used for computation \& simplification (seconds) = " ];
Write[vc, t - t0];

End of file Ymsvm.mat.

The file that follows is an example of the data file for the program Ymsvm. Again it is an empty file containing only comments. By uncommenting appropriate pieces, one can activate input data pertaining to examples given in [1], Sec. VIII.

File Ymsvm.dat:

(**** Data for program Ymsvm ****)

(**** Example B ****)

(*)

af = 0;
R11 = - (x Cos[x]^2 + Sin[x]^2);
R12 = (x - 1) Cos[x] Sin[x];
R21 = (x - 1) Cos[x] Sin[x];
R22 = - (x Sin[x]^2 + Cos[x]^2);
parrepls = {x -> 2};
*)

(* Example C.1 ***)
(*
af = 0;
R11 = x Cos[x]^2 + Sin[x]^2;
R12 = i (x - 1) Cos[x] Sin[x];
R21 = - i (x - 1) Cos[x] Sin[x];
R22 = x Sin[x]^2 + Cos[x]^2;
parrepls = {x -> 2};
*)

(* Example C.2 ***)
(*
af = 0;
R11 = - (x Cos[x]^2 + Sin[x]^2);
R12 = i (x - 1) Cos[x] Sin[x];
R21 = - i (x - 1) Cos[x] Sin[x];
R22 = - (x Sin[x]^2 + Cos[x]^2);
parrepls = {x -> 2};
*)

(* Example C.3 ***)
(*
af = 0;
R11 = - (x Cos[x]^2 + Sin[x]^2);
R12 = (1 + i)/2^(1/2) (x - 1) Cos[x] Sin[x];
R21 = (1 - i)/2^(1/2) (x - 1) Cos[x] Sin[x];
R22 = - (x Sin[x]^2 + Cos[x]^2);
parrepls = {x -> 2};
*)

(* Example C.4 ***)
(*
af = 0;
R11 = - (x Cos[x]^2 + Sin[x]^2);
R12 = (Cos[fi] + i Sin[fi]) (x - 1) Cos[x] Sin[x];
R21 = (Cos[fi] - i Sin[fi]) (x - 1) Cos[x] Sin[x];
R22 = - (x Sin[x]^2 + Cos[x]^2);
(*fi = x;*)
parrepls = {x -> 2};
*)

(* Example D ***)
(*
af = 0;
R11 = x Cos[x]^2 + Sin[x]^2;
R12 = 2 i (x - 1) Cos[x] Sin[x];
R21 = - (1/2) i (x - 1) Cos[x] Sin[x];
R22 = x Sin[x]^2 + Cos[x]^2;
parrepls = {x -> 2};
*)

(* Example E ***)
(*
af = 0;
R11 = h0[x] - h1[x];
R12 = h2[x];
R21 = h2[x];
R22 = h0[x] + h1[x];
automatic = False;
r[x_] := Sqrt[ h1[x]^2 + h2[x]^2 ];
Delta = 4 r[x]^2;
sqrtDel = 2 r[x];
signQsq = - 1;
)

(*** Example X ***)
(*
af = 0;
R11 = E1 - x^2;
R12 = x;
R21 = x;
R22 = E2 - 4 x^2;
parrepls = { x -> 3, E1 -> 1, E2 -> 2 };
*)

End of file Ymsvm.dat.

The file that follows contains an example of a program that can be appended to Ymsvm by answering y to the dialog question Append program, y/n?. This program is pertinent to Example E in the data file Ymsvm.dat. It computes and prints both the formulas in Eq. (174) and all numerical results given in Table I in [1]. For each of two eigenvalues (for the minus or plus sign in Eq. (123)), the program Ymsvm should be run twice for two possible answers to the dialog question Normalized eigenvector, y/n?. In both cases one should take mmax = 2 and answer n to the dialog questions Write results, y/n? and Simplify results, y/n?. Otherwise, the program would spend very long time in an attempt to simplify Y(x) and cT(x) which in any case are too complicated to be presented.

File ap.mat:

(***** Appended computation for program Ymsvm, Example E *****)

(*
aux = Together[ Y[1] ];
WriteString[ vc, "\n Y_1 = \n""]; Write[ vc, aux ];
(*
aux = Together[ cpf[1] ];
WriteString[ vc, "\n cp_1 = \n""]; Write[ vc, aux ];
(*
d0[x_] := 1/(4 x^2) + 4/x^4 + 38/x^6 + 748/x^8;
d1[x_] := 1/x^2 + 2/x^4 + 19/x^6 + 374/x^8;
h0[x_] := -1 - k^2 + d0[x]; h1[x_] := 2 (om + 1/x^2); h2[x_] := -1 + d1[x];
(*
parrepls = { x -> 55, k -> 4/100, om -> 26041/10^7 };
WriteString[ vc, "\n""]; Write[ vc, parrepls ];
WriteString[ vc, "\n Q = " ]; Write[ vc, N[ Q /. parrepls ] ];
WriteString[ vc, "\n eps0/2 = " ]; Write[ vc, N[ eps0/2 /. parrepls ] ];
WriteString[ vc, "\n Y_1 = " ]; Write[ vc, N[ Y[1] /. parrepls ] ];
WriteString[ vc, "\n Y_2 = " ]; Write[ vc, N[ Y[2] /. parrepls ] ];
WriteString[ vc, "\n cp_1 = " ]; Write[ vc, N[ cpf[1] /. parrepls ] ];
WriteString[ vc, "\n cp_2 = " ]; Write[ vc, N[ cpf[2] /. parrepls ] ];

End of file ap.mat.

[1] A. A. Skorupski, Phase Integral Approximation for coupled ODEs of the Schrödinger type, arXiv:0710.5868 [math-ph].