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(*-----------------------Filename: powder_MAS.nb-------------------------*)
(*      The main function powderMAS[] provides the line intensity
    of the central transition (if quanta = 1) or that of the -3-quantum
    transition (if quanta = 3) of a spin I = 3/2 system rotating at the
    magic angle, submitted to the first-order quadrupole interaction
    (if order = 1) or the first- and second-order quadrupole interactions
    (if order = 2), and excited by an x-pulse.
        This line intensity depends on
    (1) the rotor spinning speed VrotkHz (in kHz unit),
    (2) the quadrupole coupling constant QCCMHz (in MHz unit),
    (3) the asymmetry parameter η,
    (4) the three Euler angles αd, βd, and γd (in degree unit) orienting
        the rotor in the principal-axis system of the EFG tensor Σ^PAS,
    (5) the Larmor frequency ω0Mhz (in MHz unit),
    (6) the strength of the radiofrequency field ωRFkHz (in kHz unit),
    (7) the pulse duration increasing from 0 to tf (in μs unit)
        by step of tau (in μs unit),
    (8) the number maxα of summation steps of the Euler angle α
        in the 0 2π rang,
    (9) the number maxβ of summation steps of the Euler angle β
        in the 0 π rang,
    (10) the number maxγ of summation steps of the Euler angle γ
         in the 0 2π rang.

        The main function provides the parameters a_i, b_i, a2_i, b2_i,
     a4_i, and b4_i for an orientation of the rotor to the sub-function f[].

        The sub-function f[] provides the density matrix ρ(t) via
     the value of ωQ (if order = 1), and of ωQ21 and ωQ22 (if order = 2)
     by taking into account the rotor spinning speed. The spin system is
     supposed to be time-independent during each duration Δt or tau.
     It returns Table s[m] to the main function powderMAS[].           *)
(*------------------------------------------------------------------------*)
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(*------------------------------------------------------------------------*)

(* Sub-function f[] *)

f[order_, QCC_, ωRF_, Δt_, n_] := (

  For [m = 1, m ≤ n, m++,
   ωQ = QCC/(2 Sqrt[6]) (
        d1c Cos[(m - 1) Δt * ωrot]     +    d2c Cos[(m - 1) * 2 Δt * ωrot]
      + d1s Sin[(m - 1) Δt * ωrot]     +    d2s Sin[(m - 1) * 2 Δt * ωrot] );
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ωQ21 = 0;   ωQ22 = 0 ;
If [order == 2, {
  W20 =  d21c Cos[(m - 1) Δt * ωrot]     +   d22c Cos[(m - 1) * 2 Δt * ωrot]
       + d21s Sin[(m - 1) Δt * ωrot]     +   d22s Sin[(m - 1) * 2 Δt * ωrot];
  W40 =  a40
       + d44s Sin[(m - 1) * 4 Δt * ωrot]  +  d44c Cos[(m - 1) * 4 Δt * ωrot]
       + d43s Sin[(m - 1) * 3 Δt * ωrot]  +  d43c Cos[(m - 1) * 3 Δt * ωrot]
       + d42s Sin[(m - 1) * 2 Δt * ωrot]  +  d42c Cos[(m - 1) * 2 Δt * ωrot]
       + d41s Sin[(m - 1) *   Δt * ωrot]  +  d41c Cos[(m - 1) *   Δt * ωrot];
  ωQ21 = (-1/ω0) (QCC^2/36) ( (-21/(2 Sqrt[70])) W40 + (9/(2 Sqrt[5])) W00 );
  ωQ22 = (-1/ω0) (QCC^2/36) ( (27/(2 Sqrt[70])) W40 + (6/Sqrt[14]) W20 - (3/(2 Sqrt[5])) W00 );
 }]; (* End of If order == 2 *)

Ha = ( ωQ + ωQ21          -(Sqrt[3]/2) ωRF    0                    0
       -(Sqrt[3]/2) ωRF   -ωQ + ωQ22          -ωRF                 0
       0                  -ωRF                -ωQ - ωQ22           -(Sqrt[3]/2) ωRF
       0                  0                   -(Sqrt[3]/2) ωRF     ωQ - ωQ21 );

{HT, Tp} = Eigensystem[N[Ha]];                    T = Transpose[Tp];
n1 = DiagonalMatrix[Exp[-i * Δt * HT]] ;
ρ1 = T.n1.Tp;       ρ2 = T.Conjugate[n1].Tp;        ρ0 = ρ1.ρ0.ρ2;
s[m] = ρ0;
] ; (* End of For m *)

) ;  (* End of sub-function f[] *)

(* Main function powderMAS[] *)
powderMAS[order_, ω0Mhz_, QCCMHz_, ωRFkHz_,
  VrotkHz_, tf_, tau_, η_, maxα_, maxβ_, maxγ_, quanta_] := (
  ω0 = ω0Mhz * 2 π * 10^3;      QCCbis = QCCMHz * 2 π * 10^3;     ωbRFbis = ωRFkHz * 2 π;
  ωrot = VrotkHz * 2 π;         Δt = tau * 10^-3;                  ns = tf / tau;
  W00 = (Sqrt[5] / 10) (3 + η^2);

  (* Table h stores the line intensity for each pulse duration *)
  For [i = 0, i ≤ ns, i++, h[i] = 0;]; (* Clear Table h *)

  For [j = 0, j < maxα, j++, Print[j]; (* Summation on Euler angle α ∈ [0, 2π[ *)
   For [k = 1, k < maxβ, k++,           (* Summation on Euler angle β ∈ ]0,  π[ *)
                                          (* probability sin 0 ° = sin 180 ° = 0  *)
    For [c = 0, c < maxγ, c++,          (* Summation on Euler angle γ ∈ [0, 2π[ *)
     {(* Thermodynamic equilibrium of the density matrix *)
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ρ0 = DiagonalMatrix[{3/2, 1/2, -1/2, -3/2}];

cα = Cos[2 π j/maxα];   sα = Sin[2 π j/maxα];   c2α = 2 cα^2 - 1;   s2α = 2 cα sα;
cβ = Cos[π k/maxβ];     sβ = Sin[π k/maxβ];     c2β = 2 cβ^2 - 1;   s2β = 2 cβ sβ;
cγ = Cos[2 π c/maxγ];   sγ = Sin[2 π c/maxγ];   c2γ = 2 cγ^2 - 1;   s2γ = 2 cγ sγ;

(* Coefficients ai and bi involved in V(2,0) *)
a1 = -η s2α sβ / √3;            b1 = -(-3 + η c2α) s2β / (2 √3);
a2 = -η cβ s2α / √6;            b2 = -(η c2α (3 + c2β) + 6 sβ^2) / (4 √6);
d2s = a2 c2γ + b2 s2γ;          d1s = a1 cγ + b1 sγ;
d2c = a2 s2γ - b2 c2γ;          d1c = a1 sγ - b1 cγ;

If [order == 2, {
  c4α = 2 c2α^2 - 1;
  c4β = 1 - 8 cβ^2 (1 - cβ^2);     s4β = 4 cβ c2β sβ;
  c3γ = cγ (4 cγ^2 - 3);           s3γ = sγ (4 cγ^2 - 1);
  c4γ = 2 c2γ^2 - 1;               s4γ = 4 cγ c2γ sγ;
  (* Coefficients a2i and b2i involved in W(2,0) *)
  a22 = -√(2/7) η cβ s2α ;        b22 = -(η c2α (3 + c2β) + sβ^2 (-3 + η^2)) / (2 √14);
  a21 = -(2/√7) η sβ s2α ;        b21 = (-3 - 2 c2α η + η^2) s2β / (2 √7);
  d22s = a22 c2γ + b22 s2γ;       d21s = a21 cγ + b21 sγ;
  d22c = a22 s2γ - b22 c2γ;       d21c = a21 sγ - b21 cγ;
  (* Coefficients a4i and b4i involved in W(4,0) *)
  a40 = -√(7/10)/2304
     ((18 + η^2) (9 + 20 c2β + 35 c4β) + 240 η c2α (5 + 7 c2β) sβ^2 + 280 η^2 c4α sβ^4);
  a41 = (√(5/7) /72) η s2α sβ (15 + 21 c2β + 14 η c2α sβ^2);
  b41 = (√(5/7) /288) ((-18 - η^2 - 12 η c2α + 7 η^2 c4α) s2β - 7 (-3 + η c2α)^2 s4β);
  a42 = - (√(5/14) /18) η cβ s2α (-9 + 21 c2β + 14 η c2α sβ^2);
  b42 = -1/72 √(5/14)
     (3 η c2α (5 + 4 c2β + 7 c4β) + (7 η^2 c4α (3 + c2β) + (18 + η^2) (5 + 7 c2β)) sβ^2);
  a43 = -(√35 /72) η (-3 - 9 c2β + η c2α (5 + 3 c2β)) s2α sβ;
  b43 = -(√35 /288) (-18 - η^2 - 12 η c2α + 7 η^2 c4α + 2 (-3 + η c2α)^2 c2β) s2β;
  a44 = -(√(35/2) /72) η cβ s2α (η c2α (3 + c2β) + 6 sβ^2);
  b44 = -√(35/2)/2304 (η^2 c4α (35 + 28 c2β + c4β) + 48 η c2α (3 + c2β) sβ^2 + 8 (18 + η^2) sβ^4);
  d41s = a41 cγ + b41 sγ;   d41c = a41 sγ - b41 cγ;   d42s = a42 c2γ + b42 s2γ;
  d42c = a42 s2γ - b42 c2γ ;   d43s = a43 c3γ + b43 s3γ;   d43c = a43 s3γ - b43 c3γ;
  d44s = a44 c4γ + b44 s4γ;   d44c = a44 s4γ - b44 c4γ;
 }]; (* End of If order == 2 *)

f[order, QCCbis, ωbRFbis, Δt, ns]; (* Call the sub-function f[] *)

For [i = 1, i ≤ ns, i++,
 (* Normalized central-transition line intensity *)
 If [quanta == 1, {s[i] = Im[s[i][[3, 2]]], h[i] = h[i] + sβ s[i] * 2 / 5}];
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        (* -3-quantum line intensity *)
        If [quanta == 3, {s[i] = Im[s[i][[4, 1]]], h[i] = h[i] + sβ s[i]}];
      ]; (* End of For i *)

     }]; (* End of For c *)
    ]; (* End of For k *)
  ];    (* End of For j *)

  For [i = 1, i ≤ ns, i++, h[i] = h[i] / (maxα (maxβ - 1) maxγ); ];
  (* Powder normalization *)

  (*----- Provide Table crystalMAS containing ------*)
  (*------pulse duration t and line intensity ------*)
  Print["**********************************"];
  For[a = 0, a ≤ ns, a++, time[a] = a * tau;];
  powderMAS = Chop[Table[{tt, time[tt], NumberForm[h[tt], 10]}, {tt, 0, ns}]];
  Print[TableForm[powderMAS,
                 TableHeadings -> {None, {"Rang", "t(μs)", "intensity"}}]];
  (*----------------- Graph display ----------------*)
  Print["**********************************"];
  ListPlot[Table[{ tt * tau, h[tt]}, {tt, 0, ns}],
           PlotJoined → True,
           PlotLabel → "Int=f(t)",
           AxesLabel → {"t(μs)", "Int.(U.A.)"},
           PlotStyle → {Hue[0.1]},
           TextStyle → {FontFamily → "Times", FontSize → 12}];
 ); (* End of main function powderMAS *)

(* Call the main function with the corresponding numerical parameters *)
  powderMAS[ 2   , 105.8731007,  8     ,
 100  ,   15   , 20 , 1.0  , -1 ,   2 ,   3  ,  3  ,   1    ];
(* powderMAS[order_,    ω0Mhz_  , QCCMHz_, ωRFkHz_,
  VrotkHz_,tf_, tau_ , η_,maxα_,maxβ_,maxγ_,quanta_] *)

(*-----------------------------------------------------------------------------*)
(*                    Table powderMAS.m in Microsoft EXCEL format              *)
(*-----------------------------------------------------------------------------*)
Clear[writeExcel];
 writeExcel[filename_String, data_List] :=
    Module[ { file = OpenWrite[filename] },
            Scan[(
                   WriteString[file, First[#]];
                   Scan[
                        WriteString[file, "\t", #] &,
                        Rest[#]
                   ]; (* End of Scan *)
                   WriteString[file, "\n"]
                 ) &,
             data
            ]; (* End of Scan *)
            Close[file]
    ] ; (* End of Module *)
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writeExcel["powderMAS.m", powderMAS];

Remove[order, ω0Mhz, QCCMHz, ωRFkHz, VrotkHz,
 tf, tau, η, maxα, maxβ, maxγ, QCCbis, ωbRFbis, ns,
      α, β, γ, i, j, k, c, h, ρ0, f, a, powderMAS,
 n, s, m, ωQ, Ha, T, Tp, HT, n1, ωQ21, ωQ22]
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