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(*--------------------Filename: powder_MAS_rep.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 crystal file for powder summation: rep100_simp,
    (9) the number maxγ of summation steps of t he Euler angle γ
        in the 0 2π rang.

        The main function provides the parameters a_i, b_i, a_2i, b_2i,
     a_4i, and b_4i 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[].          *)
(*-------------------------------------------------------------------------*)
(* Author:  Redouane HAJJAR
   Address: Université Pierre et Marie Curie-Paris 6, UMR7142 (CNRS),
            Laboratoire des Systèmes Interfaciaux à l'Echelle Nanométrique,
            4 place Jussieu,casier 196, Paris,F-75005, FRANCE          *)
(*-------------------------------------------------------------------------*)

(* 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]);

   ωQ21 = 0;   ωQ22 = 0 ;
   If[order == 2, {
     W20 =  d21c Cos[(m - 1) Δt * ωrot]   +  d22c Cos[(m - 1) * 2 Δt * ωrot]
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        + 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 √70) W40 + 9/(2 √5) W00 );
    ωQ22 = -1/ω0 QCC^2/36 ( 27/(2 √70) W40 + 6/√14 W20 - 3/(2 √5) W00 );
  }]; (* End of If order == 2 *)

  Ha = ( ωQ + ωQ21      -√3/2 ωRF        0            0
         -√3/2 ωRF      -ωQ + ωQ22       -ωRF         0
         0              -ωRF             -ωQ - ωQ22   -√3/2 ωRF
         0              0                -√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[rep_, order_, ω0Mhz_, QCCMHz_,
  ωRFkHz_, VrotkHz_, tf_, tau_, η_, 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 = (√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 *)

  crystalfile = ReadList[rep , {Number, Number, Number}];
  fileLength = Length[crystalfile];   Print["crystalFile: ", rep];

  For [j = 1, j ≤ fileLength, j++, {Print[j];
    (* Summation on Euler angle α ∈ [0, 2π[ and β ∈ [0,  π] *)
    (* and powder normalization on α and β, because summation on proba = 1 *)
    alpha = crystalfile[[j, 1]] π / 180;
    beta = crystalfile[[j, 2]] π / 180;
    proba = crystalfile[[j, 3]];
    c2α = Cos[2 alpha];     s2α = Sin[2 alpha];
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c_β = Cos[beta];          s_β = Sin[beta];
c_2β = Cos[2 beta];       s_2β = Sin[2 beta];

For [z = 0, z < max_γ, z++, {
  (* Thermodynamic equilibrium of the density matrix *)
  ρ_0 = DiagonalMatrix[{3/2, 1/2, -1/2, -3/2}];

  c_γ = Cos[2 z π / max_γ];      s_γ = Sin[2 z π / max_γ];      c_2γ = 2 c_γ^2 - 1;      s_2γ = 2 c_γ s_γ;

  (* Coefficients a_i and b_i involved in V_(2,0) *)
  a_1 = -η s_2α s_β / √3;                b_1 = -(-3 + η c_2α) s_2β / (2 √3);
  a_2 = -η c_β s_2α / √6;                b_2 = -(η c_2α (3 + c_2β) + 6 s_β^2) / (4 √6);
  d_2s = a_2 c_2γ + b_2 s_2γ;            d_1s = a_1 c_γ + b_1 s_γ;
  d_2c = a_2 s_2γ - b_2 c_2γ;            d_1c = a_1 s_γ - b_1 c_γ;

  If [order == 2, {
    c_4α = 2 c_2α^2 - 1;
    c_4β = 1 - 8 c_β^2 (1 - c_β^2);      s_4β = 4 c_β c_2β s_β;
    c_3γ = c_γ (4 c_γ^2 - 3);            s_3γ = s_γ (4 c_γ^2 - 1);
    c_4γ = 2 c_2γ^2 - 1;                 s_4γ = 4 c_γ c_2γ s_γ;
    (* Coefficients a_2i and b_2i involved in W_(2,0) *)
    a_22 = -√(2/7) η c_β s_2α;           b_22 = -(η c_2α (3 + c_2β) + s_β^2 (-3 + η^2)) / (2 √14);
    a_21 = -(2/√7) η s_β s_2α;           b_21 = (-3 - 2 c_2α η + η^2) s_2β / (2 √7);
    d_22s = a_22 c_2γ + b_22 s_2γ;       d_21s = a_21 c_γ + b_21 s_γ;
    d_22c = a_22 s_2γ - b_22 c_2γ;       d_21c = a_21 s_γ - b_21 c_γ;
    (* Coefficients a_4i and b_4i involved in W_(4,0) *)
    a_40 = -√(7/10)/2304
      ((18 + η^2) (9 + 20 c_2β + 35 c_4β) + 240 η c_2α (5 + 7 c_2β) s_β^2 + 280 η^2 c_4α s_β^4);
    a_41 = (√(5/7)/72) η s_2α s_β (15 + 21 c_2β + 14 η c_2α s_β^2);
    b_41 = (√(5/7)/288) ((-18 - η^2 - 12 η c_2α + 7 η^2 c_4α) s_2β - 7 (-3 + η c_2α)^2 s_4β);
    a_42 = -(√(5/14)/18) η c_β s_2α (-9 + 21 c_2β + 14 η c_2α s_β^2);
    b_42 = -1/72 √(5/14)
      (3 η c_2α (5 + 4 c_2β + 7 c_4β) + (7 η^2 c_4α (3 + c_2β) + (18 + η^2) (5 + 7 c_2β)) s_β^2);
    a_43 = -(√35/72) η (-3 - 9 c_2β + η c_2α (5 + 3 c_2β)) s_2α s_β;
    b_43 = -(√35/288) (-18 - η^2 - 12 η c_2α + 7 η^2 c_4α + 2 (-3 + η c_2α)^2 c_2β) s_2β;
    a_44 = -(√(35/2)/72) η c_β s_2α (η c_2α (3 + c_2β) + 6 s_β^2);
    b_44 = -√(35/2)/2304 (η^2 c_4α (35 + 28 c_2β + c_4β) + 48 η c_2α (3 + c_2β) s_β^2 + 8 (18 + η^2) s_β^4);
    d_41s = a_41 c_γ + b_41 s_γ;   d_41c = a_41 s_γ - b_41 c_γ;   d_42s = a_42 c_2γ + b_42 s_2γ;
    d_42c = a_42 s_2γ - b_42 c_2γ; d_43s = a_43 c_3γ + b_43 s_3γ; d_43c = a_43 s_3γ - b_43 c_3γ;
    d_44s = a_44 c_4γ + b_44 s_4γ; d_44c = a_44 s_4γ - b_44 c_4γ;
  }]; (* 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 *)
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      If [quanta == 1, {s[i] = Im[s[i][[3, 2]]], h[i] = h[i] + proba s[i] * 2 / 5}];
      (* -3-quantum line intensity *)
       If [quanta == 3, {s[i] = Im[s[i][[4, 1]]], h[i] = h[i] + proba s[i]}];
     ]; (* End of For i *)

    }];(* End of For z *)
  }];  (* End of For j *)

  For [i = 1, i ≤ ns, i++, h[i] = h[i] / maxγ ]; (* Powder normalization on γ *)

  (*----- Provide Table crystalMAS containing ------*)
  (*------pulse duration t and line intensity ------*)
  Print["*********************************"];
  For[a = 0, a ≤ ns, a++, time[a] = a * tau;];
  powderMASrep = Chop[Table[{tt, time[tt], NumberForm[h[tt], 10]}, {tt, 0, ns}]];
  Print[TableForm[powderMASrep,
                  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["rep100_simp" ,  2    , 105.8731007 ,
  8    ,   100  ,   15    , 20 ,   1   ,  1 ,    3  ,   1    ];
(* powderMAS[     rep_     ,ordre_,     ω0Mhz_   , QCCMHz_,
  ωRFkHz_,VrotkHz_, tf_,  tau_, η_, maxγ_,quanta_] *)


(*-------------------------------------------------------------------------------*)
(*               Table powderMASrep.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["powderMASrep.m", powderMASrep]
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Remove[order, ω0Mhz, QCCMHz, ωRFkHz, VrotkHz, tf, tau, η, maxγ, QCCbis, ωbRFbis, ns,
        α, β, γ, i, j, k, c, h, f, a,
 powderMASrep, n, s, m, ωQ, Ha, T, Tp, HT, n1, ωQ21, ωQ22]
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