Resolution calculation

A. T. Savici
(Dated: June 26, 2010)

I. INTRODUCTION

We are interested in measuring the scattering cross section at a point in reciprocal space given by

$$\mathbf{Q}_0 = \mathbf{k}_F - \mathbf{k}_I \tag{1}$$

$$\hbar\omega_0 = \frac{\hbar^2}{2m}(\mathbf{k}_I^2 - \mathbf{k}_F^2) \tag{2}$$

However, uncertainties in positions, angles and times allow neutrons with slightly different momentum or energy transfers to be detected. The resolution of the instrument is defined as the probability to observe events differing by $\Delta\mathbf{Q}, \Delta\hbar\omega$ from $\mathbf{Q}_0, \hbar\omega_0$

II. ASSUMPTIONS

- All transmission probabilities of the guide and choppers, moderator emission time, and detection time have gaussian distribution
- The effect of the guide and moderator can be described by moderator emission time, and vertical and horizontal guide divergencies
- The angular transmission effects in the chopper are accounted for in the incident beam divergencies
- Since these type of spectrometers have fixed detectors, we will calculate resolution in the instrument frame. z axis is along the incident beam, x is in the horizontal plane, and y axis is vertical

III. CONSTRAINTS

In the calculation presented in this paper, the effect of sample size are neglected. We write all transmission probabilities in terms of $\mathbf{k}_i, \mathbf{k}_f$.

$$R(\mathbf{Q}, \hbar\omega) = R(\mathbf{Q}_0 + \Delta\mathbf{Q}, \hbar\omega_0 + \delta\hbar\omega) = \int_{constraints} P(\hbar\omega, \mathbf{Q})\mathbf{dk}_i\mathbf{dk}_f \tag{3}$$

Since the resolution function is written in terms of $\Delta\mathbf{Q}, \Delta\hbar\omega$, there must be constraints that reduce the number of independent variables from 6 to 4.

The incident beam geometry is shown in figure 1

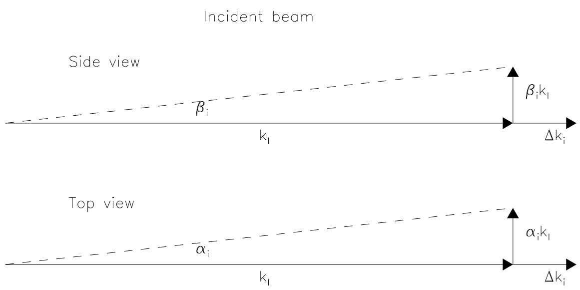

FIG. 1: Incident beam geometry

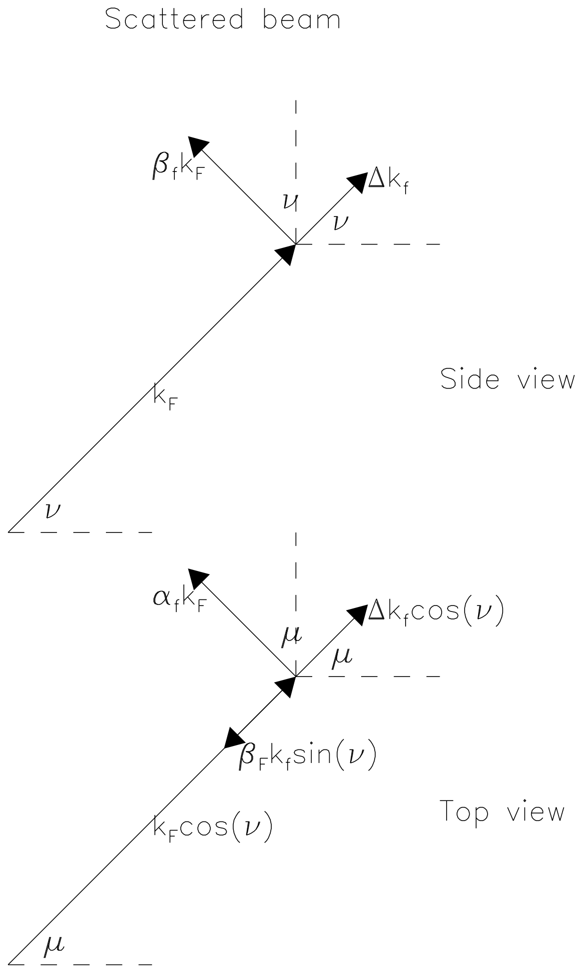

FIG. 2: Scattered beam geometry

$$\begin{aligned}
\Delta \mathbf{k}_i &= (\Delta k_{ix}, \Delta k_{iy}, \Delta k_{iz}) &(4)\\
\Delta k_{ix} &= k_I \alpha_i &(5)\\
\Delta k_{iy} &= k_I \beta_i &(6)\\
\Delta k_{iz} &= \Delta k_i &(7)
\end{aligned}$$

We can write similar equations for $\Delta \mathbf{k}_f$, on a reference frame with one axis along $\mathbf{k}_F$, one axis horizontal, and one axis perpendicular to the plane of the first two axes. The orientation of these components is shown in figure 2.

With these notations,

$$\begin{aligned}
\Delta \mathbf{k}_f &= (\Delta k_{fx}, \Delta k_{fy}, \Delta k_{fz}) &(8)\\
\Delta k_{fx} &= (\Delta k_f \cos(\nu) - k_F \beta_f \sin(\nu)) \sin(\mu) + \alpha_f k_F \cos(\mu) &(9)\\
\Delta k_{fy} &= \Delta k_f \sin(\nu) + k_F \beta_f \cos(\nu) &(10)\\
\Delta k_{fz} &= (\Delta k_f \cos(\nu) - k_F \beta_f \sin(\nu)) \cos(\mu) - \alpha_f k_F \sin(\mu) &(11)
\end{aligned}$$

Usually, the scattering angles in experiment are 2θ, andϕ, as shown in figure 3.

$$\begin{aligned}
\sin(\nu) &= \sin(2\theta) \sin(\phi) &(12)\\
\cos(\nu) &= \sqrt{1 - \sin^2(2\theta) \sin^2(\phi)} &(13)\\
\sin(\mu) &= \frac{\sin(2\theta) \cos(\phi)}{\sqrt{\cos^2(2\theta) + \sin^2(2\theta) \cos^2(\phi)}} &(14)
\end{aligned}$$

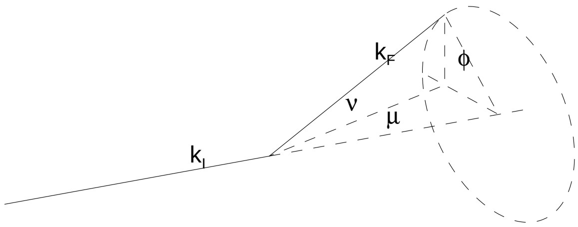

FIG. 3: Scattered beam geometry - $(2\theta, \phi)$ to (μ, ν)

$$\cos(\mu) = \frac{\cos(2\theta)}{\sqrt{\cos^2(2\theta) + \sin^2(2\theta)\cos^2(\phi)}} \tag{15}$$

Now we can write the components of $\Delta\mathbf{Q}$, and $\Delta\hbar\omega$

$$\Delta Q_x = (\Delta k_f \cos(\nu) - k_F\beta_f \sin(\nu))\sin(\mu) + \alpha_f k_F \cos(\mu) - k_I\alpha_i \tag{16}$$
$$\Delta Q_y = \Delta k_f \sin(\nu) + k_F\beta_f \cos(\nu) - k_I\beta_i \tag{17}$$
$$\Delta Q_z = (\Delta k_f \cos(\nu) - k_F\beta_f \sin(\nu))\cos(\mu) - \alpha_f k_F \sin(\mu) - \Delta k_i \tag{18}$$
$$\Delta\hbar\omega = \frac{\hbar^2}{m}(k_I\Delta k_i - k_F\Delta k_f) \tag{19}$$

If we choose to have α_i and β_i as independent variables, we rewrite $\Delta k_i, \Delta k_f, \alpha_f$, and β_f in terms of the other variables.

$$\Delta k_i = a_{00}\Delta Q_x + a_{01}\Delta Q_y + a_{02}\Delta Q_z + a_{03}\Delta\hbar\omega + a_{04}\alpha_i + a_{05}\beta_i \tag{20}$$
$$\Delta k_f = a_{10}\Delta Q_x + a_{11}\Delta Q_y + a_{12}\Delta Q_z + a_{13}\Delta\hbar\omega + a_{14}\alpha_i + a_{15}\beta_i \tag{21}$$
$$\alpha_f = a_{20}\Delta Q_x + a_{21}\Delta Q_y + a_{22}\Delta Q_z + a_{23}\Delta\hbar\omega + a_{24}\alpha_i + a_{25}\beta_i \tag{22}$$
$$\beta_f = a_{30}\Delta Q_x + a_{31}\Delta Q_y + a_{32}\Delta Q_z + a_{33}\Delta\hbar\omega + a_{34}\alpha_i + a_{35}\beta_i \tag{23}$$

$$a_{00} = \frac{k_F \sin(\mu)\cos(\nu)}{k_I - k_F\cos(\mu)\cos(\nu)} \tag{24}$$
$$a_{01} = \frac{k_F \sin(\nu)}{k_I - k_F\cos(\mu)\cos(\nu)} \tag{25}$$
$$a_{02} = \frac{k_F \cos(\mu)\cos(\nu)}{k_I - k_F\cos(\mu)\cos(\nu)} \tag{26}$$
$$a_{03} = \frac{m/\hbar^2}{k_I - k_F\cos(\mu)\cos(\nu)} \tag{27}$$
$$a_{04} = \frac{k_I k_F \sin(\mu)\cos(\nu)}{k_I - k_F\cos(\mu)\cos(\nu)} \tag{28}$$
$$a_{05} = \frac{k_I k_F \sin(\nu)}{k_I - k_F\cos(\mu)\cos(\nu)} \tag{29}$$
$$a_{10} = \frac{k_I \sin(\mu)\cos(\nu)}{k_I - k_F\cos(\mu)\cos(\nu)} \tag{30}$$
$$a_{11} = \frac{k_I \sin(\nu)}{k_I - k_F\cos(\mu)\cos(\nu)} \tag{31}$$
$$a_{12} = \frac{k_I \cos(\mu)\cos(\nu)}{k_I - k_F\cos(\mu)\cos(\nu)} \tag{32}$$
$$a_{13} = \frac{m/\hbar^2 \cos(\mu)\cos(\nu)}{k_I - k_F\cos(\mu)\cos(\nu)} \tag{33}$$
$$a_{14} = \frac{k_I^2 \sin(\mu)\cos(\nu)}{k_I - k_F\cos(\mu)\cos(\nu)} \tag{34}$$

$$a_{15} = \frac{k_I^2 \sin(\nu)}{k_I - k_F \cos(\mu)\cos(\nu)} \tag{35}$$

$$a_{20} = \frac{\lambda \cos(\mu) - \cos(\nu)}{k_I - k_F \cos(\mu)\cos(\nu)} \tag{36}$$

$$a_{21} = \frac{-\sin(\mu)\sin(\nu)}{k_I - k_F \cos(\mu)\cos(\nu)} \tag{37}$$

$$a_{22} = \frac{-\lambda \sin(\mu)}{k_I - k_F \cos(\mu)\cos(\nu)} \tag{38}$$

$$a_{23} = \frac{-m/\hbar^2 \sin(\mu)/k_F}{k_I - k_F \cos(\mu)\cos(\nu)} \tag{39}$$

$$a_{24} = \frac{k_I(\lambda \cos(\mu) - \cos(\nu))}{k_I - k_F \cos(\mu)\cos(\nu)} \tag{40}$$

$$a_{25} = \frac{-k_I \sin(\mu)\sin(\nu)}{k_I - k_F \cos(\mu)\cos(\nu)} \tag{41}$$

$$a_{30} = \frac{-\lambda \sin(\mu)\sin(\nu)}{k_I - k_F \cos(\mu)\cos(\nu)} \tag{42}$$

$$a_{31} = \frac{\lambda \cos(\nu) - \cos(\mu)}{k_I - k_F \cos(\mu)\cos(\nu)} \tag{43}$$

$$a_{32} = \frac{-\lambda \cos(\mu)\sin(\nu)}{k_I - k_F \cos(\mu)\cos(\nu)} \tag{44}$$

$$a_{33} = \frac{-m/\hbar^2 \cos(\mu)\sin(\nu)/k_F}{k_I - k_F \cos(\mu)\cos(\nu)} \tag{45}$$

$$a_{34} = \frac{-k_I \lambda \sin(\mu)\sin(\nu)}{k_I - k_F \cos(\mu)\cos(\nu)} \tag{46}$$

$$a_{35} = \frac{k_I(\lambda \cos(\nu) - \cos(\mu))}{k_I - k_F \cos(\mu)\cos(\nu)} \tag{47}$$

where $\lambda = k_I/k_F$.

IV. PROBABILITIES

At moderator, in the ideal case, all neutrons are emitted at time $t^0_{mod} = 0$. They travel parallel to k_I, and arrive at the chopper at

$$t^0_{chop} = \frac{L_1}{v_I} = \frac{L_1 m}{\hbar k_I} \tag{48}$$

then at the sample at

$$t^0_{samp} = \frac{L_1 + L_2}{v_I} = \frac{(L_1 + L_2)m}{\hbar k_I} \tag{49}$$

and at the detector at

$$t^0_{det} = \frac{L_1 + L_2}{v_I} + \frac{L_3}{k_F} = \frac{(L_1 + L_2)m}{\hbar k_I} + \frac{L_3 m}{\hbar k_F} \tag{50}$$

For the real case, the probability of neutron emission at time τ is given by

$$P_{mod}(\tau) = \frac{1}{\sqrt{2\pi t_m^2}} e^{-\frac{\tau^2}{2t_m^2}} \tag{51}$$

where t_m^2 is the variance of the moderator time pulse.

Neutrons arrive at the chopper at

$$t_{chop} = \tau + \frac{L_1}{v_I} - \frac{L_1}{v_I^2}\Delta v_i = \tau + \frac{L_1 m}{\hbar k_I} - \frac{L_1 m}{\hbar k_I^2}\Delta k_i \quad (52)$$

For parallel beam, the maximum transmission probability through the chopper occurs at t^0_{chop}. If the beam is divergent, the maximum probability for neutrons traveling at angle α_i occurs at $t^0_{chop} + \alpha_i/(2\pi f)$, where f is the rotation frequency of the chopper. The transmission probability through chopper with standard deviation t_c is then

$$P_{chop}(\tau, \Delta k_i, \alpha_i) = P_c e^{-\frac{\left(\tau - \frac{L_1 m}{\hbar k_I^2}\Delta k_i - \frac{\alpha_i}{2\pi f}\right)^2}{2t_c^2}} \quad (53)$$

The value of P_c depends on the construction of the chopper, and it can be included in the flux calculation.

Similar to previous calculations, it is easy to show that neutrons arrive at the neutrons arrive at the detector at

$$t_{det} = \tau + \frac{(L_1+L_2)m}{\hbar k_I} - \frac{(L_1+L_2)m}{\hbar k_I^2}\Delta k_i + \frac{L_3 m}{\hbar k_F} - \frac{L_3 m}{\hbar k_F^2}\Delta k_f \quad (54)$$

and that the detection probability is

$$P_{det}(\tau, \Delta k_i, \Delta k_f) = \frac{P_D}{\sqrt{2\pi t_d^2}} e^{-\frac{\left(\tau - \frac{(L_1+L_2)m}{\hbar k_I^2}\Delta k_i - \frac{L_3 m}{\hbar k_F^2}\Delta k_f\right)^2}{2t_d^2}} \quad (55)$$

where P_D is the detector efficiency.

In addition to transmission probabilities as a function of time, we also need to consider the geometrical transmission probabilities:

$$P_g^I(\alpha_i, \beta_i) = \frac{1}{2\pi\gamma_I\delta_I} e^{-\frac{\alpha_i^2}{2\gamma_I^2} - \frac{\beta_i^2}{2\delta_I^2}} \quad (56)$$

$$P_g^F(\alpha_f, \beta_f) = \frac{1}{2\pi\gamma_F\delta_F} e^{-\frac{\alpha_f^2}{2\gamma_F^2} - \frac{\beta_f^2}{2\delta_F^2}} \quad (57)$$

where $\gamma_I, \delta_I, \gamma_F, \delta_F$ are the vertical and horizontal divergencies of the incident and scattered beams. The values for the incident beam are obtained from the simulations of the guide (and are slightly dependent on k_I), while the values for the scattered beam are given by the angular sizes of the detector pixels.

The total detection probability is then given by the product of each individual transmission/detection probabilities:

$$P(\tau, \Delta k_i, \Delta k_f, \alpha_i, \alpha_f, \beta_i, \beta_f) = P_{mod}(\tau) P_{chop}(\tau, \Delta k_i, \alpha_i) P_{det}(\tau, \Delta k_i, \Delta k_f) P_g^I(\alpha_i, \beta_i) P_g^F(\alpha_f, \beta_f) \quad (58)$$

V. RESOLUTION FUNCTION

With the probability in equation 58, one needs to replace $\Delta k_i, \Delta k_f, \alpha_f$, and β_f in terms of $\Delta Q_x, \Delta Q_y, \Delta Q_z, \Delta\hbar\omega, \alpha_i, \beta_i$, and integrate over τ, α_i, β_i. What we are left with is

$$R(\Delta\mathbf{Q}, \Delta\hbar\omega) = R_0 e^{-\frac{1}{2}X^T M X} \quad (59)$$

where $X^T = (\Delta Q_x, \Delta Q_y, \Delta Q_z, \Delta\hbar\omega)$

From equation 58,

$$\begin{aligned} P(\tau, \Delta k_i, \Delta k_f, \alpha_i, \alpha_f, \beta_i, \beta_f) &= \frac{1}{\sqrt{2\pi t_m^2}} e^{-\frac{\tau^2}{2t_m^2}} P_c e^{-\frac{\left(\tau - \frac{L_1 m}{\hbar k_I^2}\Delta k_i - \frac{\alpha_i}{2\pi f}\right)^2}{2t_c^2}} \frac{P_D}{\sqrt{2\pi t_d^2}} e^{-\frac{\left(\tau - \frac{(L_1+L_2)m}{\hbar k_I^2}\Delta k_i - \frac{L_3 m}{\hbar k_F^2}\Delta k_f\right)^2}{2t_d^2}} \cdot \\ & \frac{1}{2\pi\gamma_I\delta_I} e^{-\frac{\alpha_i^2}{2\gamma_I^2} - \frac{\beta_i^2}{2\delta_I^2}} \frac{1}{2\pi\gamma_F\delta_F} e^{-\frac{\alpha_f^2}{2\gamma_F^2} - \frac{\beta_f^2}{2\delta_F^2}} \end{aligned} \quad (60)$$

$$= \frac{P_c P_D}{(2\pi)^3 \gamma_I \gamma_F \delta_I \delta_f t_m t_d} \exp\left\{-\frac{1}{2}\left[\frac{\tau^2}{t_m^2} + \frac{\left(\tau - \frac{L_1 m}{\hbar k_I^2}\Delta k_i - \frac{\alpha_i}{2\pi f}\right)^2}{t_c^2} + \frac{\left(\tau - \frac{(L_1+L_2)m}{\hbar k_I^2}\Delta k_i - \frac{L_3 m}{\hbar k_F^2}\Delta k_f\right)^2}{t_d^2} + \frac{\alpha_i^2}{\gamma_I^2} - \frac{\beta_i^2}{\delta_I^2} + \frac{\alpha_f^2}{\gamma_F^2} - \frac{\beta_f^2}{\delta_F^2}\right]\right\} \quad (61)$$

$$= P_0 \exp\left\{-\frac{1}{2} Y^T B Y\right\} \quad (62)$$

where $Y^T = (\Delta k_i, \Delta k_f, \alpha_f, \beta_f, \alpha_i, \beta_i, \tau)$, and B is a 7×7 symmetric matrix with the following elements:

$$b_{00} = \frac{L_1^2 m^2}{\hbar^2 k_I^4 t_c^2} + \frac{(L_1+L_2)^2 m^2}{\hbar^2 k_I^4 t_d^2} \quad (63)$$

$$b_{01} = \frac{(L_1+L_2) L_3 m^2}{\hbar^2 k_I^2 k_F^2 t_d^2} \quad (64)$$

$$b_{02} = 0 \quad (65)$$

$$b_{03} = 0 \quad (66)$$

$$b_{04} = \frac{L_1 m}{2\pi f \hbar k_I^2 t_c^2} \quad (67)$$

$$b_{05} = 0 \quad (68)$$

$$b_{06} = -\frac{L_1 m}{\hbar k_I^2 t_c^2} - \frac{(L_1 + L2) m}{\hbar k_I^2 t_d^2} \quad (69)$$

$$b_{11} = \frac{L_3^2 m^2}{\hbar^2 k_F^4 t_d^2} \quad (70)$$

$$b_{12} = 0 \quad (71)$$

$$b_{13} = 0 \quad (72)$$

$$b_{14} = 0 \quad (73)$$

$$b_{15} = 0 \quad (74)$$

$$b_{16} = -\frac{L_3 m}{\hbar k_F^2 t_d^2} \quad (75)$$

$$b_{22} = \frac{1}{\gamma_F^2} \quad (76)$$

$$b_{23} = 0 \quad (77)$$

$$b_{24} = 0 \quad (78)$$

$$b_{25} = 0 \quad (79)$$

$$b_{26} = 0 \quad (80)$$

$$b_{33} = \frac{1}{\delta_F^2} \quad (81)$$

$$b_{34} = 0 \quad (82)$$

$$b_{35} = 0 \quad (83)$$

$$b_{36} = 0 \quad (84)$$

$$b_{44} = \frac{1}{(2\pi f t_c)^2} + \frac{1}{\gamma_I^2} \quad (85)$$

$$b_{45} = 0 \quad (86)$$

$$b_{46} = -\frac{1}{2\pi f t_c^2} \quad (87)$$

$$b_{55} = \frac{1}{\delta_I^2} \quad (88)$$

$$b_{56} = 0 \quad (89)$$

$$b_{66} = \frac{1}{t_m^2} + \frac{1}{t_c^2} + \frac{1}{t_d^2} \tag{90}$$

$$b_{ij} = b_{ji} \tag{91}$$

If we create vector X_3 such as $X_3^T = (\Delta Q_x, \Delta Q_y, \Delta Q_z, \Delta\hbar\omega, \alpha_i, \beta_i, \tau)$, we can write

$$Y = AX_3 \tag{92}$$

with most of the coefficients discussed previously (equations 20-47). The remaining coefficients are equal to 0, except

$$a_{44} = a_{55} = a_{66} = 1 \tag{93}$$

We can now rewrite equation 62 as:

$$P(\tau, \Delta k_i, \Delta k_f, \alpha_i, \alpha_f, \beta_i, \beta_f) = P(\Delta Q_x, \Delta Q_y, \Delta Q_z, \Delta\hbar\omega, \alpha_i, \beta_i, \tau) = P_0 \exp\left\{-\frac{1}{2} X_3^T A^T B A X_3\right\} \tag{94}$$

Integration over τ, β_i, α_i is straightforward, and can be done algebraically. Let

$$M_3 = A^T B A \tag{95}$$

and

$$X_2^T = (\Delta Q_x, \Delta Q_y, \Delta Q_z, \Delta\hbar\omega, \alpha_i, \beta_i) \tag{96}$$

Then

$$\int_{-\infty}^{\infty} d\tau P(\Delta Q_x, \Delta Q_y, \Delta Q_z, \Delta\hbar\omega, \alpha_i, \beta_i, \tau) = P_0 \sqrt{\frac{2\pi}{m_{3,66}}} \exp\left\{-\frac{1}{2} X_2^T M_2 X_2\right\} \tag{97}$$

The elements of M_2 are calculated using

$$m_{2,ij} = m_{3,ij} - \frac{m_{3,i6} m_{3,j6}}{m_{3,66}^2}, i, j = \overline{0,5} \tag{98}$$

Similarly, we proceed with integration over β_i and α_i.

$$\int_{-\infty}^{\infty} d\beta_i \exp\left\{-\frac{1}{2} X_2^T M_2 X_2\right\} = \sqrt{\frac{2\pi}{m_{2,55}}} \exp\left\{-\frac{1}{2} X_1^T M_1 X_1\right\} \tag{99}$$

$$X_2^T = (\Delta Q_x, \Delta Q_y, \Delta Q_z, \Delta\hbar\omega, \alpha_i) \tag{100}$$

$$m_{1,ij} = m_{2,ij} - \frac{m_{2,i5} m_{2,j5}}{m_{2,55}^2}, i, j = \overline{0,4} \tag{101}$$

$$\int_{-\infty}^{\infty} d\alpha_i \exp\left\{-\frac{1}{2} X_1^T M_1 X_1\right\} = \sqrt{\frac{2\pi}{m_{1,44}}} \exp\left\{-\frac{1}{2} X^T M X\right\} \tag{102}$$

$$X^T = (\Delta Q_x, \Delta Q_y, \Delta Q_z, \Delta\hbar\omega) \tag{103}$$

$$m_{ij} = m_{1,ij} - \frac{m_{1,i4} m_{1,j4}}{m_{1,44}^2}, i, j = \overline{0,3} \tag{104}$$

VI. SUMMARY

In order to calculate the resolution function, we need to execute the following steps:

1. Calculate sine and cosine of angles μ, ν (Eq 12-15)
2. Calculate matrix A (Eq 24-47, 93)
3. Calculate matrix B (Eq 63-91)
4. $M_3 = A^T B A$
5. Calculate M_2, M_1, M using equations 98, 101, 104
6. $R_0 = \frac{P_c P_D}{(2\pi)^3 \gamma_I \gamma_F \delta_I \delta_f t_m t_d} \sqrt{\frac{2\pi}{m_{3,66}}} \sqrt{\frac{2\pi}{m_{2,55}}} \sqrt{\frac{2\pi}{m_{1,44}}}$