372(8). New General Results in Quantum Mechanics For All Materials.

In general, for all atoms and molecules on the non-relativistic level:

$$i\hbar \frac{\partial \phi}{\partial t} = E\phi \quad -(1)$$

$$-i\hbar \frac{\partial \phi}{\partial r} = m\dot{r}\phi \quad -(2)$$

$$-i\hbar \frac{\partial \phi}{\partial \theta} = mr^2\dot{\theta}\phi \quad -(3)$$

$$-i\hbar \frac{\partial \phi}{\partial \phi} = mr^2\dot{\phi}\sin^2\theta\,\phi \quad -(4)$$

From the Lagrangian theory on the classical level:

$$L_Z = mr^2\dot{\phi}\sin^2\theta \quad -(5)$$

and

$$L^2 = m^2r^4\left(\dot{\theta}^2 + \dot{\phi}^2\sin^2\theta\right) \quad -(6)$$

For all atoms and molecules:

$$L^2\phi = \hbar^2 l(l+1)\phi \quad -(7)$$

and

$$L_Z\phi = \hbar m_l\phi \quad -(8)$$

where

$$m_l = -l, \ldots, l \quad -(9)$$

By classical quantum equivalence:

$$\hat{L}_Z\phi = \hbar m_l\phi = mr^2\dot{\phi}\sin^2\theta\,\phi \quad -(10)$$

$$\left\langle mr^2\dot{\phi}\sin^2\theta\right\rangle = \hbar m_l \quad -(10a)$$

2) and

$$\ell(\ell+1)\hbar^2 = \left\langle m^2 r^4 \left(\dot{\theta}^2 + \dot{\phi}^2 \sin^2\theta\right)\right\rangle \quad (11)$$

$$= \left\langle m^2 r^4 \dot{\theta}^2 \right\rangle + m_\ell^2 \hbar^2$$

So

$$\left\langle \dot{\theta} \right\rangle = \left\langle \frac{d\theta}{dt} \right\rangle = \frac{\hbar}{mr^2}\left(\ell(\ell+1) - m_\ell^2\right)^{1/2} \quad (12)$$

i.e. $$\left\langle mr^2 \dot{\theta} \right\rangle = \hbar\left(\ell(\ell+1) - m_\ell^2\right)^{1/2} \quad (13)$$

However, from Lagrangian theory on the classical level:

$$mr^2\dot{\theta} = \left(L^2 - \frac{L_z^2}{\sin^2\theta}\right)^{1/2} \quad (14)$$

So $$\boxed{\left\langle L^2 - \frac{L_z^2}{\sin^2\theta} \right\rangle = \hbar^2\left(\ell(\ell+1) - m_\ell^2\right)} \quad (15)$$

Eq (15) is true generally in non-relativistic quantum mechanics for all atoms and molecules.

From Eq (15):

$$\left\langle \sin^2\theta \right\rangle = \frac{L_z^2}{L^2 - \hbar^2\left(\ell(\ell+1) - m_\ell^2\right)} \quad (16)$$

and using expectation value definitions:

3) $$\int \phi^* m r^2 \dot{\theta} \phi \, d\tau = \hbar \left(l(l+1) - m_l^2 \right)^{1/2} \quad -(17)$$

$$\int \phi^* m r^2 \dot{\phi} \sin^2\theta \, \phi \, d\tau = \hbar m_l \quad -(18)$$

$$\int \phi^* \sin^2\theta \, \phi \, d\tau = \frac{L_z^2}{L^2 - \hbar^2 \left(l(l+1) - m_l^2 \right)} \quad -(19)$$

Fm eqns (3) and (17):

$$\boxed{ -i \int \phi^* \frac{\partial \phi}{\partial \theta} \, d\tau = \left(l(l+1) - m_l^2 \right)^{1/2} } \quad -(20)$$

Fm eqs. (4) and (18):

$$\boxed{ -i \int \phi^* \frac{\partial \phi}{\partial \phi} \, d\tau = m_l } \quad -(21)$$

Fm eqs. (15) and (20):

$$-i \int \phi^* \frac{\partial \phi}{\partial \theta} \, d\tau = \frac{1}{\hbar^2} \left\langle L^2 - \frac{L_z^2}{\sin^2\theta} \right\rangle \quad -(22)$$

i.e. $$\boxed{ L^2 - \frac{L_z^2}{\sin^2\theta} = -i\hbar^2 \int \phi^* \frac{\partial \phi}{\partial \theta} \, d\tau } \quad -(23)$$