## Appendix A: Rigid body algebra and the problem of cross-talk between parameters

Main text Eqns. (1) and (2) describe the computation of motion correction by minimization of the squared difference between a selected reference frame, $I_0$, and all other frames, indexed by $i$. Thus,

$$\varepsilon_i^2 = \langle\left(gI_0(T(\vec{x})) - I_i(\vec{x})\right)^2\rangle, \qquad \text{(A1.1)}$$

where $I(\vec{x})$ is the image intensity at locus $\vec{x}$ and $g$ is a scalar factor that compensates for fluctuations in mean signal intensity, spatially averaged over the whole brain (angle brackets). Each transform is represented as a 4 × 4 matrix combining rotations and displacements. Thus,

$$T_i = \begin{bmatrix} R_i & \vec{d}_i \\ 0 & 1 \end{bmatrix}, \qquad \text{(A2)}$$

where $R_i$ is a 3 × 3 rotation matrix and $\vec{d}_i$ is 3 × 1 column vector of displacements (in mm). Ideally, in the absence of true head motion, factitious head motion in the phase encoding direction should appear as an isolated translation along one axis (here assumed to be y). Thus, $R_i$ would be the 3 × 3 identity matrix ($I_{3\times3}$) and $\vec{d}_i$ would be a column vector of form

$$\begin{bmatrix} 0 \\ \Delta_{iy} \\ 0 \end{bmatrix}. \qquad \text{(A3)}$$

This ideal representation will not, in general, be obtained unless two conditions are met. First, the coordinate transform, $T_i$, must be applied to frame $i$ rather than the reference frame as written in Eqn. A1.1. In other words, the error must be computed as

$$\varepsilon_i^2 = \langle\left(gI_i(T_i(\vec{x})) - I_0(\vec{x})\right)^2\rangle. \qquad \text{(A1.2)}$$

This condition is semi-trivially achievable as the transforms in Eqns. A1.1 and A1.2 are algebraic inverses.

Second, but less trivially, cross-talk between rotations and translations occurs unless the coordinate origin is at the center of mass of the object being rotated (in the present case, the head). In algebraic terms, consider the case in which the coordinate origin initially is at the center of the head but subsequently is arbitrarily shifted by displacement $\vec{s}$. Then, the coordinate at which image intensities are read out shifts and Eqn. A1.2 reads

$$\varepsilon_i^2 = \langle\left(gI_i(T_i(\vec{x} - \vec{s})) - I_0(\vec{x} - \vec{s})\right)^2\rangle. \qquad \text{(A1.2')}$$

In the absence of rotation, the displacement component of the rigid body transform simply compensates for the coordinate origin shift. However, if rotation is involved, cross-talk occurs. To see this, represent the coordinate origin shift as an affine transform. Thus, $\vec{x}' = D\vec{x}$, where

$$D = \begin{bmatrix} I_{3\times3} & -\vec{s} \\ 0 & 1 \end{bmatrix}.$$

The coordinate transform acting on frame $i$ reads $T_i(\vec{x}') = T_i D\vec{x}$. Composing $T_i$ with $D$ yields

$$T_i D = \begin{bmatrix} R_i & \vec{d}_i \\ 0 & 1 \end{bmatrix} \begin{bmatrix} I_{3\times 3} & -\vec{s} \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} R_i & -R_i \vec{s} + \vec{d}_i \\ 0 & 1 \end{bmatrix}. \tag{A4}$$

Thus, rotations may "bleed" into translations and the magnitude of this effect is proportional to how far the coordinate origin is from the center of the head.