APPENDIX A
GRADIENTS OF RESIDUAL FUNCTIONS FOR AC POWER FLOW CONSTRAINTS

In this section, we derive the gradients of residual functions corresponding to the AC power flow constraints, which are used to construct the gradient guidance terms within the diffusion sampling procedure described in Sec. IV. Specifically, we focus on the equality constraints imposed by nodal active and reactive power balance constraints. Analogous guidance terms for inequality constraints such as generator output limits, voltage limits, and line thermal ratings can be easily derived. In this regard, we first consider the active power balance constraint at bus $b \in \mathcal{B}$:

$$\mathcal{H}_b^p(\mathbf{p}, \mathbf{q}, \mathbf{v}, \boldsymbol{\theta}) = p_b - \sum_{l \in \mathcal{L}: i=b} f_{l,i\to j}^p - \sum_{l \in \mathcal{L}: j=b} f_{l,j\to i}^p, \quad \forall b \in \mathcal{B}. \tag{A.1}$$

where

$$f_{l,i\to j}^p = v_i v_j \big[g_l \cos(\theta_i - \theta_j) + b_l \sin(\theta_i - \theta_j) \big]. \tag{A.2}$$

Similarly, the reactive power balance constraint at bus b is given by

$$\mathcal{H}_b^q(\mathbf{p}, \mathbf{q}, \mathbf{v}, \boldsymbol{\theta}) = q_b - \sum_{l \in \mathcal{L}: i=b} f_{l,i\to j}^q - \sum_{l \in \mathcal{L}: j=b} f_{l,j\to i}^q, \quad \forall b \in \mathcal{B}. \tag{A.3}$$

where

$$f_{l,i\to j}^q = v_i v_j \big[g_l \sin(\theta_i - \theta_j) - b_l \cos(\theta_i - \theta_j) \big]. \tag{A.4}$$

Now, we define the residual functions for the active power balance and reactive power balance constraints at bus $b \in \mathcal{B}$, respectively:

$$\mathcal{R}_b^p(\mathbf{p}, \mathbf{q}, \mathbf{v}, \boldsymbol{\theta}) = \|\mathcal{H}_b^p(\mathbf{p}, \mathbf{q}, \mathbf{v}, \boldsymbol{\theta})\|_2^2 = \left\| p_b - \sum_{l \in \mathcal{L}: i=b} f_{l,i\to j}^p - \sum_{l \in \mathcal{L}: j=b} f_{l,j\to i}^p \right\|_2^2, \quad \forall b \in \mathcal{B}. \tag{A.5}$$

$$\mathcal{R}_b^q(\mathbf{p}, \mathbf{q}, \mathbf{v}, \boldsymbol{\theta}) = \|\mathcal{H}_b^q(\mathbf{p}, \mathbf{q}, \mathbf{v}, \boldsymbol{\theta})\|_2^2 = \left\| q_b - \sum_{l \in \mathcal{L}: i=b} f_{l,i\to j}^q - \sum_{l \in \mathcal{L}: j=b} f_{l,j\to i}^q \right\|_2^2, \quad \forall b \in \mathcal{B}. \tag{A.6}$$

A. *Derivatives of $\mathcal{R}_b^p$*

- With Respect to Active Power Injection $\mathbf{p}$

$$\frac{\partial \mathcal{R}_b^p}{\partial p_b} = \frac{\partial \|\mathcal{H}_b^p\|_2^2}{\partial p_b} = 2\mathcal{H}_b^p \frac{\partial \mathcal{H}_b^p}{\partial p_b}, \quad \forall b \in \mathcal{B}, \tag{A.7}$$

  where

$$\frac{\partial \mathcal{H}_b^p}{\partial p_b} = 1, \quad \forall b \in \mathcal{B}. \tag{A.8}$$

  Therefore, we have

$$\frac{\partial \mathcal{R}_b^p}{\partial p_b} = \frac{\partial \|\mathcal{H}_b^p\|_2^2}{\partial p_b} = 2\mathcal{H}_b^p, \quad \forall b \in \mathcal{B}. \tag{A.9}$$

- With Respect to Reactive Power Injection $\mathbf{q}$

$$\frac{\partial \mathcal{R}_b^p}{\partial q_b} = 0, \quad \forall b \in \mathcal{B}. \tag{A.10}$$

- With Respect to Voltage Magnitude $\mathbf{v}$

$$\frac{\partial \mathcal{R}_b^p}{\partial v_b} = \frac{\partial \|\mathcal{H}_b^p\|_2^2}{\partial v_b} = 2\mathcal{H}_b^p \frac{\partial \mathcal{H}_b^p}{\partial v_b}, \tag{A.11}$$

  where

$$\frac{\partial \mathcal{H}_b^p}{\partial v_b} = -\sum_{l \in L} \left(\frac{\partial f_{l,i\to j}^p}{\partial v_b} + \frac{\partial f_{l,j\to i}^p}{\partial v_b} \right). \tag{A.12}$$

  The derivatives of the active power flow components with respect to the voltages magnitude are given by:

$$\frac{\partial f_{l,i\to j}^p}{\partial v_b} = \begin{cases} -v_j \left(g_l \cos(\theta_b - \theta_j) + b_l \sin(\theta_b - \theta_j) \right), & \text{if } b = i \\ -v_i \left(g_l \cos(\theta_i - \theta_b) + b_l \sin(\theta_i - \theta_b) \right), & \text{if } b = j \\ 0, & \text{o.w.} \end{cases} \tag{A.13}$$

$$\frac{\partial f^p_{l,j\to i}}{\partial v_b} = \begin{cases} -v_j\left(g_l\cos(\theta_j-\theta_b)+b_l\sin(\theta_j-\theta_b)\right), & \text{if } b=i \\ -v_i\left(g_l\cos(\theta_b-\theta_i)+b_l\sin(\theta_b-\theta_i)\right), & \text{if } b=j \\ 0, & \text{o.w.} \end{cases} \tag{A.14}$$

- Derivative with Respect to Voltage Angle $\boldsymbol{\theta}$

$$\frac{\partial \mathcal{R}^p_b}{\partial \theta_b} = \frac{\partial \|\mathcal{H}^p_b\|_2^2}{\partial \theta_b} = 2\mathcal{H}^p_b \frac{\partial \mathcal{H}^p_b}{\partial \theta_b}, \tag{A.15}$$

where

$$\frac{\partial \mathcal{H}^p_b}{\partial \theta_b} = -\sum_{l\in L}\left(\frac{\partial f^p_{l,i\to j}}{\partial \theta_b} + \frac{\partial f^p_{l,j\to i}}{\partial \theta_b}\right). \tag{A.16}$$

The derivatives of the active power flow components with respect to the voltages angle are given by:

$$\frac{\partial f^p_{l,i\to j}}{\partial \theta_b} = \begin{cases} v_b v_j\left(g_l\sin(\theta_b-\theta_j)-b_l\cos(\theta_b-\theta_j)\right), & \text{if } b=i \\ -v_i v_b\left(g_l\sin(\theta_i-\theta_b)-b_l\cos(\theta_i-\theta_b)\right), & \text{if } b=j \\ 0, & \text{o.w.} \end{cases} \tag{A.17}$$

$$\frac{\partial f^p_{l,j\to i}}{\partial \theta_b} = \begin{cases} -v_j v_b\left(g_l\sin(\theta_j-\theta_b)-b_l\cos(\theta_j-\theta_b)\right), & \text{if } b=i \\ v_b v_i\left(g_l\sin(\theta_b-\theta_i)-b_l\cos(\theta_b-\theta_i)\right), & \text{if } b=j \\ 0, & \text{o.w.} \end{cases} \tag{A.18}$$

To obtain the full gradient of $\mathcal{R}^p_b$ with respect to the input vector $\mathbf{x} = (\mathbf{p}, \mathbf{q}, \mathbf{v}, \boldsymbol{\theta})$, we stack the partial derivatives with respect to each component:

$$\nabla_{\mathbf{x}}\mathcal{R}^p_b = \begin{bmatrix} \nabla_{\mathbf{p}}\mathcal{R}^p_b \\ \nabla_{\mathbf{q}}\mathcal{R}^p_b \\ \nabla_{\mathbf{v}}\mathcal{R}^p_b \\ \nabla_{\boldsymbol{\theta}}\mathcal{R}^p_b \end{bmatrix} = \begin{bmatrix} \frac{\partial \mathcal{R}^p_b}{\partial \mathbf{p}} \\ \frac{\partial \mathcal{R}^p_b}{\partial \mathbf{q}} \\ \frac{\partial \mathcal{R}^p_b}{\partial \mathbf{v}} \\ \frac{\partial \mathcal{R}^p_b}{\partial \boldsymbol{\theta}} \end{bmatrix} \in \mathbb{R}^{4B}. \tag{A.19}$$

B. Derivatives of $\mathcal{R}^q_b$

- With Respect to Active Power Injection $\mathbf{p}$

$$\frac{\partial \mathcal{R}^q_b}{\partial p_b} = 0, \quad \forall b \in \mathcal{B}. \tag{A.20}$$

- With Respect to Reactive Power Injection $\mathbf{q}$

$$\frac{\partial \mathcal{R}^q_b}{\partial q_b} = \frac{\partial \|\mathcal{H}^q_b\|_2^2}{\partial q_b} = 2\mathcal{H}^q_b \frac{\partial \mathcal{H}^q_b}{\partial q_b}, \quad \forall b \in \mathcal{B}, \tag{A.21}$$

where

$$\frac{\partial \mathcal{H}^q_b}{\partial q_b} = 1, \quad \forall b \in \mathcal{B}. \tag{A.22}$$

Therefore, we have

$$\frac{\partial \mathcal{R}^q_b}{\partial q_b} = \frac{\partial \|\mathcal{H}^q_b\|_2^2}{\partial q_b} = 2\mathcal{H}^q_b, \quad \forall b \in \mathcal{B}. \tag{A.23}$$

- With Respect to Voltage Magnitude $\mathbf{v}$

$$\frac{\partial \mathcal{R}^q_b}{\partial v_b} = \frac{\partial \|\mathcal{H}^q_b\|_2^2}{\partial v_b} = 2\mathcal{H}^q_b \frac{\partial \mathcal{H}^q_b}{\partial v_b}, \tag{A.24}$$

where

$$\frac{\partial \mathcal{H}^q_b}{\partial v_b} = -\sum_{l\in L}\left(\frac{\partial f^q_{l,i\to j}}{\partial v_b} + \frac{\partial f^q_{l,j\to i}}{\partial v_b}\right). \tag{A.25}$$

The derivatives of the reactive power flow components with respect to the voltages magnitude are given by:

$$\frac{\partial f^q_{l,i\to j}}{\partial v_b} = \begin{cases} v_j\left(b_l\cos(\theta_b-\theta_j)-g_l\sin(\theta_b-\theta_j)\right), & \text{if } b=i \\ v_i\left(b_l\cos(\theta_i-\theta_b)-g_l\sin(\theta_i-\theta_b)\right), & \text{if } b=j \\ 0, & \text{o.w.} \end{cases} \tag{A.26}$$

$$\frac{\partial f^q_{l,j\to i}}{\partial v_b} = \begin{cases} v_j\left(b_l\cos(\theta_j-\theta_b)-g_l\sin(\theta_j-\theta_b)\right), & \text{if } b=i \\ v_i\left(b_l\cos(\theta_b-\theta_i)-g_l\sin(\theta_b-\theta_i)\right), & \text{if } b=j \\ 0, & \text{o.w.} \end{cases} \tag{A.27}$$

- Derivative with Respect to Voltage Angle $\boldsymbol{\theta}$

$$\frac{\partial \mathcal{R}^q_b}{\partial \theta_b} = \frac{\partial \|\mathcal{H}^q_b\|_2^2}{\partial \theta_b} = 2\mathcal{H}^q_b \frac{\partial \mathcal{H}^q_b}{\partial \theta_b}, \tag{A.28}$$

where

$$\frac{\partial \mathcal{H}^q_b}{\partial \theta_b} = -\sum_{l\in L}\left(\frac{\partial f^q_{l,i\to j}}{\partial \theta_b} + \frac{\partial f^q_{l,j\to i}}{\partial \theta_b}\right). \tag{A.29}$$

The derivatives of the reactive power flow components with respect to the voltages angle are given by:

$$\frac{\partial f^q_{l,i\to j}}{\partial \theta_b} = \begin{cases} -v_b v_j\left(b_l\sin(\theta_b-\theta_j)+g_l\cos(\theta_b-\theta_j)\right), & \text{if } b=i \\ v_i v_b\left(b_l\sin(\theta_i-\theta_b)+g_l\cos(\theta_i-\theta_b)\right), & \text{if } b=j \\ 0, & \text{o.w.} \end{cases} \tag{A.30}$$

$$\frac{\partial f^q_{l,j\to i}}{\partial \theta_b} = \begin{cases} v_j v_b\left(b_l\sin(\theta_j-\theta_b)+g_l\cos(\theta_j-\theta_b)\right), & \text{if } b=i \\ -v_b v_i\left(b_l\sin(\theta_b-\theta_i)+g_l\cos(\theta_b-\theta_i)\right), & \text{if } b=j \\ 0, & \text{o.w.} \end{cases} \tag{A.31}$$

To obtain the full gradient of $\mathcal{R}^q_b$ with respect to the input vector $\mathbf{x} = (\mathbf{p}, \mathbf{q}, \mathbf{v}, \boldsymbol{\theta})$, we stack the partial derivatives with respect to each component:

$$\nabla_{\mathbf{x}}\mathcal{R}^q_b = \begin{bmatrix} \nabla_{\mathbf{p}}\mathcal{R}^q_b \\ \nabla_{\mathbf{q}}\mathcal{R}^q_b \\ \nabla_{\mathbf{v}}\mathcal{R}^q_b \\ \nabla_{\boldsymbol{\theta}}\mathcal{R}^p_b \end{bmatrix} = \begin{bmatrix} \frac{\partial \mathcal{R}^q_b}{\partial \mathbf{p}} \\ \frac{\partial \mathcal{R}^q_b}{\partial \mathbf{q}} \\ \frac{\partial \mathcal{R}^q_b}{\partial \mathbf{v}} \\ \frac{\partial \mathcal{R}^q_b}{\partial \boldsymbol{\theta}} \end{bmatrix} \in \mathbb{R}^{4B}. \tag{A.32}$$