From the DVR solution we have

$$\Psi^{DVR}_{(r)} = \sum_{\alpha=0}^{N-1} A_\alpha^{DVR} \phi_\alpha^{DVR}(r) + \mathcal{R}_0(r) + \mathcal{L}^{DVR} \mathcal{R}_1(r)$$

Then the second order estimate for $\mathcal{L}$ is

$$[\mathcal{L}]^{DVR} = \mathcal{L}^{DVR} - \frac{2}{\det(\mu)} \langle \Psi^{DVR} | H-E | \Psi^{DVR} \rangle$$

The integral

$$\Delta = \langle \Psi^{DVR} | H-E | \Psi^{DVR} \rangle$$

has to be calculated accurately. <u>NOT</u> using quadratures. A tentative to calculate

$$\Delta_q = \sum_{\alpha=0}^{N-1} \Psi^{DVR}_{(x_\alpha)} \left[ (H-E) \Psi^{DVR} \right]_{x_\alpha}$$

<u>fails</u> to produce a converge result.