Blog Entry © Tuesday, October 29, 2024, by James Pate Williams, Jr. Quantum Mechanical Perturbation Calculation

Reference: Microsoft PowerPoint - Lesson 23 Perturbation theory.pptx

The unperturbed Hamiltonian operator is:

$$H_0 = -\frac{1}{\pi^2}\frac{d^2}{d\xi^2}$$

The perturbation is as follows:

$$H_p = f\left(\xi - \frac{1}{2}\right)$$

The Schrödinger equation is shown next:

$$H_0\psi = -\frac{1}{\pi^2}\frac{d^2\psi_0}{d\xi^2} = E\psi$$

$$\frac{d^2\psi_0}{d\xi^2} + \pi^2 E\psi_0 = 0$$

$$\psi_0(\xi) = A\sin\left(\pi\sqrt{E}\xi\right)$$

$$\frac{d\psi_0}{d\xi} = A\pi\sqrt{E}\cos\left(\pi\sqrt{E}\xi\right)$$

$$\frac{d^2\psi_0}{d\xi^2} = -A\pi^2 E\sin\left(\pi\sqrt{E}\xi\right)$$

$$\psi_0(0) = 0$$

$$\psi_0(1) = 0 \rightarrow \sqrt{E} = n$$

$$\int_0^1 \psi_0(\xi)\psi_0(\xi)d\xi = A^2\int_0^1 [\sin(n\pi\xi)]^2 d\xi = 1$$

$$e^{in\pi\xi} = \cos(n\pi\xi) + i\sin(n\pi\xi)$$

$$e^{-in\pi\xi} = \cos(n\pi\xi) - i\sin(n\pi\xi)$$

$$\sin(n\pi\xi) = \frac{e^{in\pi\xi} - e^{-in\pi\xi}}{2i}$$

$$[\sin(n\pi\xi)]^2 = -\frac{e^{2in\pi\xi} + e^{-2in\pi\xi} - 2}{4}$$

$$A^2\int_0^1[\sin(n\pi\xi)]^2d\xi=-\frac{A^2}{8n\pi}\left(e^{2in\pi}-1\right)+\frac{A^2}{8n\pi}\left(e^{-2in\pi}-1\right)+\frac{2A^2}{4}$$

$$=-\frac{A^2}{8n\pi}\left(e^{2in\pi}-e^{-2in\pi}\right)+\frac{A^2}{2}=-\frac{2i}{8n\pi}\sin(2n\pi)+\frac{A^2}{2}$$

$$e^{2in\pi}-e^{-2in\pi}=2i\sin(2n\pi)$$

$$\sin(2n\pi)=0\forall n\in\{0,1,2,\dots\}$$

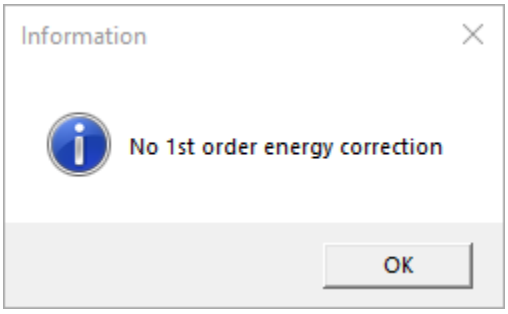
$$A^2=2$$

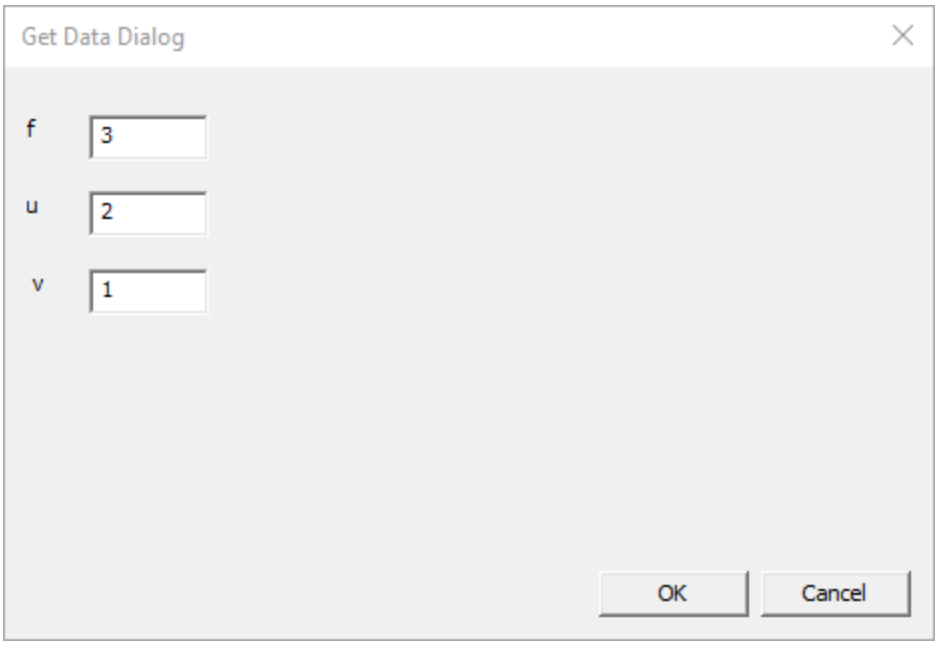
$$A=\sqrt{2}$$

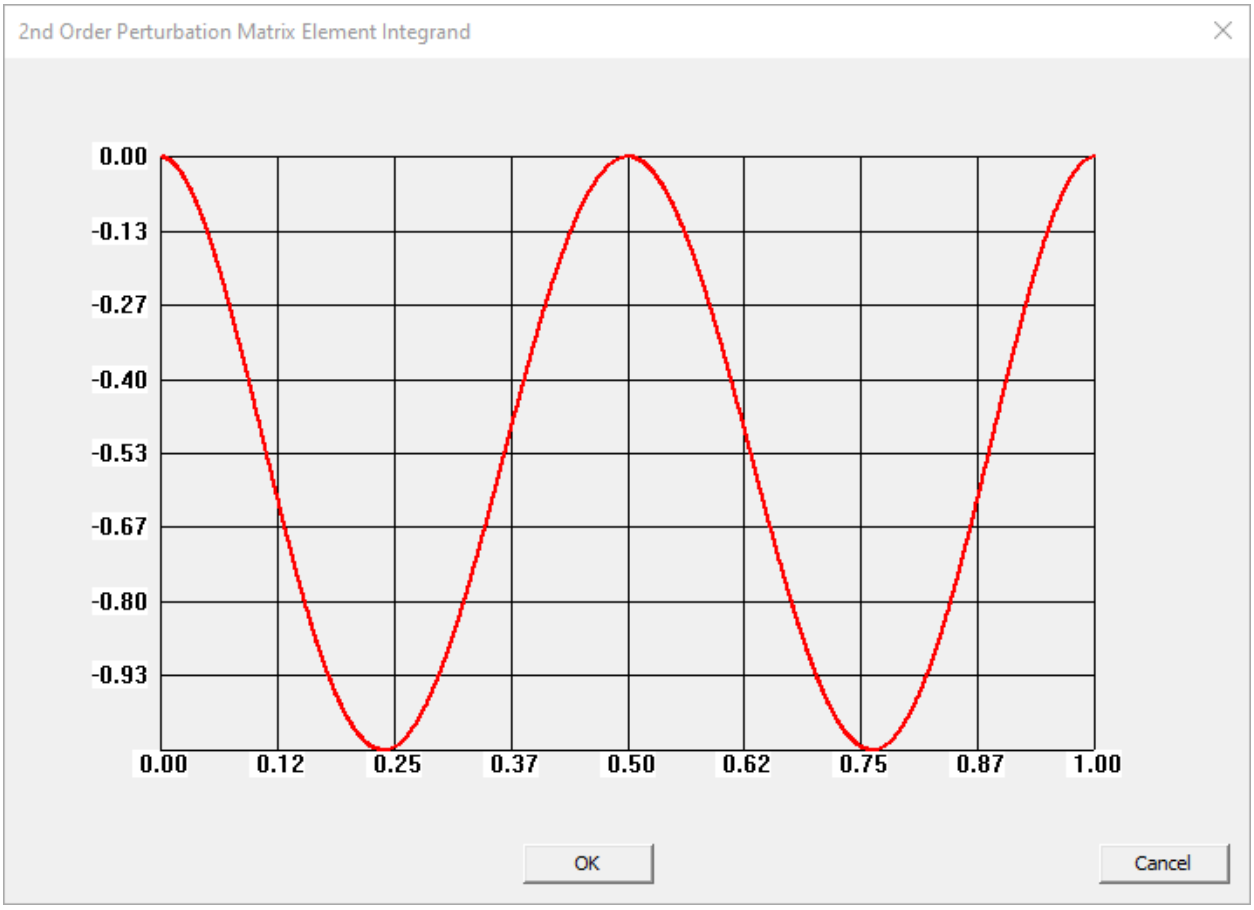
$$\psi_0(\xi)=\sqrt{2}\sin(n\pi\xi)$$

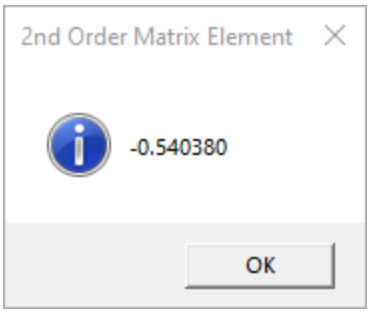
$$\langle\psi_0(\xi)|H_p|\psi_0(\xi)\rangle=f\int_0^1\psi_0(\xi)\left(\xi-\frac{1}{2}\right)\psi_0(\xi)d\xi=2f\int_0^1\sin(m\pi\xi)\left(\xi-\frac{1}{2}\right)\sin(n\pi\xi)\,d\xi$$

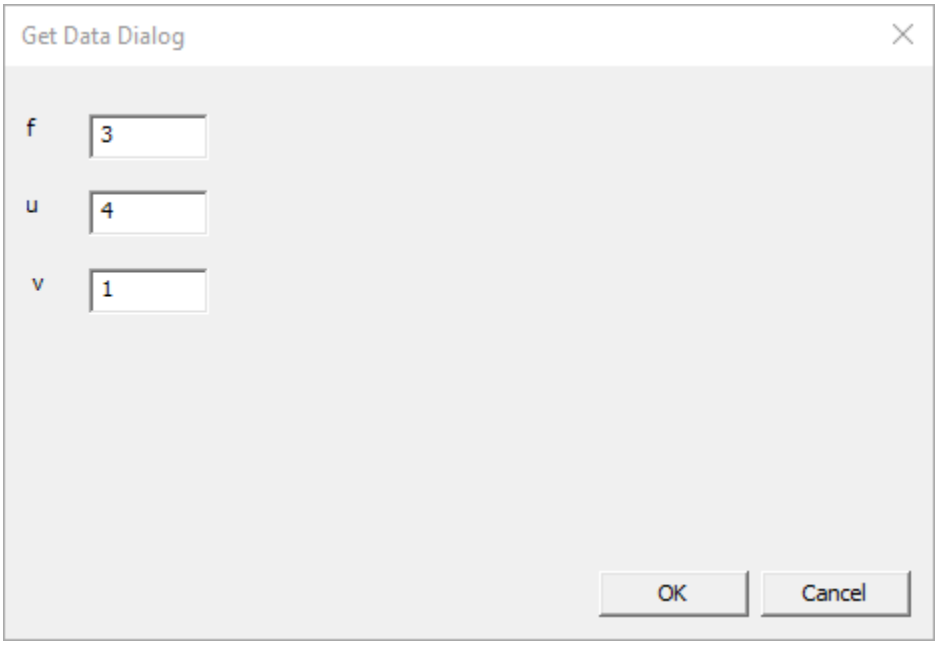
I wrote a little C++ Win32 program to graph the first and second order perturbation results. The integrals are zero for m = n and m or n must be even and the other odd.

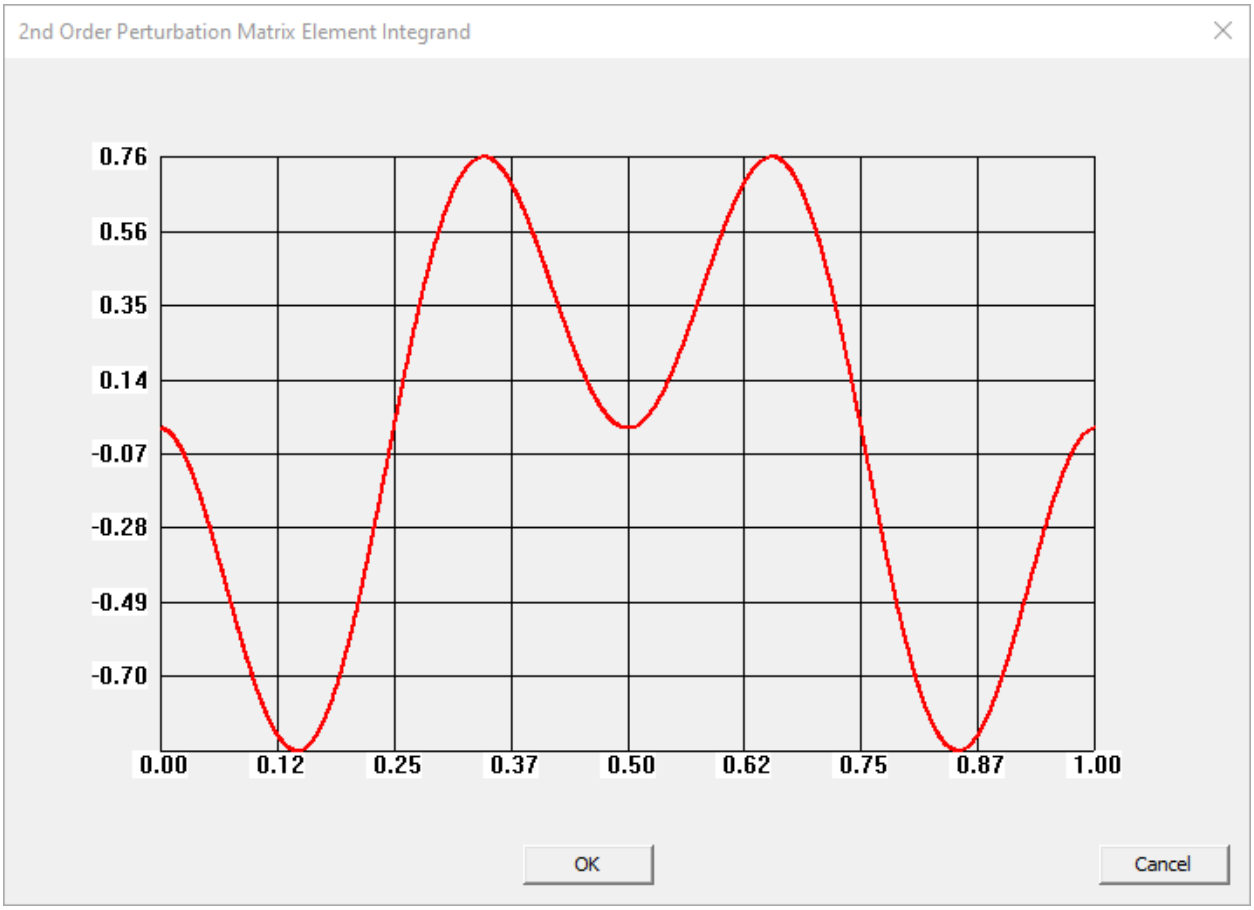


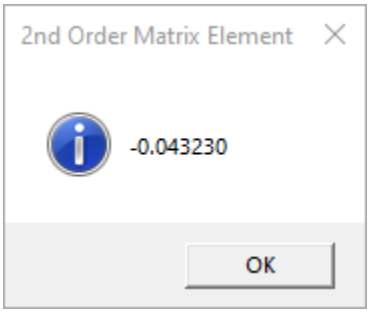

Get Data Dialog
f
3
u
2
v
1
OK
Cancel

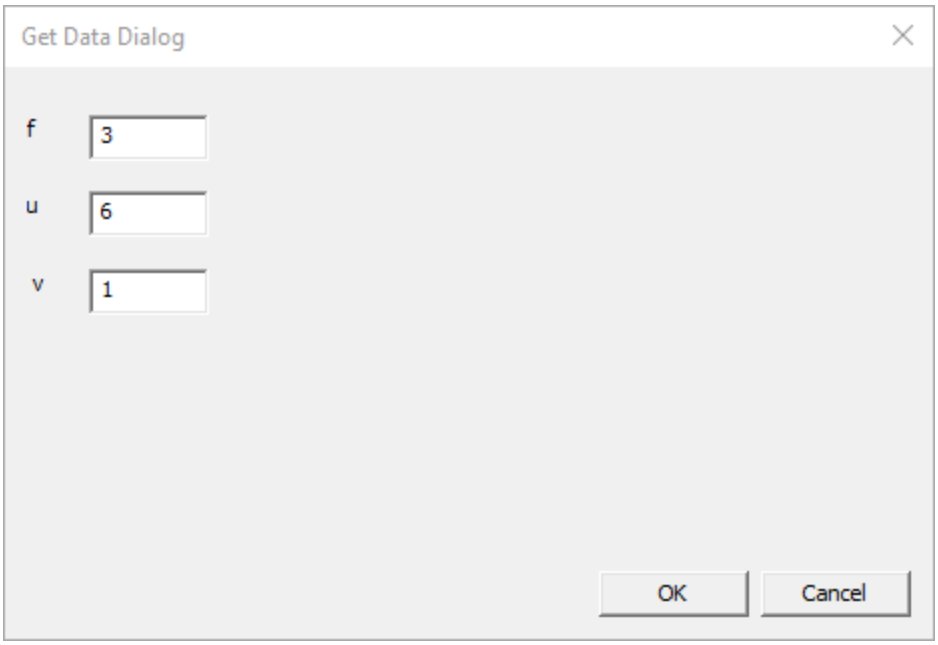

2nd Order Perturbation Matrix Element Integrand
0.00
-0.13
-0.27
-0.40
-0.53
-0.67
-0.80
-0.93
0.00
0.12
0.25
0.37
0.50
0.62
0.75
0.87
1.00
OK
Cancel

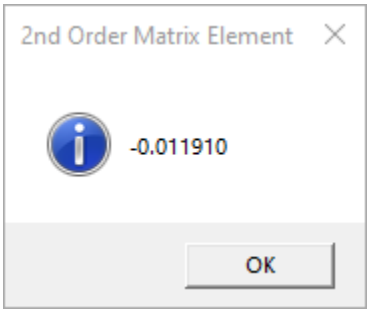

2nd Order Matrix Element
-0.540380
OK

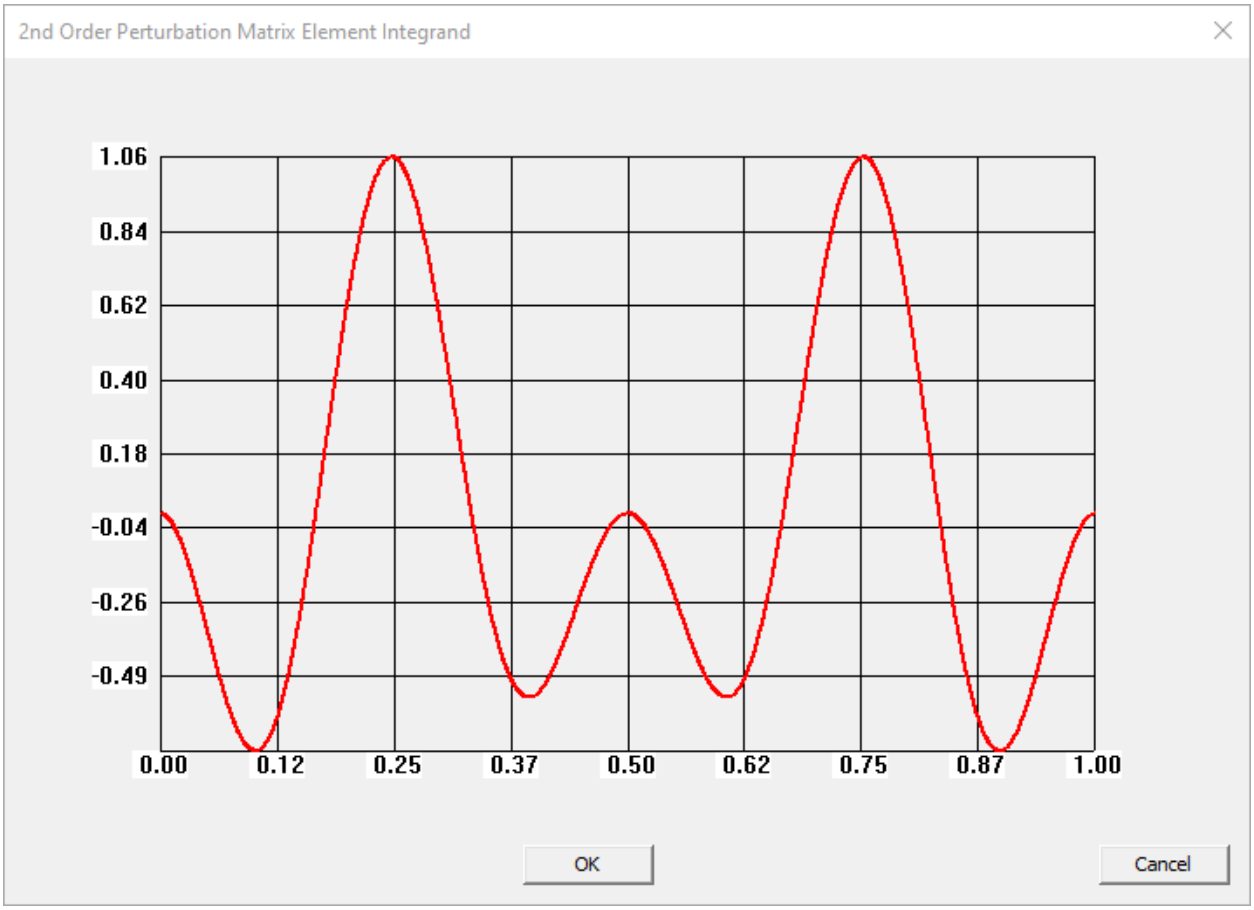

Get Data Dialog
f
3
u
4
v
1
OK
Cancel

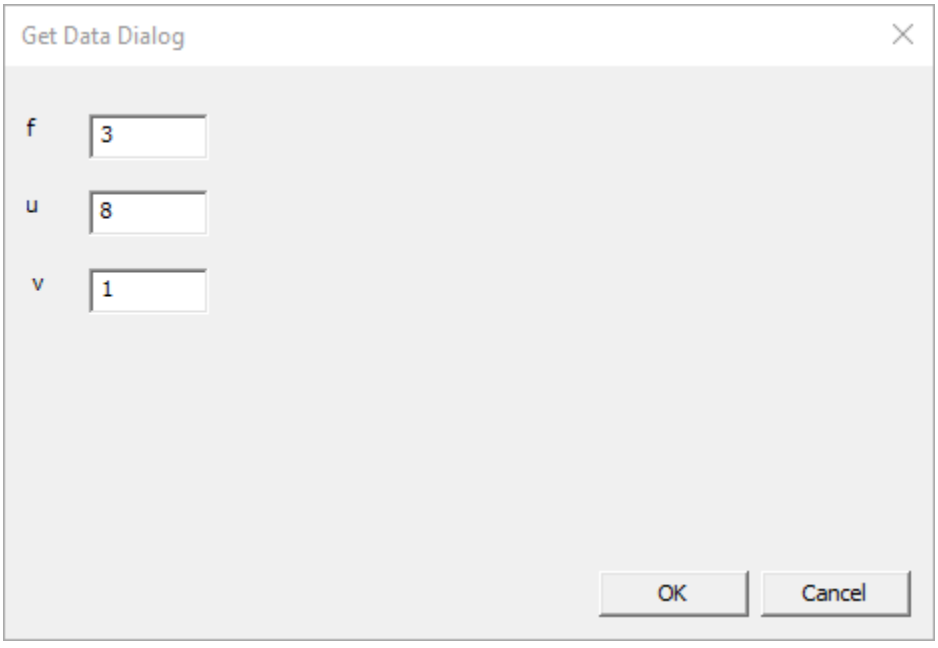

2nd Order Perturbation Matrix Element Integrand
0.76
0.56
0.35
0.14
-0.07
-0.28
-0.49
-0.70
0.00
0.12
0.25
0.37
0.50
0.62
0.75
0.87
1.00
OK
Cancel

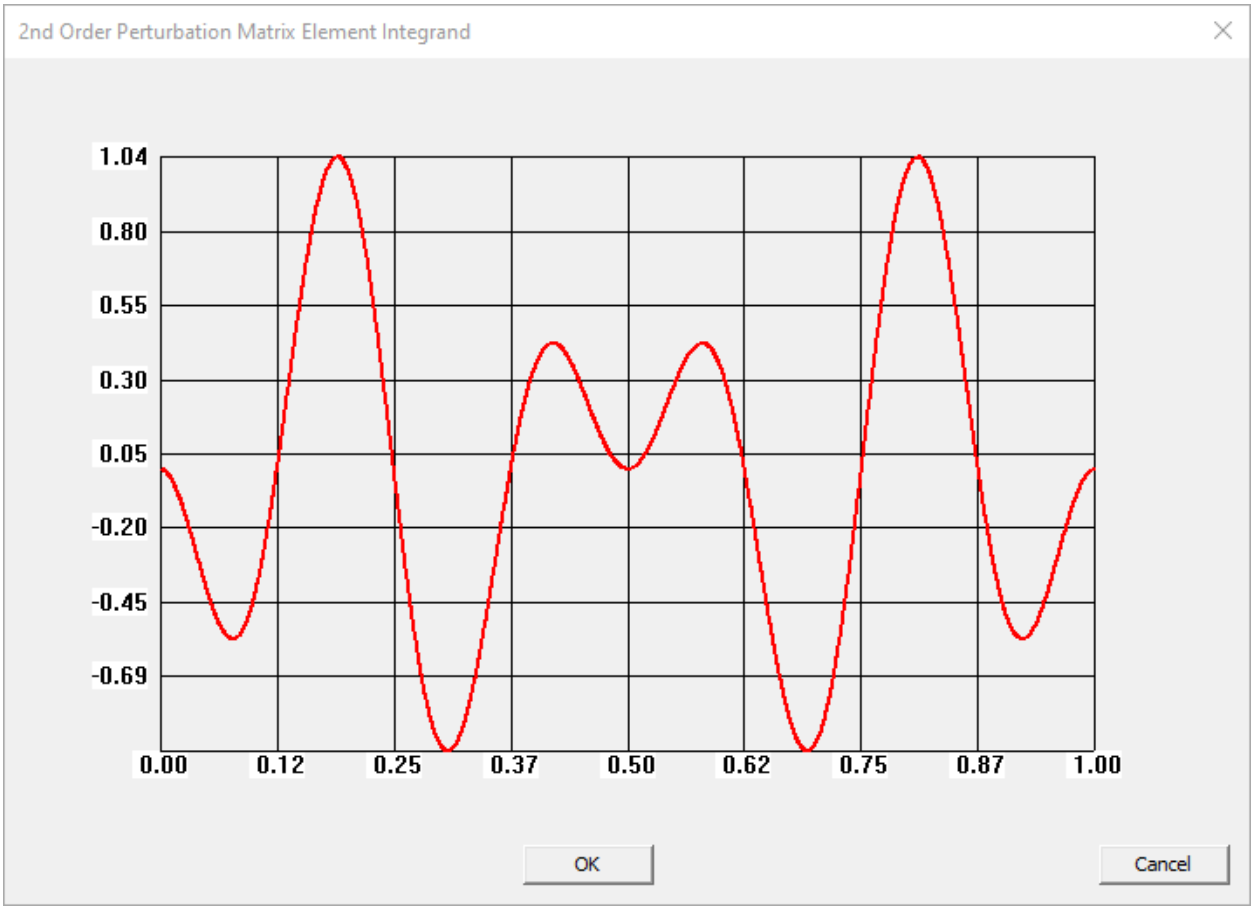

2nd Order Matrix Element
-0.043230
OK

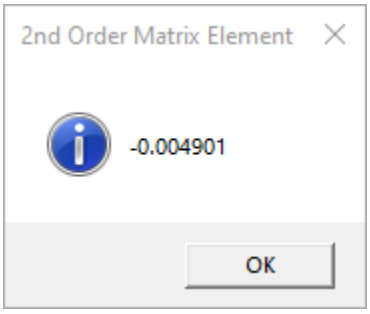

Get Data Dialog
f
3
u
6
v
1
OK
Cancel


2nd Order Matrix Element
-0.011910
OK


2nd Order Perturbation Matrix Element Integrand
1.06
0.84
0.62
0.40
0.18
-0.04
-0.26
-0.49
0.00
0.12
0.25
0.37
0.50
0.62
0.75
0.87
1.00
OK
Cancel


Get Data Dialog
f
3
u
8
v
1
OK
Cancel


2nd Order Perturbation Matrix Element Integrand
1.04
0.80
0.55
0.30
0.05
-0.20
-0.45
-0.69
0.00
0.12
0.25
0.37
0.50
0.62
0.75
0.87
1.00
OK
Cancel


2nd Order Matrix Element
-0.004901
OK