Code_Aster

Version default

Titre : ZZZZ399 – Fréquences d'un oscillateur harmonique q[...]
Responsable : ABBAS Mickaël

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ZZZZ399 – Frequencies of a quantum harmonic oscillator to a dimension

Summary:

The objective of this test is of to calculate the frequencies of a quantum harmonic oscillator[1] with a dimension, for the stationary solution.

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1 http://fr.wikipedia.org/wiki/Oscillateur_harmonique_quantique

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1 Problem of reference

1.1 Geometry

The problem, while being unidimensional, is modelled in two dimensions (there is not currently a modeling 1D for thermics in Code_Aster).
For reasons of setting in scale, one uses the System of atomic units[2].
A band length is considered $L=10,0\,a_0$ and thickness $L/100\,a_0$, centered at the origin of the axes, to represent space.

A particle charged (in this case, an electron), subjected to a potential, can assume only specific values of energy, which one can obtain by resolution of the equation of Schroedinger:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_n(x)+\frac{1}{2}kx^2\psi_n(x)=E_n\psi_n(x)$$
$$n=0,1,\cdots$$
$$\omega=\sqrt{\frac{k}{m}}$$

It is about a problem to the clean functions[3]: the values should be found E_n (autovaleurs).
The equation is of standard diffusion (in analogy with the calculation of thermal balance), the resolution of the clean functions will be made by a modal calculation.

1.2 Materials

The test uses two materials: for the resolution of the equation of diffusion ($\lambda=1,\rho_{cp}=1$) and the other to affect the potential, with ρ_{cp} variable according to a value of a field, calculated with the formula of the potential.

1.3 Boundary conditions

One imposes zero value at the ends of the field. There does not need really this condition, which is put to also test this setting in data but which perhaps removed without modifications.

1.4 Initial conditions

Nothing.

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2 http://fr.wikipedia.org/wiki/Syst%C3%A8me_d%27unit%C3%A9s_atomiques
3 http://fr.wikipedia.org/wiki/Fonction_propre

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2   Reference solution

An exact solution is known for this problem:

$$E_n = \left(n + \frac{1}{2}\right) \hbar \omega \tag{1}$$

2.1   Bibliographical references

[1]   ATKINS P.W. Molecular Mechanics Quantum

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3 Modeling A

3.1 Characteristics of modeling

A modeling is used PLAN.

3.2 Characteristics of the grid

The grid contains 212 elements of the type TRIA8.

3.3 Sizes tested and results

One tests the values of energy calculated from " frequencies " obtained by modal calculation, compared to the exact solution.

Place	Type of reference	VALE_REFE	Précision
Difference between analytical solution (1) and calculation	'ANALYTICAL'	0	5.0E-4

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4   Summary of the results

Here a visualization of the real part of the clean functions calculated. One notices an alternation of symmetrical and antisymmetric functions, typical of the solution of this problem.