A NUMERICAL SOLUTION SCHEME OF THE KLEIN-GORDON EQUATION BY THE FINITE ELEMENT METHOD

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(Communicated by F. C. Auluck, F. N. A.)

(*Received 10 September 1973; after revision January 1974*)

A finite element solution scheme of Klein-Gordon equation is obtained by first getting the equivalent variational integral of the problem and then discretized by the methods used for discrete element (finite element) analysis.

INTRODUCTION

Recently, the finite element methods are used for the analysis of problems in structures, elastoplastic bodies, heat conduction, hydrodynamics and other areas of continuum mechanics (cf. Zienkiewicz 1971). Hitherto, the difference equation methods were applied for the discretization of the differential equations, however this method is not suitable for the numerical analysis of practical technical problems in the case of arbitrarily shaped boundaries. On the other hand, the finite element methods are preferable in the case of complex boundaries, so that this method are now widely applied to the numerical calculation of various differential equations (cf. Aguirre-Ramirez *et al.* 1970). The problems of applied physics can be specified in two ways (cf. Crandall 1956). In the first differential equations governing the behaviour of a typical, infinitesimal, region are given. In the second a variational (extremum) principle valid over the whole region is postulated and then applied finite element method. It seems that the finite element techniques can also be used effectively for the solution of quantum mechanical problem. In this paper, we are concerned with Klein-Gordon equation and formulate the equivalent variational principle and then apply finite element method. The object of this paper is to formulate the numerical solution scheme for the Klein-Gordon equation. We also formulate the discrete equivalent of Hamiltonian density in terms of finite elements.

Variational Formulation

In quantum mechanics, a charged scalar meson having rest mass m_0 may be described by the field component ψ satisfying the Klein-Gordon equation (cf. Morse and Feshback 1953)

$$\nabla^2 \psi - \frac{1}{c^2} \frac{\partial^2 \psi}{\partial t^2} = \frac{m_0^2 c^2}{\hbar^2} \psi \tag{1}$$

where the wave function ψ is a complex quantity, so that its real and imaginary parts can be considered as independent variables, or what is same thing, ψ and its complex conjugate $\bar{\psi}$ can be considered as seperate field variables, which can be varied independently. The product $\psi \bar{\psi}$ is real and will be equal to the probability density. c is the velocity of the particle and $\hbar$ the Planck's constant.

We seek a restatement of eqn. (1) in the form of variational (extremum) principle and then to make an attempt for numerical solution by finite element method.

The variational principle for (1) is given by

$$I = \int_R L \, d \, R \tag{2}$$

where L is the Lagrangian density function defined by

$$L = -\frac{\hbar^2}{2m_0} (\text{grad } \bar{\psi}) (\text{grad } \psi) + \frac{\hbar^2}{2m_0 c^2} \dot{\bar{\psi}} \dot{\psi} - \frac{m_0 c^2}{2} \bar{\psi} \psi. \tag{3}$$

Here the dot donotes the differentiation with respect to t. The function L depends upon both ψ and $\bar{\psi}$ and varied independently until I is a minimum.

Finite Element method of Solution

Since the wave function ψ is complex and hence defined as

$$\psi (\bar{X}, t) = u (\bar{X}, t) + i \, v (\bar{X}, t)$$

where

$$\bar{X} = (x, y, z), \; i = \sqrt{-1}. \tag{4}$$

Then the complex conjugate of ψ is defined as

$$\bar{\psi} (\bar{X}, t) = u (\bar{X}, t) - i \, v (\bar{X}, t). \tag{5}$$

Now the product $\psi \bar{\psi}$ represent the configuration of the system specified by the co-ordinates $\bar{X}$.

Let us consider a typical finite element (e) and approximate the real and imaginary parts of $\psi (\bar{X}, t)$ locally by

$$\left.\begin{aligned} u^{(e)} (\bar{X}, t) &= \phi_N (\bar{X}) \, u^N_{(e)} \\ v^{(e)} (\bar{X}, t) &= \phi_N (\bar{X}) \, v^N_{(e)} \end{aligned}\right\} \tag{6}$$

where $u^N_{(e)}$ and $v^N_{(e)}$ are time-dependent nodal values of $u\ (\bar{X}, t)$ and $v\ (\bar{X}, t)$ respectively and $\phi_N\ (\bar{X})$ is the local interpolation function of $\bar{X}$. Therefore,

$$\left.\begin{aligned} \psi^{(e)}\ (\bar{X}, t) &= \psi^N_{(e)}\ \phi^{(e)}_N\ (\bar{X}) \\ \bar{\psi}^{(e)}\ (\bar{X}, t) &= \bar{\psi}^N_{(e)}\ \phi^{(e)}_N\ (\bar{X}) \end{aligned}\right\} \tag{7}$$

where

$$\left.\begin{aligned} \psi^N_{(e)} &= u^N_{(e)} + i\, v^N_{(e)} \\ \bar{\psi}^N_{(e)} &= u^N_{(e)} - i\, v^N_{(e)}. \end{aligned}\right\} \tag{8}$$

Now for a typical element (e) eqn. (3) becomes

$$L^{(e)} = -\frac{h^2}{2m_0}\ (\text{grad}\ \bar{\psi}^{(e)})\ (\text{grad}\ \psi^{(e)}) + \\ + \frac{h^2}{2m_0c^2}\ \dot{\bar{\psi}}^{(e)}\ \dot{\psi}^{(e)} - \frac{m_0c^2}{2}\ \bar{\psi}^{(e)}\ \psi^{(e)}. \tag{9}$$

Substituting (7) in (9), we have

$$L^{(e)} = -\frac{h^2}{2m_0}\ (\bar{\psi}^M_{(e)}\ \phi^{(e)}_{M,i})\ (\psi^N_{(e)}\ \phi^{(e)}_{N,i}) + \\ + \frac{h^2}{2m_0c^2}\ (\dot{\bar{\psi}}^M_{(e)}\ \phi^{(e)}_M)\ (\dot{\psi}^N_{(e)}\ \phi^{(e)}_N) - \\ - \frac{m_0c^2}{2}\ (\bar{\psi}^M_{(e)}\ \phi^{(e)}_M)\ (\psi^N_{(e)}\ \phi^{(e)}_N). \tag{10}$$

Thus, for a typical element

$$I^{(e)} = \int_{R^{(e)}} L^{(e)}\ dR^{(e)}. \tag{11}$$

Substituting (10) in (11), we have

$$I^{(e)} = -\frac{h^2}{2m_0}\ a^{(e)}_{MNi}\ \bar{\psi}^M_{(e)}\ \psi^N_{(e)} + \frac{h^2}{2m_0c^2}\ b^{(e)}_{MN} \\ \dot{\bar{\psi}}^M_{(e)}\ \dot{\psi}^N_{(e)} - \frac{m_0c^2}{2}\ b^{(e)}_{MN}\ \bar{\psi}^M_{(e)}\ \psi^N_{(e)} \tag{12}$$

where

$$a^{(e)}_{MNi} = \int_{R^{(e)}} \phi^{(e)}_{M,i}\ \phi^{(e)}_{N,i}\ dR^{(e)} \tag{13}$$

$$b^{(e)}_{MN} = \int_{R^{(e)}} \phi^{(e)}_M\ \phi^{(e)}_N\ dR^{(e)}. \tag{14}$$

For a local minimum $I^{(e)}$, condition is

$$\delta I^{(e)} = 0$$

or,

$$\frac{\partial I^{(e)}}{\partial \psi^N_{(e)}}\ \delta \psi^N_{(e)} = 0 \tag{15}$$

and

$$\frac{\partial I^{(e)}}{\partial \bar{\psi}^N_{(e)}} \delta \bar{\psi}^N_{(e)} = 0. \tag{16}$$

Substituting (12) in (15)–(16) we arrive at a pair of equations

$$\frac{h^2}{2m_0} a^{(e)}_{MNi} \bar{\psi}^M_{(e)} + \frac{m_0 c^2}{2} b^{(e)}_{MN} \bar{\psi}^M_{(e)} = 0 \tag{17}$$

$$\frac{h^2}{2m_0} a^{(e)}_{MNi} \psi^M_{(e)} + \frac{m_0 c^2}{2} b^{(e)}_{MN} \psi^M_{(e)} = 0. \tag{18}$$

Upon connecting the elements together (in space and time) and applying approximate boundary and initial conditions, equations (17)—(18) lead to a system of linear equations in $\psi^N_{(e)}$ and $\bar{\psi}^N_{(e)}$ that must be solved simultaneously.

We now formulate the equations for generalized canonical momenta and Hamiltonian density H in terms of finite elements (e). H represents the total energy of the system.

The momenta canonically conjugate to ψ and $\bar{\psi}$ are defined as

$$\pi = \frac{\partial L}{\partial \dot{\psi}} = \frac{h^2}{2m_0 c^2} \dot{\bar{\psi}} \tag{19}$$

and

$$\bar{\pi} = \frac{\partial L}{\partial \dot{\bar{\psi}}} = \frac{h^2}{2m_0 c^2} \dot{\psi}. \tag{20}$$

Then the Hamiltonian density takes the form

$$H = \pi \dot{\psi} + \bar{\pi} \dot{\bar{\psi}} - L. \tag{21}$$

Now applying the previous procedure, we have for a typical finite element, the canonical momenta and Hamiltonian density as

$$\pi^{(e)} = \frac{h^2}{2m_0 c^2} \dot{\bar{\psi}}^M_{(e)} \phi^{(e)}_M \tag{22}$$

and

$$\bar{\pi}^{(e)} = \frac{h^2}{2m_0 c^2} \dot{\bar{\psi}}^N_{(e)} \phi^{(e)}_N. \tag{23}$$

Therefore, substituting (22), (23) and (9) in (21), we have

$$H^{(e)} = \frac{h^2}{2m_0 c^2} \alpha^{(e)}_{MN} \dot{\bar{\psi}}^M_{(e)} \dot{\psi}^N_{(e)} + \frac{h^2}{2m_0} \beta^{(e)}_{MNi} \times$$

$$\times \bar{\psi}^M_{(e)} \psi^N_{(e)} + \frac{m_0 c^2}{2} \alpha^{(e)}_{MN} \bar{\psi}^M_{(e)} \psi^N_{(e)} \tag{24}$$

where

$$\alpha_{MN}^{(e)} = \phi_M^{(e)}\ \phi^{(e)}$$
$$\beta_{MNi}^{(e)} = \phi_{M,}^{(e)}{}_i\ \phi_{N,i}^{(e)} . \tag{25}$$

Thus, eqns. (22) and (23) give the generalized canonical momenta at the node N of the finite element (e) and eqn. (24) represent the discrete equivalent of Hamiltonian density in terms of finite elements.

ACKNOWLEDGEMENT

The author would like to thank Prof. P. C. Jain for suggesting many valuable improvements. Also he takes pleasure in expressing his appreciation and gratitude to the referee for useful comments. Sincere thanks are due to the Council of Scientific and Industrial Research, New Delhi, for financial support.

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