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THE TIME DEPENDENT VARIATIONAL DESCRIPTION OF ONE-DIMENSIONAL INELASTIC SCATTERING

by

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ABSTRACT

The time dependent variational principle is applied to generate semi-classical approximations in the description of inelastic collisions in one-dimension. This is achieved by using appropriately parametrized trial wave functions. The method is applied to an exactly solvable model and the results are fairly good, in general much better than other approximate calculations.

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The time dependent variational principle (TDVP) was introduced by Dirac (1930) but its application to nuclear physics problems is rather recent. One of the methods deriving from it is the time dependent Hartree-Fock (TDHF) method used extensively for describing fission and fusion of nuclei (Negele 1982, Davies et al. 1982). The main disadvantage of the TDHF method is the non existence of a practical way of extracting quantum information from it (besides the large amount of numerical calculations required). Another way of using the TDVP is through the parametrization of the variational wave function. The parametrized wave function should span a collective subspace of a given system and the use of the TDVP obtains classical equations of motion for the chosen parameters (Kramer and Saraceno 1981). This form of the TDVP has the semiclassical character of the TDHF method but at the same time allows the computation of quantities having quantum interpretation and this is its main advantage (it also involves a large amount of numerical calculation). This parametrized TDVP has been successfully applied for describing vibrational and rotational modes in nuclei (Cohen 1984, Kramer 1984). Also it has proved to be a useful tool for describing elastic scattering of light nuclei at low energies (Saraceno 1982) and this stimulated us to trying to extend this method so as to allow for excitations during the collision. In this work we investigate the possibility of using the TDVP for describing inelastic scattering by solving a one-dimensional problem: collision of an excitable system with a potential. By appropriately parametrizing the trial wave function we can calculate transition probabilities.

In section 2 we briefly describe the TDVP using parametrized trial wave function and obtain the classical equations of motion for the parameters. In section 3 we propose a parametrization of the trial function for describing the collision of an excitable system with a particle. The equations of motion for the parameters are obtained and in section 4 they are solved for an exactly solvable system. We make comparisons with the exact results and with the results of other approximation schemes. In section 5 we summarize the conclusions.

2. TDVP AND THE CLASSICAL EQUATIONS OF MOTION

In its usual formulation the TDVP is derived from the action functional

$$S = \int_{t_1}^{t_2} L(\psi,\bar{\psi})\, dt \quad , \tag{2.1}$$

with the Lagrangian given by

$$L(\psi,\bar{\psi}) = \frac{i\hbar}{2}\frac{\langle\psi|\dot{\psi}\rangle - \langle\dot{\psi}|\psi\rangle}{\langle\psi|\psi\rangle} - \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} \quad , \tag{2.2}$$

where H is the Hamiltonian of the system and $|\psi\rangle$ unormalized (but normalizable) wave function (the dot means time derivative).

Imposing stationarity of S with respect to arbitrary variations of $|\psi\rangle$ and $\langle\psi|$ obtains an equation which is the analog of the Schrödinger equation for unormalized

wave function. Approximations in this scheme are naturally obtained by considering restricted variations of $|\psi\rangle$ and $\langle\psi|$. A simple way of doing restricted variations of the wave function is by parametrizing it. Considering a time dependent parametrization of the function, when imposing stationarity of the action S with respect to variations of the parameters will result in Hamilton type equations of motion for the parameters instead of a Schrödinger type equation of motion for $|\psi\rangle$. Of course the particular choice of parameters depends on the problem to be solved and at the present time there is no practical procedure for assessing the suitability of the chosen parameters. At the moment the best way of checking the validity of the approximation resulting from some particular choice of parameters is by enlarging the subspace spanned by the variational function and then recalculate the relevant quantities. If no essential change is observed we can be reasonably sure of the appropriateness of the choice of parameters.

If $z = (z_1, z_2, \ldots, z_r)$ are the chosen parameters and $|z\rangle$ is the trial function that depends only on $\bar{z}$ (complex conjugate of z) the Lagrangian (2.2) can be written as

$$L(z,\bar{z}) = \frac{i\hbar}{2}\sum_{i=1}^{r}\left(\dot{\bar{z}}_i\frac{\partial}{\partial\bar{z}_i} - \dot{z}_i\frac{\partial}{\partial z_i}\right)\ln N - H \quad , \tag{2.4}$$

where

$$N(z,\bar{z}) = \langle z|z\rangle \tag{2.5a}$$

and

$$H(z,\bar{z}) = \frac{\langle z|H|z\rangle}{\langle z|z\rangle} \quad . \tag{2.5b}$$

Imposing stationarity of S with respect to variations of z_i and $\bar{z}_i$ obtains the following equations of motion for the parameters

$$\sum_k i\hbar\, g_{jk}\, \dot{\bar{z}}_k = \frac{\partial H(z,\bar{z})}{\partial z_j} \quad , \tag{2.6a}$$

$$-\sum_k i\hbar\, g_{kj}\, \dot{z}_k = \frac{\partial H(z,\bar{z})}{\partial \bar{z}_j} \quad , \tag{2.6b}$$

where

$$g_{jk} = \frac{\partial^2 \ell n\, N(z,\bar{z})}{\partial z_j\, \partial \bar{z}_k} \quad . \tag{2.7}$$

If g is non-degenerate ($\det g \neq 0$) equations (2.6) can be inverted and Hamilton type equations of motion are obtained for $\bar{z}_i$ and z_i

$$i\hbar\, \dot{\bar{z}}_i = \sum_j (g^{-1})_{ij}\, \frac{\partial H(z,\bar{z})}{\partial z_j} \quad \text{and c.c.} \quad . \tag{2.8}$$

Defining the simpletic structure (or generalized Poisson brackets) of functions $F(z,\bar{z})$ and $G(z,\bar{z})$ as

$$\{F,G\} = \sum_{ij} \left\{ \frac{\partial F}{\partial \bar{z}_i} (g^{-1})_{ij} \frac{\partial G}{\partial z_j} - \frac{\partial G}{\partial \bar{z}_i} (g^{-1})_{ij} \frac{\partial F}{\partial z_j} \right\} \quad , \tag{2.9}$$

equations (2.8) take the form

$$i\hbar\, \dot{\bar{z}}_k = \{z_k, H\} \quad . \tag{2.10}$$

3. ONE-DIMENSIONAL COLLISION OF A PARTICLE WITH AN EXCITABLE SYSTEM

We shall now apply the method presented in the previous section to the system shown in fig. 3.1: a particle of mass m_1 collides with the system consisting of a particle of mass m_2 submitted to a potential $U(y)$. The interaction between the particles is given by $V(x-y)$.

The Hamiltonian for this problem can be written as

$$H = \frac{K_x^2}{2m_1} + \frac{K_y^2}{2m_2} + U(y) + V(x-y) \quad . \tag{3.1}$$

The first step to use the method described in section 2 is to choose the trial wave function. In the case of elastic scattering the coherent state has proved to be a good choice (Saraceno 1982), so in this case of inelastic collision we propose the following variational function

$$|z,\alpha\rangle_N = \sum_{n=0}^{N} \bar{\alpha}_n(t)\, |z(t),n\rangle \quad , \tag{3.2}$$

where

$$|z(t),n\rangle = e^{\bar{z}b^\dagger} |0\rangle \otimes ||n\rangle \equiv |z\rangle \otimes ||n\rangle \tag{3.3}$$

and

$$z = \sqrt{\frac{m_1}{2}}\left(x - i\frac{K_x}{m_1}\right) ,$$

$$\hat{b} = \sqrt{\frac{m_1}{2}}\left(\hat{x} + i\frac{\hat{K}_x}{m_1}\right) ,$$

$$\hat{a} = \sqrt{\frac{m_2}{2}}\left(\hat{y} + i\frac{\hat{K}_y}{m_2}\right) , \qquad (3.4)$$

$$\hat{a}\,|0\rangle = 0 ,$$

$$\hat{b}\,|0\rangle = 0 .$$

In other words, $\hat{a}^\dagger$ and $\hat{a}$ are the creation and annihilation operators for the system of mass m_2 and $e^{\bar{z}\hat{b}^\dagger}|0\rangle$ is an unormalized gaussian wave packet which describes the motion of the particle m_1 relative to the equilibrium position of m_2.

The number of terms N in (3.2) is suitably chosen so as to have $|\alpha_{N+1}|^2 << |\alpha_N|^2$. The coefficients $\alpha_n(t)$ are the unormalized probability amplitudes of finding the system in the state $|z(t),n\rangle$ (eq. (3.3)) at time t.

The equations of motion for the parameters (namely z and $\alpha_0,\ldots,\alpha_N$) are obtained from equations (2.8). So, the first thing we must do is to calculate the matrix g (2.7). It is easy to see that this matrix is non diagonal so that the parameters are not canonical variables. But in this case canonical variables are obtained by defining the normalized probability amplitudes

$$\beta_n = \frac{\alpha_n}{\sqrt{\sum_{\ell=0}^{N} |\alpha_\ell|^2}} . \qquad (3.5)$$

With this, the Lagrangian (2.4) takes the simple form

$$L = \frac{i\hbar}{2}(\dot{\bar{w}}w - \dot{w}\bar{w}) - H(w,\bar{w}) , \qquad (3.6a)$$

where

$$w = (z,\beta_0,\ldots,\beta_N) ,$$

$$H(w,\bar{w}) = H(z,\bar{z},\alpha(\beta,\bar{\beta}),\bar{\alpha}(\beta,\bar{\beta})) , \qquad (3.6b)$$

and the equations (2.6) turn into

$$i\hbar\,\dot{\bar{w}}_k = \frac{\partial H(w,\bar{w})}{\partial w_k} \quad \text{and} \quad \text{c.c.} . \qquad (3.7)$$

Given potentials $U(y)$ and $V(x-y)$ we can calculate $H(w,\bar{w})$ and solve equations (3.7) for any given initial condition. The transition probabilities will be given by

$$P^{TDVP}_{n_i \to n_f} = \left|\lim_{t\to\infty} \beta_{n_f}(t)\right|^2 , \qquad (3.8)$$

where n_i and n_f are the initial and final states of the system of mass m_2.

It is interesting to note that the same equations may be obtained by using a normalized trial function and taking

only z and $\bar{z}$ as variational parameters. The equations for the other parameters $(\beta_0,\ldots,\beta_N)$ are obtained imposing the time dependent Schrödinger equation to the wave function.

In the next section equations (3.7) will be solved for a simple case which is exactly solvable: the system of mass m_2 is a harmonic oscillator.

4. COLLISION WITH A HARMONIC OSCILLATOR

The model we shall solve using the method developed in the previous section was introduced by Jackson and Mott (1932) for understanding the colinear collision of a diatomic molecule with an atom. The molecule is represented by a harmonic oscillator (see fig. 4.1) and during the collision we disregard the interaction between the atoms that are furthest apart (A and C in fig. 4.1).

The Hamiltonian is given by

$$H = \frac{p_A^2}{2m_A} + \frac{p_B^2}{2m_B} + \frac{p_C^2}{2m_C} + V_{BC}(q_B-q_C) + V_{AB}(q_A-q_B) \quad , \qquad (4.1)$$

with V_{BC} a harmonic oscillator potential of elastic constant k.

Introducing the center of mass coordinate X of the whole system

$$X = \frac{m_A q_A + m_B q_B + m_C q_C}{m_A + m_B + m_C} \quad ,$$

and the relative coordinates $\tilde{x}$ and $\tilde{y}$ (see fig. 4.1)

$$\tilde{x} = q_A - \frac{m_B q_B + m_C q_C}{m_B + m_C} \quad ,$$

$$\tilde{y} = q_B - q_C \quad ,$$

together with their respective canonically conjugate momenta $p_{\tilde{x}}$, $p_{\tilde{y}}$ and P_X, the Hamiltonian (4.1) can be written as

$$H = \frac{P_X^2}{2M} + \frac{p_{\tilde{x}}^2}{2\mu_A} + \frac{p_{\tilde{y}}^2}{2\mu_{BC}} + V_{BC}(\tilde{y}) + V_{AB}(\tilde{x} - \frac{m_C}{m_B + m_C}\tilde{y}) \quad , \qquad (4.2)$$

where

$$M = m_A + m_B + m_C \quad ,$$

$$\mu_A = \frac{m_A(m_B + m_C)}{M} \quad ,$$

$$\mu_{BC} = \frac{m_B m_C}{m_B + m_C} \quad .$$

The harmonic oscillator potential $V_{BC}(\tilde{y})$ is given by

$$V_{BC}(\tilde{y}) = \frac{1}{2} k \, (\tilde{y} - \tilde{y}_{eq})^2 \quad .$$

In order to eliminate the constant $\tilde{y}_{eq}$ we define the relative coordinates x and y by

$$\tilde{y} = \left[\frac{\hbar}{\sqrt{k\mu_{BC}}}\right]^{\frac{1}{2}} y + \tilde{y}_{eq} \quad ,$$

$$\bar{x} = \frac{m_C}{m_B + m_C}\left[\left(\frac{\hbar}{\sqrt{k\mu_{BC}}}\right)^{\frac{1}{2}} x + \bar{y}_{eq}\right] ,$$

for which the Hamiltonian of the system (with the center of mass kinetic energy removed) H_{rel} is simply written as:

$$H_{rel} = \hbar\omega\left[\frac{K_x^2}{2m} + \frac{K_y^2}{2} + \frac{y^2}{2} + V(x-y)\right] , \qquad (4.3)$$

with $p_x = \hbar K_x$ and $p_y = \hbar K_y$ being the momenta canonically conjugated to x and y respectively and where we have defined

$$V(x-y) = \frac{1}{\hbar\omega} V_{AB}\left(\frac{m_C}{m_B + m_C}\left(\frac{\hbar}{\sqrt{k\mu_{BC}}}\right)^{\frac{1}{2}} (x-y)\right) ,$$

$$m = \frac{m_A m_C}{M m_B} ,$$

$$\omega = \sqrt{\frac{k}{\mu_{BC}}} .$$

Using the Hamiltonian in form (4.3) energy will be measured in terms of $\hbar\omega$ and the formalism of section 3 can be used directly by putting $m_2 = 1$ and $m_1 = m$ (see eq. (3.1)). In terms of the creation and annihilation operators (3.4) the Hamiltonian H_{rel} (4.3) can be written as

$$H_{rel} = -\frac{(\hat{b}-\hat{b}^\dagger)^2}{4} + \hat{a}\hat{a}^\dagger + V\left(\frac{\hat{b}+\hat{b}^\dagger}{\sqrt{2m}} - \frac{\hat{a}+\hat{a}^\dagger}{\sqrt{2}}\right) . \qquad (4.4)$$

The potential $V(x-y)$ will be chosen as

$$V(x-y) = V_0' e^{-\gamma(x-y)} \qquad (4.5)$$

in order to compare our results with the results of the exact calculation performed by Secrest and Johnson (1976).

The relevant matrix elements needed for the numerical calculation via the parametrized TDVP can be calculated straightforwardly. The result is

$$N = {}_N\langle z,\alpha | z,\alpha\rangle_N = e^{z\bar{z}} \sum_{n=0}^{N} |\alpha_n|^2 ,$$

$$\langle z,n_2|H_{rel}|z,n_1\rangle = e^{z\bar{z}}\left(\frac{K_x^2}{2m} + n_1 + \frac{3}{4}\right)\delta_{n_1 n_2} + V_{n_1 n_2} e^{z\bar{z}} , \qquad (4.6)$$

where

$$V_{n_1 n_2} = e^{-z\bar{z}} \langle z,n_2|V(x-y)|z,n_1\rangle =$$

$$= V_0 e^{-\gamma x} \sum_{\ell=0}^{\infty} \langle n_2|| \frac{\gamma^\ell \hat{y}^\ell}{\ell!} ||n_1\rangle$$

and

$$V_0 = V_0' e^{\frac{\gamma^2}{4m}} .$$

Even though the terms $V_{n_1 n_2}$ can be calculated analytically

it will instead be calculated by making a series expansion because we shall consider the case $\gamma << 1$.

In terms of the normalized parameters β_n (3.5) we have

$$H = \sum_{n=0}^{N} n|\beta_n|^2 + \frac{3}{4} + \frac{K_x^2}{2m} + \sum_{n_1 n_2} \beta_{n_2} \bar{\beta}_{n_1} V_{n_1 n_2} \quad , \tag{4.7}$$

and equations (3.7) are explicitly given by

$$i\hbar \dot{\bar{\beta}}_j = j \bar{\beta}_j + \sum_{n=0}^{2} \bar{\beta}_n V_{nj} \quad \text{and} \quad \text{c.c.} \quad , \tag{4.8a}$$

$$\dot{x} = \frac{K_x}{m} \tag{4.8b}$$

$$\dot{K}_x = \gamma V_0 e^{-\gamma x} \sum_{n_1 n_2}^{N} \beta_{n_2} \bar{\beta}_{n_1} \left\{ \sum_{\ell=0}^{\infty} \langle n_2 | | \frac{\hat{\gamma}^{\ell} \hat{y}^{\ell}}{\ell!} | | n_1 \rangle \right\} \quad , \tag{4.8c}$$

where x and K_x are related to z and $\bar{z}$ by equations (3.4).

We shall consider small transition amplitudes and the equations of motion for K_x is in this case approximated by

$$\dot{K}_x = \gamma V_0 e^{-\gamma x} \tag{4.8d}$$

thus decoupling from equations for β_n.

Tables 1 and 2 show the results for the transition probabilities $P_{i\to f}^{TDVP}$ obtained solving equations (4.8a), (4.8b), and (4.8d). Comparisons are made with the exact results $P_{i\to f}'$ (Secrest and Johnson 1976) and with the results of other two

approximate methods due to Jackson and Mott (1932), $P_{i\to f}^{JM}$ and to Sharp and Rapp (1963), $P_{i\to f}^{SR}$.

In equation (4.8a) we have considered terms up to γ^3 so that $(f-i) \leq 3$. As it can be seen, the results of the calculations using the parametrized TDVP are in most cases in good agreement with the results of the exact calculations. In general our results are better than the results of the other approximate calculations shown in the tables. Therefore we conclude that the choice made of parametrization was appropriate for the problem we investigated. However, as it can also be seen, our results do not have the desirable symmetry $P_{i\to f}^{TDVP} = P_{f\to i}^{TDVP}$. The origin of this problem lies in the approximation we made of small transition amplitudes. When this approximation is made an average trajectory $z(t)$ is assumed. But in fact, after the collision with the particle, the oscillator wave function is in a combination of all possible states, each of them having a different internal energy and should correspond to a different trajectory of the particle. If instead of taking an average trajectory we allow for different trajectories this problem of lack of symmetry is eliminated.

As the energy difference between the levels considered becomes small compared to the total energy the average trajectory approximation should be good and indeed, in this case the lack of symmetry becomes small.

5. CONCLUSION

We have presented an approximative method using parametrized trial function in the TDVP so as to allow for internal excitation of colliding systems (in one dimension). The method was applied to the problem of collinear collision of a particle (atom) with a harmonic oscillator (diatomic molecule). Our results do compare fairly well with the results of an exact calculations. Therefore we conclude that the formalism developed by M. Saraceno and P. Kramer (1982) for treating elastic collision is also applicable to describing inelastic collisions. However, the problem of fusion remains an open question. In this case a re-quantization of the closed paths "a la" Bohr-Sommerfeld, will probably be required. Another problem is its applicability to real nuclear inelastic collisions.

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TABLE CAPTIONS

TABLE 1 - Transition probabilities as a function of the total energy for $m = 1/13$ and $\gamma = 0.1287$. The columns I and F are the initial and final states of the oscillator, respectively. $P_{i\to f}$ is the exact result, $P^{TDVP}_{i\to f}$ is our calculations, $P^{JM}_{i\to f}$ and $P^{SR}_{i\to f}$ are the results of Jackson and Mott (1932) and Sharp and Rapp (1963), respectively.

TABLE 2 - Transition probabilities as a function of the total energy for $m = 13/37$ and $\gamma = 0.1287$. (See caption of Table 1).

FIGURE CAPTIONS

Fig. 3.1 - Coordinates for the one-dimensional collision of a particle with an excitable system.

Fig. 4.1 - Coordinates for the collinear collision of an atom with a diatomic molecule.

TABLE 1

E_{Total}	I	F	$P_{i\to f}$	$P^{TDVP}_{i\to f}$	$P^{JM}_{i\to f}$	$P^{SR}_{i\to f}$
6.418	0	1	3.17×10^{-1}	2.89×10^{-1}	4.75×10^{-1}	5.74×10^{-1}
6.418	1	0	3.17×10^{-1}	2.23×10^{-1}	4.75×10^{-1}	3.87×10^{-1}
6.418	1	2	3.35×10^{-1}	3.76×10^{-1}	6.02×10^{-1}	7.73×10^{-1}
6.418	0	2	4.86×10^{-2}	7.26×10^{-2}	7.97×10^{-5}	–
6.418	0	3	2.50×10^{-3}	6.26×10^{-3}	–	–
6.418	1	3	4.47×10^{-2}	4.73×10^{-2}	–	–
6.418	2	3	–	1.97×10^{-1}	–	–
7.418	0	1	3.78×10^{-1}	3.32×10^{-1}	6.73×10^{-1}	7.81×10^{-1}
7.418	1	0	3.78×10^{-1}	2.28×10^{-1}	6.73×10^{-1}	5.74×10^{-1}
7.418	1	2	3.76×10^{-1}	4.45×10^{-1}	9.50×10^{-1}	1.15
7.418	0	2	9.49×10^{-2}	1.22×10^{-1}	1.74×10^{-4}	–
7.418	0	3	9.68×10^{-3}	1.37×10^{-2}	–	–
7.418	1	3	1.10×10^{-1}	8.20×10^{-2}	2.39×10^{-4}	–
7.418	2	3	–	2.47×10^{-1}	–	–
8.418	0	1	4.09×10^{-1}	3.53×10^{-1}	8.90×10^{-1}	1.01
8.418	1	0	4.09×10^{-1}	3.32×10^{-1}	8.90×10^{-1}	7.81×10^{-1}
8.418	1	2	3.43×10^{-1}	4.92×10^{-1}	1.35	1.56
8.418	2	1	3.43×10^{-1}	4.56×10^{-1}	1.35	1.15
8.418	2	3	3.21×10^{-1}	2.60×10^{-1}	1.42	1.72
8.418	0	2	1.50×10^{-1}	1.79×10^{-1}	3.17×10^{-4}	–
8.418	0	3	2.50×10^{-2}	2.48×10^{-2}	–	–
8.418	1	3	1.88×10^{-1}	1.16×10^{-1}	5.22×10^{-4}	–

TABLE 2

E_{Total}	I	F	$P_{i\to f}$	$P^{TDVP}_{i\to f}$	$P^{JM}_{i\to f}$	$P^{SR}_{i\to f}$
6.418	0	1	4.87×10^{-2}	6.30×10^{-2}	8.89×10^{-2}	1.31×10^{-1}
6.418	1	0	4.87×10^{-2}	2.76×10^{-2}	8.89×10^{-2}	5.80×10^{-2}
6.418	1	2	3.71×10^{-2}	3.03×10^{-2}	6.88×10^{-2}	1.16×10^{-1}
6.418	0	2	4.73×10^{-4}	9.97×10^{-4}	8.61×10^{-8}	–
7.418	0	1	9.96×10^{-2}	1.14×10^{-1}	1.82×10^{-1}	2.47×10^{-1}
7.418	1	0	9.96×10^{-2}	6.28×10^{-2}	1.82×10^{-1}	1.31×10^{-1}
7.418	1	2	9.14×10^{-2}	4.99×10^{-2}	1.78×10^{-1}	2.62×10^{-1}
7.418	0	2	2.47×10^{-3}	2.71×10^{-3}	4.51×10^{-7}	–
7.418	1	3	1.37×10^{-3}	5.29×10^{-4}	2.58×10^{-7}	–
8.418	0	1	1.62×10^{-1}	1.76×10^{-1}	3.21×10^{-1}	4.10×10^{-1}
8.418	1	0	1.62×10^{-1}	1.14×10^{-1}	3.21×10^{-1}	2.47×10^{-1}
8.418	1	2	1.71×10^{-1}	6.15×10^{-2}	3.64×10^{-1}	4.94×10^{-1}
8.418	2	1	1.71×10^{-1}	5.01×10^{-2}	3.64×10^{-1}	2.62×10^{-1}
8.418	2	3	1.28×10^{-1}	2.29×10^{-2}	2.67×10^{-1}	3.94×10^{-1}
8.418	0	2	8.66×10^{-3}	5.54×10^{-3}	1.64×10^{-6}	–

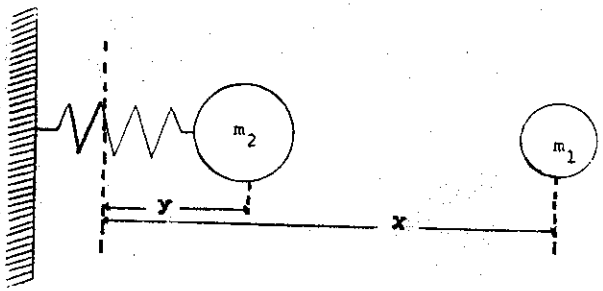

Figure 3.1

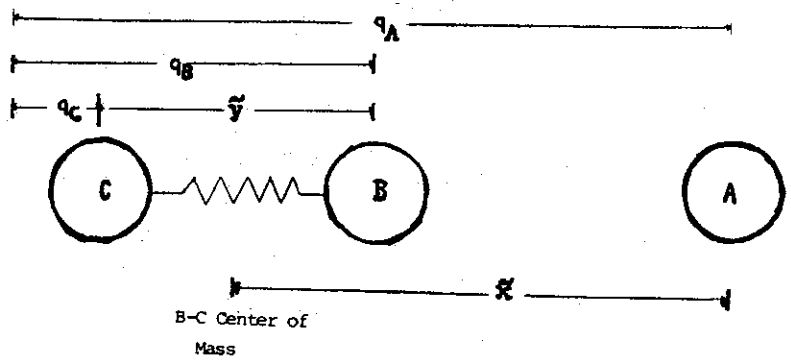

Figure 4.1