The Simulation of Quantum Friction

G. J. Ibeh* and E. D. Mshelia**

*Department of Physics, Nigerian Defence Academy, Kaduna, Nigeria. E-mail: gjibeh@nda.edu.ng
**Department of Physics, University of Abuja, Nigeria. E-mail: edmshelia@yahoo.com.

Abstract—A model for the dissipation of energy from a collective degree of freedom represented by free motion into intrinsic excitations is presented here. It is shown that by approximating the Hamiltonian of a system of interacting particles as a sum of two Hamiltonians, the quantum mechanical version of frictional effects on the system can be studied.

Keywords: energy dissipation, collective degree of freedom, intrinsic excitations, normal coordinates, probability amplitude, Friction, heavy-ion, Hermite polynomial.

1 INTRODUCTION

Friction or dissipation in a physical system is a classical physics concept. In quantum mechanics dissipation is considered to be the conversion of energy of collective degrees of freedom into intrinsic excitations [1]. Examples of dissipative systems are the damping of a particle while moving in a viscous medium; the noisy interaction observed when atoms or molecules traverse cavities irradiated by microwaves or the phonon field in superconducting quantum interference devices (SQUIDs)[2],[3],[4],[5],[6]. Dissipation has been shown to exist in nuclear physics, particularly in reactions where large scale collective motions are involved such as in nuclear fission, deep-inelastic heavy-ion reactions and giant resonance excitations [7],[8],[9],[10],[11],[12],[13],[14],[15]. There are basically two different methods used to quantify dissipative systems. The first method, by Kanai [16] consists of starting with Newton's equations of motion for the system with dissipation, due to a velocity-dependent force, finding the Lagrangian which leads to these equations of motion, and then proceeding to quantization by conventional formal methods. This method is invalid because it violates the uncertainty principle. Senitzky [17] assumed dissipation as due to the interaction of two systems—the lossless oscillator and the loss mechanism—and used an approximation method to solve the problem. This second method is the appropriate one because the result obtained is consistent with the principles of quantum mechanics. Another method by Kan and Griffin [18] consists of quantizing the linear harmonic oscillator with friction under the condition that in the classical limit a frictional force is obtained, and that at any time the total energy is equal to the sum of the expectation values of the kinetic and potential energies. This could only be achieved if in addition to the frictionless Hamiltonian a friction term and a counter-term were present. This however, leads to a nonlinear Schrödinger equation with two sets of solutions: damped and undamped ones.

Mshelia et al. [1] developed a quantum mechanical description of the energy that is lost or dissipated from the kinetic energy of the two bombarding nuclei into intrinsic excitations. They consider the energy dissipation as caused by the coupling of relative motion of the two ions to intrinsic degrees of freedom. This idea led to the solution of some integro-differential equations for the functions which determine the probability of finding the intrinsic energy within some energy interval. This paper considers the application of the above theory of energy dissipation to a model of three oscillators coupled to free motion, the bases for this application is given in Mshelia et al., [19]. In section 2 the model of the coupled harmonic oscillators is given. Section 3 is the solutions of the eigenvalue equations for the total and intrinsic Hamiltonians. Section 4 is a derivation of the probability amplitude for the intrinsic excitation, while section 5 deals with the numerical calculations and discussion of the results and finally in section 6 is the conclusion and the future outlook.

2 METHOD: THE MODEL

The model considered in this work consists of three oscillators coupled to translational motion. The oscillators described by the coordinates \(x_1, x_2\) and \(x_3\), represent the intrinsic degrees of freedom, and the translational motion, described by \(x\), the collective degree of freedom. According to Mshelia et al. [19] and Mshelia [20], the total Hamiltonian is split into the collective and intrinsic parts as given by

\[
H = H_{\text{int}} \left( x_1, x_2, x_3, x \right) + H_{\text{col}} \left( x \right) \tag{1}
\]

where \(x_1, x_2\) and \(x_3\) are the set of intrinsic coordinates and \(x\) the collective variable. The collective Hamiltonian \(H_{\text{col}}\) depends only on the collective variable while the intrinsic Hamiltonian \(H_{\text{int}}\) depends on both the intrinsic and collective variables, however independent of the momentum canonically conjugate to \(x\).

The terms on the right-hand side of (1) are explicitly stated as

\[
H_{\text{col}} = -\frac{\hbar^2}{2M} \frac{\partial^2}{\partial x^2} \tag{2}
\]

\[
H_{\text{int}} = -\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2} \right) + \frac{1}{2} c \left( x_1 - x \right)^2 + \frac{1}{2} c \left( x_2 - x \right)^2 + \frac{1}{2} c \left( x_3 - x \right)^2. \tag{3}
\]
The collective Hamiltonian is assumed to be that of a free particle with mass M. The three oscillators in (3) have the same mass m and are coupled to the collective motion via the same coupling constant c. The coupling of the intrinsic coordinates to the collective coordinate simulates the dissipation of energy from the collective degree of freedom to intrinsic excitation.

Using (2) and (3) the total Hamiltonian (1) is explicitly written as

\[ H = -\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2} \right) - \frac{\hbar^2}{2M} \frac{\partial^2}{\partial^2 x} + \frac{1}{2} c \left( x_1^2 + x_2^2 + 3x^2 - 2(x_1 + x_2 + x_3)x \right) \]  

This Hamiltonian shows that the kinetic energy operator is diagonal in the coordinates, while the potential energy is non-diagonal due to the products \( x_1 x, x_2 x, \) and \( x_3 x \). These off-diagonal terms give rise to the coupling of the collective and intrinsic motions.

To study the different modes of the motions, Mshelia et al. [19] and Mshelia [20] showed, that a transformation to normal coordinates results in:

\[ H = -\frac{\hbar^2}{2} \left( \frac{1}{\mu_1} \frac{\partial^2}{\partial g_1^2} + \frac{1}{\mu_2} \frac{\partial^2}{\partial g_2^2} + \frac{1}{\mu_3} \frac{\partial^2}{\partial g_3^2} + \frac{1}{\mu_4} \frac{\partial^2}{\partial g_4^2} \right) \]

This shows the normal modes of vibration.

2.1 Time Independent Schrödinger Equation for the Total and Intrinsic Hamiltonians

The eigenvalue problem of the total Hamiltonian (9) is

\[ H\Psi(g_1, g_2, g_3, g_4) = E\Psi(g_1, g_2, g_3, g_4). \]  

The introduction of the normal coordinates \( g_1, g_2, g_3, g_4 \) decouples the vibration of the system into normal modes of vibration and a free translational motion of the centre of mass; hence the eigenvalues and eigenfrequencies may be obtained as

\[ E_{k\mu r s} = \frac{\hbar^2 k^2}{2\mu_s} + h\omega_1 \left( r_1 + \frac{1}{2} \right) + h\omega_2 \left( r_2 + \frac{1}{2} \right) \]

\[ + h\omega_3 \left( r_3 + \frac{1}{2} \right), \]  

\[ \Psi_{k\mu r s} (g_1, g_2, g_3, g_4) = \psi_{\mu} (g_1) \psi_{r} (g_2) \psi_{s} (g_3) \]

\[ \times U_k (g_4), \]  

\[ U_k (g_4) = \frac{1}{\sqrt{2\pi}} \exp(ikg_4), \]

where the quantum numbers are \( r_1, r_2, r_3 = 0,1,2, \ldots, \) and \( k \) is the wave number of the plane wave (13), normalised by the Dirac \( \delta \) - function. The normalised eigenfunctions of the harmonic oscillator are defined by

\[ \psi_i (g_i) = N_i \exp \left( -\frac{1}{2} \alpha_i^2 g_i^2 \right) H_i (\alpha_i g_i) \]  

The quantity \( H_i (\alpha_i g_i) \) is a Hermite polynomial of order \( r_i \) and the inverse oscillation lengths and the normalization constant occurring in (14) are respectively defined by:
\[ \alpha_i = \sqrt{\frac{\mu_i \omega_i}{\hbar}} \] and \[ N_i = \sqrt{\frac{\alpha_i}{\sqrt{\pi^2 2^6} i!}}, \quad i = 1, 2, \ldots, n \] (15)

The total wave function (12) is normalized as follows:

\[
\int \ldots \int \phi^*_{k_{1,2,3}} \Psi_{k_{1,2,3}} \, dg_1 \, dg_2 \, dg_3 \, dg_4 = \delta(k - k')
\]
\[ \times \delta_{r_{1,2}} \delta_{r_{1,3}} \delta_{r_{2,3}}. \] (16)

The eigenvalue problem of the intrinsic Hamiltonian is solved as follows:

Defining the following change of variables

\[ \xi_i = x_i - x, \quad \xi_2 = x_2 - x, \quad \xi_3 = x_3 - x \] (17)

the eigenvalue equation takes the form

\[
\frac{-\hbar^2}{2m} \left( \frac{\partial^2}{\partial \xi_1^2} + \frac{\partial^2}{\partial \xi_2^2} + \frac{\partial^2}{\partial \xi_3^2} \right) + \frac{c}{2} \left( \xi_1^2 + \xi_2^2 + \xi_3^2 \right) \nabla \phi_{n_1 n_2 n_3} \left( \xi_1, \xi_2, \xi_3 \right) = \varepsilon \phi_{n_1 n_2 n_3} \left( \xi_1, \xi_2, \xi_3 \right) \] (18)

resulting in the following set of eigenvalues and eigenfunctions of the harmonic oscillator:

\[ \varepsilon_{n_1 n_2 n_3} = \hbar \omega \left( n_1 + n_2 + n_3 + \frac{3}{2} \right) \]
\[ = \hbar \omega \left( N + \frac{3}{2} \right) \] (19a)

\[ \phi_{n_1 n_2 n_3} \left( \xi_1, \xi_2, \xi_3 \right) = \psi_{n_1} \left( \xi_1 \right) \psi_{n_2} \left( \xi_2 \right) \psi_{n_3} \left( \xi_3 \right) \] (19b)

\[ \psi_{n_i} \left( \xi_i \right) = N_{n_i} \exp \left( -\frac{1}{2} \frac{\gamma^2}{\xi_i^2} \right) \frac{\partial^{n_i}}{\partial \xi_i^{n_i}} \] (19c)

\[ \gamma = \frac{m \omega}{\hbar}, \quad \omega^2 = \frac{c}{m}, \]
\[ N_{n_i} = \frac{\gamma}{\sqrt{\pi^2 2^6} \xi_i^!}. \] (19d)

2.2 The Distribution Function for Intrinsic Excitation

The total wave function may be expanded in terms of the eigenfunctions of the intrinsic Hamiltonian, since these eigenfunctions form a complete set. Therefore by the completeness relation [22]

\[ \Psi_{k_{1,2,3}} = \sum_{n_1 n_2 n_3} f_{k_{1,2,3}}^{n_1 n_2 n_3} \phi_{n_1 n_2 n_3} \left( \xi_1, \xi_2, \xi_3 \right) \] (20)

The expansion coefficients \( f_{k_{1,2,3}}^{n_1 n_2 n_3} \) are the collective wave functions and represents the probability amplitude for the excitation of the intrinsic motion. Multiplying from the left by the complex conjugate function \( \phi^*_{n_1 n_2 n_3} \) and integrating over intrinsic coordinates the probability amplitude becomes

\[ f_{k_{1,2,3}}^{n_1 n_2 n_3} \left( x \right) = \sum_{n_1 n_2 n_3} \int \phi^*_{n_1 n_2 n_3} \left( \xi_1, \xi_2, \xi_3 \right) \Psi_{k_{1,2,3}} \left( n_1, n_2, n_3, g_1, g_2, g_3, g_4 \right) \]
\[ \times dx_1 dx_2 dx_3. \] (21)

The integral above can be analytically evaluated after inserting the wave functions from (12) and (19c) and taking the expressions (8) for the normal coordinates into account. The resulting integral is

\[ f_{k_{1,2,3}}^{n_1 n_2 n_3} \left( x \right) = \frac{1}{\sqrt{2\pi}} \int N_{n_1} N_{n_2} N_{n_3} \int \exp \left[ -\frac{\gamma^2}{6} \left( 5 + \frac{1}{\delta} \right) \left( x_1^2 + x_2^2 + x_3^2 \right) \right] \]
\[ - \frac{3}{2} \frac{\gamma^2}{3} \left( 5 + \frac{1}{\delta} \right) x^2 + \left\{ x \gamma^2 \left( 1 + \frac{1}{\delta} \right) \right\} \]
\[ \times \left( x_1 + x_2 + x_3 \right) + \left( \frac{M}{m} \right) x \]
\[ \times H_{n_1} \left( y \left( x_1 - x \right) \right) H_{n_2} \left( y \left( x_2 - x \right) \right) \]
\[ \times H_{n_3} \left( y \left( x_3 - x \right) \right) \frac{\gamma}{\sqrt{2}} \left( x_1 - x_3 \right) \]
\[ \times \frac{\gamma}{\sqrt{3\delta}} \left( x_1 - x_2 - x_3 + 3x \right) \]
\[ \times \frac{\gamma}{\sqrt{6}} \left( x_1 - 2x_2 + x_3 \right) \]
\[ dx_1 dx_2 dx_3. \] (22)

where the constants

\[ \delta = \left( \frac{3m/M}{3m/M} + 1 \right)^{1/3} \quad \text{and} \quad b = \frac{ikm}{3m/M} \] (23)

Using the method of completing the square of a quadratic equation and application of the addition theorem for Hermite polynomials [23], [24]

\[ H_n \left( x + y \right) = 2^{-n} \sum_{m=0}^{n} \binom{n}{m} H_m \left( x \sqrt{2} \right) H_{n-m} \left( y \sqrt{2} \right) \] (24)

The final form of the collective amplitudes is
The physical meaning of the quantity \( \sum_{i_{1}\cdots i_{4}} |f_{x_{1}x_{2}x_{3}}(x)|^{2} \) is the probability that in the state \( \Psi \) the intrinsic energy will have one of the energy values of the discrete spectrum. That is, it is a measure for the internal excitation.

3 RESULTS: NUMERICAL CONSIDERATION

The amplitude given in (25) leads to the following graphical values of probability distributions for the intrinsic excitations. In the numerical calculation the final formulae contain only varied dimensionless quantities, such as the ratio of oscillator mass \( m \) to the central mass \( M \); the ratio of the energy of free motion \( E_{k} \) to the energy of oscillator spacing, \( \tilde{E}_{k} = E_{k}/\hbar \omega = \hbar k^{2}/(3m+M)\omega \); and the ratio of the intrinsic excitation energy to the energy of the oscillator spacing, \( \tilde{E}_{N} = E_{N}/\hbar \omega \).

The plot of Fig.1 is that of \( 2\pi |f_{x_{1}x_{2}x_{3}}(x)|^{2} \), as functions of the energy \( \tilde{E}_{k} \) of free motion, for various quantum numbers, \( s_{1}, s_{2}, s_{3}, r_{1}, r_{2}, r_{3} \) and for fixed ratio of masses \( m/M = 1 \).
Curves for the set of collective quantum numbers \( r_1 = r_2 = r_3 = 0 \) and \( r_2 = r_3 = 2, r_3 = 0 \) and their intrinsic numbers, which for Fig.1a are: (i). \( s_1 = s_2 = s_3 = 0 \); (ii). \( s_1 = 1, s_2 = s_3 = 0 \); (iii). \( s_1 = s_2 = 1, s_3 = 0 \); (iv). \( s_1 = 1, s_2 = 2, s_3 = 1 \); (v). \( s_1 = 1, s_2 = 3, s_3 = 1 \); (vi). \( s_1 = 1, s_2 = 7, s_3 = 1 \), and Fig.1b is that of: (i). \( s_1 = s_2 = s_3 = 1 \); (ii). \( s_1 = s_2 = 1, s_3 = 0 \); (iii). \( s_1 = 1, s_2 = s_3 = 0 \).

The following Fig.3 depicts the plot of probabilities as functions of the intrinsic quantum numbers. Here \( s_3 \) is kept constant and \( s_1 \) is varied to obtain the probability distributions.
for different values of $s_2$.

Fig. 3: Probability density against intrinsic quantum numbers for $E_1 = 1$ and mass ratios $m/M = 1$

Fig.4 shows the plot of the probability density against the mass ratio $m/M = \mu$, for varying values of $r_1$ and $s_2$ and constant values of the intrinsic and collective quantum numbers. For Fig.4a: $s_1 = s_2 = s_3 = 0$ and $r_2 = r_3 = 0$. And for Fig.4b: $s_1 = s_3 = 0$ and $r_1 = r_2 = r_3 = 0$

Fig. 4a: Probability density against the mass
Fig. 4b: probability density against the mass ratio $m/M = \mu$, for varying $s_2$

4 DISCUSSIONS

Fig.1 shows that the excitation of intrinsic states $(s_1, s_2, s_3)$ has an increasing width with increasing energy $\tilde{E}_k$. We observe also that the distributions are all peaked except that of the ground state, Fig.1a, (i) which has a maximum value of about 0.47 at around $\tilde{E}_k = 0$. Also, the results of Fig.1 show that the probability for intrinsic excitation is highest only for specific energy ratios $\tilde{E}_k$.

Fig.2a shows that the widths of the probability distributions decreases with increasing ratio $m/M$; the peaks, at specific value of $\tilde{E}_k$ for each ratio $m/M$, decreases with decreasing ratio $m/M$ and is shifted to a higher $\tilde{E}_k$ value. It is noticeable that the plots exhibits lower peaks and fast vanishing probability amplitudes with increasing quantum number.

In Fig.3 the probability amplitudes exhibit oscillatory features. This structure reveals that intrinsic states can be excited or deexcited in any higher-lying energy states other than zero.

Fig.4 implies that the intrinsic excitation is possible for small ratios of masses when in their ground states while excitation is possible for large ratios of masses when they are in states other than their ground states.

5 CONCLUSION

This paper has demonstrated the problem of energy dissipation from a collective coordinate into internal degrees of freedom by using an analytically solvable two oscillators coupled to free motion. The results obtained here are in agreement with similar models calculated previously [19], [26]. The model can be extended to the more realistic but more complex case of heavy-ion collisions, where energy dissipation plays an important role in deciding whether the fusion of superheavy elements is possible or not. To achieve this extension we shall have to solve the time-dependent Schrödinger equation in the future.

REFERENCES


