STUDY OF MANY-BODY APPROXIMATION TECHNIQUES IN SIMPLE NON-LINEAR COUPLED SYSTEM OF FERMIONS AND OSCILLATORS

by

VENKATARAMANAIAH KRISHNAMURTHY

B.Sc., Mysore University, India
(1968)

B.Sc. (Honours), Bangalore University, India
(1969)

M.Sc., Bangalore University, India
(1971)

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Signature redacted

Signature of Author. . . . . .
Department of Physics, Jan 27, 1978

Signature redacted

Certified by. . . . . .
Thesis Supervisor

Signature redacted

Accepted by. . . . . .
Chairman, Departmental Committee

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ABSTRACT

The application of many-body approximation techniques to study quantum mechanical non-linear systems is discussed. General methods of calculation are developed first by studying the example of an anharmonic oscillator. Using time-dependent variational method, the ground state energy and a few excited state energies are obtained. The second method used is the Kerman-Klein method based on studying the matrix elements of the equations of motion. Systematic and self-consistent calculational schemes are developed. The results in both these approximations are shown to agree well with the exact results.

The time-dependent variational method is extended to study a system of one fermion coupled to an oscillator from a meson field theoretical point of view. Next, a system of two fermions coupled to an oscillator is studied to find ways to calculate the two-nucleon interaction. These variation calculations are shown to agree well with the exact results. The perturbation results are shown to be far inadequate.

Thesis Supervisor: Arthur Kerman
Title: Professor of Physics

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TABLE OF CONTENTS

CHAPTER 1

INTRODUCTION

As first proposed by Yukawa, the nucleon-nucleon interaction is described as the exchange of quanta associated with the meson field. Numerous calculations have been made to derive the potential due to the two-body interaction of the nucleons using the perturbation theory in an expansion in the coupling constant. There is also the so-called static approximation in which the nuclear recoil is neglected. It has been found that, in the perturbation theory, the resulting two-nucleon potential has a strong singularity. The situation becomes worse by including the higher terms in the expansion. The renormalization process, introduced to remove these infinities, still does not able us to calculate the renormalized mass, charge and coupling constant. These renormalized quantities are identified with the physically observed ones and the experimental values are borrowed. There is no information obtained regarding the dynamics of the meson since the meson is treated to have a constant mass in deriving the two-nucleon potential.

If we can derive the two-nucleon potential, we should then be interested in the effective two-body interactions in many-nucleon systems to gain insights into its properties [1] . But, till now, most of the nuclear structure calculations are based on phenomenological potentials. The phenomenological potentials still do not give the

correct mean binding energy per nucleon. The other calculations are based on direct two-nucleon interactions without any reference to the dynamics of the meson. The retardation effect in the two-body interaction is neglected by considering only the dynamics of the two nucleons. As mentioned earlier, the attempts to include the dynamics of the meson introduces singularity problems in the perturbation theory. The important higher order terms are usually neglected in such cases.

The correct way to find the characteristics of a many-nucleon system consists of two phases. First we have to deduce the two-nucleon interaction from the dynamical equations of motion of a coupled meson-nucleon system. The interaction potential should then be used to calculate the properties of the many-body systems. Because of the problems posed by the perturbation theory, it is desirable to use some non-perturbative approximation techniques.

In this work, we attempt to find ways to derive the two-nucleon potential from a meson field theoretical point of view in a variational scheme. We will not be concerned with the full field theoretical problem. Instead, we solve a non-linear system of fermions interacting with a quantum mechanical oscillator by using the many-body variational approximation technique. In such a system, the basic features of the field theory problem are still present but with reduced complexity. It is also possible to find exact solutions by diagonalizing the hamiltonian in a suitable basis so that the results of the approximate solutions can be tested for their accuracy.

Coming back to the variational approximation technique, we adopt a method based on the time-dependent Hartree-Fock approximation for the nuclear many-body systems. It has been shown by Kerman and Koonin [2] that the time-dependent variation associated with the Schrodinger equation can be cast into a canonical Hamiltonian formulation. The Schrodinger equation is transcribed into equations for classical fields and their conjugate momenta. This method enables us to obtain the ground state energy as well as the energies of the low-lying excited states. The variation parameters introduced in the oscillator part of the trial wavefunction will ensure that the mass of the meson (i.e., the frequency of the quanta of the oscillator) is not kept constant. Thus we will be studying the dynamics of the meson also. Specifically, we expect to extract such information as the exchange energy, the binding energy and the role of the meson.

We also attempt to apply another approximation method which is an equations-of-motion method of generalized Hartree-Fock approximation due to Kerman and Klein [3] . Here, we study the matrix elements of the equations of motion and of the commutation relations. The method is developed for general non-linear systems by studying the anharmonic oscillator. The approximation involved is the truncation of the intermediate states, after a finite number of terms, in the sum decomposition of the matrix elements of the dynamical variables with non-linear powers. The dynamics of a non-linear system can be studied in a systematic way.

In Chapter 2, the two approximation techniques are illustrated by studying a quantum mechanical anharmonic oscillator which is one of the simplest non-linear systems. With this example, systematic calculational schemes are developed for later application to the system consisting of fermions coupled to oscillators. Another motivation to consider the particular example of the anharmonic oscillator is that it has received quite an amount of attention in the context of the non-perturbative methods in quantum field theory [4] . All the approximate results are compared with the exact solutions.

Chapter 3 deals with a system of one fermion coupled to an oscillator. The time-dependent variational method of Chapter 1 is extended to include the fermion nature of the system. The results of this discussion will also be useful in calculating the binding energy of the two-fermion system.

In Chapter 4, we treat the system of two fermions interacting through an oscillator in the time-dependent variational scheme. The ground state energy and the energies of the low-lying excited states are calculated and compared to the exact solutions. The binding energy is this approximation is compared to the interaction potential energy found by the ordinary perturbation theory.

Chapter 5 presents some comments on the two-fermion interaction and approximation techniques that were used.

CHAPTER 2

THE ANHARMONIC OSCILLATOR

In this chapter, we discuss the application of the two different nuclear many-body approximation techniques, mentioned in the Introduction, to general quantum mechanical non-linear systems. For clarity, we study the simple case of an anharmonic oscillator with quartic interaction and described by the hamiltonian

$$H = \frac{1}{2}\pi^2 + \frac{1}{2}\phi^2 + \frac{1}{4}\lambda\phi^4 \qquad (2.1)$$

Complete calculational schemes are developed, in the two approximation schemes, to obtain the energy eigenvalues and the matrix elements of the dynamical variables.

2.1 TIME-DEPENDENT VARIATION

The general time-dependent variational principle associated with the Schrodinger equation can be cast into hamiltonian formulation as discussed by Kerman and Koonin [2]. The quantal equation for the evolution of the system is transcribed into equations for classical fields and their conjugate momenta. This helps us to use all the approximation methods available to classical problems.

Consider a quantum system, say, a many-body system, described by a time-dependent wavefunction $\Psi(\omega;t)$ where the generalized coordinate may denote such variables as spatial position, spin. The

evolution of $\Psi(r;t)$ is given by the time-dependent Schrodinger equation:

$$i\dot{\Psi} = H\Psi \tag{2.2}$$

where H is the hamiltonian defining the system.

To express the Schrodinger equation in terms of a variational principle, a time-dependent lagrangian, which is a functional of Ψ and Ψ^*, is defined as

$$\mathcal{L}[\Psi,\Psi^*] = \int dr\, \Psi^*(r,t)\left(i\frac{\partial}{\partial t} - H\right)\Psi(r;t) \tag{2.3}$$

$$= \int dr\, i\Psi^*\dot{\Psi} - \mathcal{H}[\Psi,\Psi^*] \tag{2.4}$$

where $\mathcal{H}$ is defined to be the real hamiltonian:

$$\mathcal{H}[\Psi,\Psi^*] = \int dr\, \Psi^*(r,t)\, H\, \Psi(r;t) \tag{2.5}$$

The action S corresponding to the lagrangian $\mathcal{L}$ for evolution between times t_1 and t_2 is

$$S = \int_{t_1}^{t_2} dt \left(\int dr\, i\Psi^*\dot{\Psi} - \mathcal{H}[\Psi,\Psi^*]\right) \tag{2.6}$$

The equations of motion, obtained by requiring S to be stationary with respect to the variations of Ψ and Ψ^* between t_1 and t_2, are given by

$$\begin{aligned} i\dot{\Psi} &= \delta\mathcal{H}/\delta\Psi^* \\ i\dot{\Psi}^* &= -\delta\mathcal{H}/\delta\Psi \end{aligned} \tag{2.7}$$

where $\delta/\delta\Psi$ denotes a functional derivative.

To obtain a classical interpretation of the equations (2.7) in

terms of field coordinates and momenta, define the multi-coordinate fields $\mathbf{\Phi}$ and $\mathbf{\Pi}$ by

$$\mathbf{\Psi} = \frac{1}{\sqrt{2}} (\mathbf{\Phi} + i\mathbf{\Pi}) \tag{2.8}$$

so that

$$\mathbf{\Phi} = \sqrt{2}\, \mathrm{Re}\, \mathbf{\Psi} \qquad \text{and} \qquad \mathbf{\Pi} = \sqrt{2}\, \mathrm{Im}\, \mathbf{\Psi} \tag{2.9}$$

The equations (2.7) become

$$\dot{\mathbf{\Phi}} = \delta \mathcal{H} / \delta \mathbf{\Pi} \tag{2.10a}$$

$$\dot{\mathbf{\Pi}} = -\delta \mathcal{H} / \delta \mathbf{\Phi} \tag{2.10b}$$

Thus, the Schrodinger equation is transformed into a classical equation for a field and its conjugate momentum. The lagrangian is

$$\mathcal{L}\,[\mathbf{\Phi}, \mathbf{\Pi}] = \int dr\, \mathbf{\Pi}\, \dot{\mathbf{\Phi}} - \mathcal{H}\,[\mathbf{\Phi}, \mathbf{\Pi}] \tag{2.11}$$

We can now attempt to find approximate solutions by parametrizing the wavefunction in terms of several time-dependent parameters and determine their time evolution. With such a parametrized wavefunction, we perform a variational calculation, in the next two sections, to obtain the energies of the ground state and a few low-lying excited states of the anharmonic oscillator.

2.1.1 The Ground State Energy

For the hamiltonian given by (2.1), we choose a trial wavefunction in the form of a gaussian wavepacket described by

$$\Psi(\phi,t) = N \exp\left[-\frac{(\phi-\varphi)^2}{4G^2}\right] \tag{2.12}$$

Here, N is the normalization constant and φ (center of the wavepacket) and G (width of the wavepacket) are the variation parameters.

To begin with, let us take only φ to be time-dependent keeping G independent of time. As noted earlier, the parametrized wavefunction $\Psi(\phi,t)$ must also be complex and so we define

$$\varphi \longrightarrow \varphi + iP$$

Substituting this in (2.12) and discarding the unnecessary real factor, we get the trial wavefunction to be

$$\Psi = N \exp\left[-\frac{(\phi-\varphi)^2}{4G^2} + iP(\phi-\varphi)\right] \tag{2.13}$$

Using the normalization relation, $\int \Psi^* \Psi \, d\phi = 1$, the normalized trial wavefunction is given by

$$\Psi = \left(\frac{1}{2\pi G^2}\right)^{1/4} \exp\left[-\frac{(\phi-\varphi)^2}{4G^2} + iP(\phi-\varphi)\right] \tag{2.14}$$

Notice that this wavefunction, representing a minimum uncertainty wavepacket, happens to be an eigenfunction of the harmonic oscillator and hence seems to be the best choice for the anharmonic oscillator.

Before finding the classical hamiltonian, let us identify the canonical variables that are implicit in (2.14). Consider

$$\langle \Psi | (i\partial/\partial t) | \Psi \rangle = \int d\phi \; \Psi^* \, i(\partial \Psi/\partial t)$$

$$= P\dot{\varphi} \qquad (2.15)$$

which indicates that φ is the canonical coordinate and P its conjugate momentum. The classical hamiltonian corresponding to (2.1) is obtained by evaluating $\langle \Psi | H | \Psi \rangle$. Thus

$$\mathcal{H} = \int \Psi^* H \Psi \, d\phi$$

$$= \tfrac{1}{2} P^2 + \tfrac{1}{2}\varphi^2 + \tfrac{1}{2} G^2 + \tfrac{1}{4}\lambda\varphi^4 + \tfrac{3}{4}\lambda G^4$$

$$+ \tfrac{3}{2}\lambda\varphi^2 G^2 + \frac{1}{8G^2} \qquad (2.16)$$

In order to find the ground state energy, we minimize $\mathcal{H}$ with respect to the parameters P, φ and G and obtain the minimum values P_0, φ_0 and G_0 as follows.

$$\frac{\partial \mathcal{H}}{\partial \varphi} = 0 \longrightarrow \varphi_0 = 0 \qquad (2.17a)$$

$$\frac{\partial \mathcal{H}}{\partial P} = 0 \longrightarrow P_0 = 0 \qquad (2.17b)$$

$$\frac{\partial \mathcal{H}}{\partial G} = 0 \longrightarrow 3\lambda G_0^6 + G_0^4 - \tfrac{1}{4} = 0 \qquad (2.17c)$$

Substituting these minimum values in eq (2.16), we obtain the ground state energy as

$$E_0 = \frac{1}{8G_0^2} + \tfrac{1}{2} G_0^2 + \tfrac{3}{4}\lambda G_0^4$$

$$= G_0^2 + \tfrac{9}{4}\lambda G_0^4 \qquad (2.18)$$

Treating G also to be time-dependent and complex, i.e., putting $G \to G + i\Gamma$, the trial wavefunction (2.12), after discarding the unnecessary real factor, becomes

$$\Psi = \left(\frac{1}{2\pi G^2}\right)^{1/4} \exp\left[\frac{-(\phi-\varphi)^2}{4G^2} + iP(\phi-\varphi) + i\frac{\Gamma}{2G}(\phi-\varphi)^2\right] \qquad (2.19)$$

Notice that the normalization constant is also time-dependent.

It can easily be shown that the lagrangian is

$$\mathcal{L} = P\dot{\varphi} + \Gamma\dot{G} - \mathcal{H}$$

which indicates that φ and G to be canonical coordinates and P and Γ their respective conjugate momenta. Here the classical hamiltonian $\mathcal{H}$ is given by

$$\mathcal{H} = \tfrac{1}{2}P^2 + \tfrac{1}{2}\Gamma^2 + \tfrac{1}{2}\varphi^2 + \tfrac{1}{2}G^2 + \tfrac{1}{4}\lambda\varphi^4 + \tfrac{3}{4}\lambda G^4 + \tfrac{3}{2}\lambda\varphi^2 G^2 + \frac{1}{8G^2} \qquad (2.20)$$

The variation of $\mathcal{H}$ with respect to these new parameters gives the minimum value of Γ to be zero and the rest of the parameters still have the same minimum values as given by eqs (2.17). The ground state energy is again given by eq (2.18). This additional time-dependent parameter will, however, contribute to the information regarding the excited states of the system. The discussion regarding the excited states will be the topic of the next section.

2.1.2 Near Equilibrium Dynamics

As a function of the variation parameters, the hamiltonian

has an absolute minimum at the ground state. The small amplitude motion of the system about this minimum can be described by a linearized version of the equations of motion which represent a set of coupled harmonic oscillators. The normal modes of this set will correspond to the Random Phase Approximation (RPA) solutions.

The near equilibrium motion is investigated by assuming

$$\begin{aligned} \varphi &= \varphi_0 + \delta\varphi \\ P &= P_0 + \delta P \\ G &= G_0 + \delta G \\ \Gamma &= \Gamma_0 + \delta\Gamma \end{aligned} \tag{2.21}$$

with $\delta\varphi$, δP, δG and $\delta\Gamma$ small and time-dependent. As the ground state wavefunction may be chosen to have no dependence on time, (2.21) represents a time-dependent canonical transformation to the new variables $\delta\varphi$, δP, δG and $\delta\Gamma$. Inserting eq (2.21) in eq (2.20), the hamiltonian becomes

$$\begin{aligned} \mathcal{H} = E_0 &+ \tfrac{1}{2}\delta P^2 + \tfrac{1}{2}\delta\Gamma^2 + \tfrac{1}{2}\left(1+3\lambda G_0^2\right)\delta\varphi^2 \\ &+ \tfrac{1}{2}\left(1+9\lambda G_0^2 + \frac{3}{4G_0^4}\right)\delta G^2 + \mathcal{O}(\delta\varphi^4) + \mathcal{O}(\delta\varphi^2\delta G) \\ &+ \mathcal{O}(\delta\varphi^2\delta G^2) + \mathcal{O}(\delta G^3) + \mathcal{O}(\delta G^4) \end{aligned} \tag{2.22}$$

where eqs (2.17) and (2.18) have been used. Neglecting the third- and fourth-order terms in eq (2.22), the linearized equations of motion which follow from the Hamilton's equations, are

$$\frac{d}{dt}(\delta\varphi) = \delta P \tag{2.23}$$

$$\frac{d}{dt}(\delta P) = -(1+3\lambda G_0^2)\delta\varphi$$

$$\frac{d}{dt}(\delta G) = \delta\Gamma \qquad (2.23)$$

$$\frac{d}{dt}(\delta\Gamma) = -\left(1+9\lambda G_0^2+\frac{3}{4G_0^4}\right)\delta G$$

Because of the one-dimensional nature of the system under consideration, the linearized equations of motion (2.23) turned out to be those of two separate harmonic oscillators. The solutions of eq (2.23) for the case of harmonic time dependence for δP, $\delta\varphi$, $\delta\Gamma$ and δG are the RPA eigenfrequencies. The frequencies are

$$\omega_1 = \left(1+3\lambda G_0^2\right)^{1/2} \qquad (2.24a)$$

$$\omega_2 = \left(1+9\lambda G_0^2+\frac{3}{4G_0^4}\right)^{1/2} \qquad (2.24b)$$

These frequencies are, in the RPA treatment, usually identified with the energies of some "collective" excited states of the system.

In Table (2,3), the ground state energy E_0, the two excited state energies $E_1 = E_0+\omega_1$ and $E_2 = E_0+\omega_2$ for several different values of are given. In a later section, we will compare these values with the exact values of the energies and examine which excited states correspond to E_1 and E_2.

2.2 THE KERMAN-KLEIN METHOD

In this section, we discuss another approximation method developed by Kerman and Klein [3] in the context of nuclear many-body systems. The method consists of studying the matrix elements of the equations of motion and of the commutation relations. The approximation involved is the truncation of the intermediate states, after a finite number of terms, in the sum decomposition of the matrix elements of the dynamical variables with non-linear powers. This truncation results in solving, in a self-consistent manner, a closed set of non-linear equations of the matrix elements of the dynamical variables.

2.2.1 Equations of Motion and Commutation Relations

Let us denote the exact eigenstates of the hamiltonian (eq 2.1) by $|n\rangle$ with $n = 0,1,2,.....$

i.e., $$H|n\rangle = E_n|n\rangle \tag{2.25}$$

where E_n is the energy of the th eigenstate. The Heisenberg equations of motion for this system are

$$[\phi, H] = i\pi \tag{2.26a}$$

$$[\pi, H] = -i(\phi + \lambda\phi^3) \tag{2.26b}$$

and the commutation relation is

$$[\phi, \pi] = i \tag{2.27}$$

We now take matrix elements of these relations between the eigenstates of H defined in eq (2.25). Therefore, eqs(2.26) become

$$\omega_{mn} \langle n|\phi|m\rangle = i \langle n|\pi|m\rangle \tag{2.28a}$$

$$\omega_{mn} \langle n|\pi|m\rangle = -i \left(\langle n|\phi|m\rangle + \lambda \langle n|\phi^3|m\rangle\right) \tag{2.28b}$$

where $\omega_{mn} = E_m - E_n$.

Eliminating ω_{mn}, the two equations of motion combine to form

$$\langle n|\pi|m\rangle^2 + \langle n|\phi|m\rangle^2 + \lambda \langle n|\phi|m\rangle\langle n|\phi^3|m\rangle = 0 \tag{2.29}$$

Similarly, from eq (2.27), we obatain

$$\langle n|\phi\pi|m\rangle - \langle n|\pi\phi|m\rangle = i\,\delta_{mn} \tag{2.30}$$

2.2.2 The Approximations

Before going into the approximation scheme, we note the following. From the definite parities of the eigenstates of H, we have

$$\begin{aligned} &\langle n|\phi|m\rangle = 0 \\ &\langle n|\pi|m\rangle = 0 \qquad \text{for} \quad |m-n| \ \text{even} \end{aligned} \tag{2.31}$$

From the invariance under time reversal, we have

$$\begin{aligned} &\langle n|\phi|m\rangle = \langle m|\phi|n\rangle \\ &\langle n|\pi|m\rangle = -\langle m|\pi|n\rangle \end{aligned} \tag{2.32}$$

In order to solve eqs (2.29) and (2.30), we have to expand the matrix element $\langle n|\phi^3|m\rangle$ in a complete set of eigenstates of H as follows.

$$\langle n|\phi^3|m\rangle = \sum_r \sum_s \langle n|\phi|r\rangle\langle r|\phi|s\rangle\langle s|\phi|m\rangle \qquad (2.33)$$

This will generate an infinite number of non-linear equations in $\langle n|\phi|m\rangle$ and $\langle n|\pi|m\rangle$. If we assume that the sum (2.33) is saturated by a suitable finite number of states, the problem will be reduced to a closed set of equations. The basis for this assumption is that $\langle n|\phi|m\rangle$ and $\langle n|\pi|m\rangle$ decrease rapidly with increasing $|m-n|$ For example, consider the matrix element $\langle 0|\phi^3|1\rangle$ which can be written as

$$\langle 0|\phi^3|1\rangle = \langle 0|\phi|1\rangle\langle 1|\phi|0\rangle\langle 0|\phi|1\rangle + \langle 0|\phi|1\rangle\langle 1|\phi|2\rangle\langle 2|\phi|1\rangle + \langle 0|\phi|1\rangle\langle 1|\phi|4\rangle\langle 4|\phi|1\rangle + \cdots\cdots\cdots \qquad (2.34)$$

The matrix elements $\langle 0|\phi|1\rangle$ and $\langle 1|\phi|2\rangle$ are of the same order, but $\langle 1|\phi|4\rangle$ is a small term. In the case of a harmonic oscillator, all the matrix elements except $\langle 0|\phi|1\rangle$ and $\langle 1|\phi|2\rangle$ will be zero. Thus, the most significant contribution comes from the first two terms in eq (2.34).

2.2.3 Calculational Scheme

Starting from the ground state $|0\rangle$ and going up in energy, we can build an approximation scheme up to the desired accuracy. As seen from eq (2.34) and the subsequent discussion, the lowest or the first order of approximation involves considering only the states $|0\rangle, |1\rangle, |2\rangle$. From the parity considerations, two more successive states must be included for each further order of approximation.

i.e., First order: $|0\rangle, |1\rangle, |2\rangle$

Second order: $|0\rangle, |1\rangle, |2\rangle, |3\rangle, |4\rangle$

$\hat{j}$ th order: $|0\rangle, |1\rangle, |2\rangle, \ldots\ldots, |2\hat{j}-1\rangle, |2\hat{j}\rangle$

Thus, in the $\hat{j}$ th order of approximation, there are $(2\hat{j}+1)$ states and $2\hat{j}(\hat{j}+1)$ matrix elements. However, from eqs (2.29) and (2.30), we see that there are more than $2\hat{j}(\hat{j}+1)$ equations available. One should be careful to omit such equations which involve the matrix elements in the boundary region since a part of the most significant terms will appear in the next order of approximation. The condition $\langle n|H|m\rangle = 0$, for $n \neq m$, can be used as a self-consistency check.

The numerical technique used to solve these non-linear equations is the standard iteration process based on the Gauss elimination method. This technique is briefly described in Appendix (A). Since this process depends sensitively on the initial values of the variables, some approximate solutions of the non-linear equations must be found. In the first order of approximation, the initial values are taken to be the solutions of eqs (2.29) and (2.30) in the harmonic oscillator limit i.e., in the limit $\lambda = 0$. If λ is large, one can obtain an approximate solution by neglecting the terms small compared to the λ-term in eq (2.29). In the next order, all the quantities that were found in the previous order are used as the initial values. The rest of the dominant matrix elements are found by solving the eqs (2.29) and 2.30) neglecting the matrix elements for which $|m-n|$ is greater than 2. These approximate values are used as the initial values and the iteration process is carried out.

Table (1) gives the matrix elements calculated in various orders of approximations for $\lambda = 1.0$ showing the fast convergence of the method.

In each order of approximation, the energy eigenvalues are found as follows. The ground state energy is

$$\begin{aligned} E_0 &= \langle 0|H|0\rangle \\ &= \tfrac{1}{2}\langle 0|\pi^2|0\rangle + \tfrac{1}{2}\langle 0|\phi^2|0\rangle + \tfrac{1}{4}\lambda\langle 0|\phi^4|0\rangle \\ &= \tfrac{1}{2}\sum_r \langle 0|\pi|r\rangle\langle r|\pi|0\rangle + \tfrac{1}{2}\sum_r \langle 0|\phi|r\rangle\langle r|\phi|0\rangle \\ &\quad + \tfrac{1}{4}\sum_r\sum_s\sum_t \langle 0|\phi|r\rangle\langle r|\phi|s\rangle\langle s|\phi|t\rangle\langle t|\phi|0\rangle \end{aligned} \tag{2.35}$$

The energy of the nth state, using eq (2.28a), is given by

$$E_n = E_0 + i\,\frac{\langle 0|\pi|n\rangle}{\langle 0|\phi|n\rangle} \tag{2.36a}$$

$$E_n = E_1 + i\,\frac{\langle 1|\pi|n\rangle}{\langle 1|\phi|n\rangle} \tag{2.36b}$$

E_n can also be found by evaluating

$$E_n = \langle n|H|n\rangle \tag{2.37}$$

which serves as a self-consistency check to the values obtained by using eqs (2.36).

The numerical results for the energies calculated for different values of λ, in various orders of approximation, are shown in Table (2,3). The rapid convergence of the energies justify, once again, the assumptions made regarding the matrix elements.

2.3 COMPARISON OF APPROXIMATE RESULTS TO THE EXACT CALCULATIONS

2.3.1 Exact Calculations

The method for exact calculations, developed within the framework of the harmonic oscillator representation, is elementary in principle [5] . The hamiltonian (2.1) is written in a suitable Heisenberg harmonic oscillator representation. We introduce a basis by defining

$$H_0 = \frac{1}{2}\pi^2 + \frac{1}{2}\alpha^2\phi^2 \tag{2.38}$$

If $|\nu\rangle$ is an exact ν th eigenstate of H_0, then

$$\langle\nu|\, H_0 \,|\mu\rangle = E_0^{\nu}\,\delta_{\nu\mu} \tag{2.39}$$

In this representation, the eigenvalue equation for the hamiltonian (2.1) is

$$\sum_{\mu}\langle\nu|\, H \,|\mu\rangle\langle\mu|\,\rangle = E\,\langle\nu|\,\rangle \tag{2.40}$$

where E is the eigenvalue of H .

To obtain the eigenvalues of H , we have to diagonalize the matrix $H' = \langle\nu|H|\mu\rangle$ with a suitable α . The numerical method of diagonalization is briefly described in Appendix ($\mathcal{B}$). The size of the matrix H' , i.e., the number of basis states of H_0 spanning the subspace, to be considered depends on the number of energy eigenvalues of H we are interested in and on the value of the anharmonicity λ . As the value of λ increases, we have to include more and more higher basis states. The exactness of the energy eigenvalues are ensured by

performing the diagonalization process in several steps. At each step, the size of the matrix H' is increased by including a finite number of next higher basis states. The process is continued till we are assured of the convergence of the desired energy eigenvalues.

2.3.2 Comparison of the Approximate Calculations

Table (2) shows the ground state energy, for various values of λ, calculated by the time-dependent variation and the Kerman-Klein methods and compared to the exact results. Similarly, Table (3a, 3b) lists the energies of the first two excited states.

Compared to the exact values, the RPA solutions in the TDV correspond very closely to the first two excited states. The ground state energies also come close to the exact values. The converged energy values of the Kerman-Klein calculations are almost exact.

Another noticeable feature is the identical results in the case of the TDV and first order Kerman-Klein calculations. To understand this, consider the following discussion of the first order Kerman-Klein calculation with only three states, viz, $|0\rangle$, $|1\rangle$ and $|2\rangle$. From eqs (2.29) and (2.30), we obtain

$$\langle 0|\pi|1\rangle^2 + \langle 0|\phi|1\rangle^2 + \lambda \langle 0|\phi|1\rangle\langle 0|\phi^3|1\rangle = 0 \qquad (2.42)$$

$$\langle 0|\pi|1\rangle = -\frac{i}{2\langle 0|\phi|1\rangle} \qquad (2.43)$$

Using (2.43), eq (2.42) becomes

$$\lambda \langle 0|\phi^3|1\rangle \langle 0|\phi|1\rangle^3 + \langle 0|\phi|1\rangle^4 - \tfrac{1}{4} = 0 \qquad (2.44)$$

In the first order of approximation,

$$\langle 0|\phi^3|1\rangle = \langle 0|\phi|1\rangle^3 + \langle 0|\phi|1\rangle \langle 1|\phi|2\rangle^2 \qquad (2.45)$$

By considering only the states $|0\rangle$, $|1\rangle$ and $|2\rangle$, we are essentially working in a harmonic oscillator basis in which case $\langle n|\phi|m\rangle$ is nonvanishing only when $m = n+1$. It is well known that, for a harmonic oscillator,

$$\langle n|\phi|n+1\rangle = \sqrt{n+1}\ \langle 0|\phi|1\rangle \qquad (2.46)$$

Therefore, eq (2.45) becomes

$$\langle 0|\phi^3|1\rangle = 3\langle 0|\phi|1\rangle^3 \qquad (2.47)$$

Using this value in eq (2.44), we obtain

$$3\lambda \langle 0|\phi|1\rangle^6 + \langle 0|\phi|1\rangle^4 - \tfrac{1}{4} = 0 \qquad (2.48)$$

The ground state energy is

$$E_0 = \frac{1}{8\langle 0|\phi|1\rangle^2} + \tfrac{1}{2}\langle 0|\phi|1\rangle^2 + \tfrac{3}{4}\lambda \langle 0|\phi|1\rangle^4 \qquad (2.49)$$

Using eqs (2.28), the frequency ω_{10} is given by

$$\omega_{10} = \left[1 + 3\lambda \langle 0|\phi|1\rangle^2\right]^{1/2} \qquad (2.50)$$

If we replace $\langle 0|\phi|1\rangle$ by , the equations (2.48), (2.49) and (2.50) are identical respectively to (2.17c), (2.18) and (2.24a) of the TDV calculations. Extending this, we can conclude that

$$\varphi = 0 = \langle 0|\phi|0\rangle$$

This should not be surprising since the trial wavefunction Ψ in (2.14) represents the ground state of a harmonic oscillator.

CHAPTER 3

A SYSTEM OF ONE FERMION (ORBIT) COUPLED TO AN OSCILLATOR

After gaining the experience, in the previous chapter, of applying the many-body approximation techniques to simple quantum mechanical non-linear systems, we now proceed to extend the application of the time-dependent variational method to the case of relativistic fermions coupled to oscillators. Though the ultimate aim is to solve the two-fermion problem, let us begin with a system of one fermion interacting with an oscillator. This less difficult case will contribute to the development of general methods to be employed to the general fermion systems. This example is also necessary to find the binding energy of the two-fermion system.

3.1 THE MODEL

In field theory, a fermion field interacting with a neutral scalar boson field through a Yukawa coupling is described by the hamiltonian

$$H = \psi^{\dagger}(-i\alpha\cdot\nabla + \beta M)\psi + \tfrac{1}{2}\pi^2 + \tfrac{1}{2}\nabla^2\phi + \tfrac{1}{2}\mu^2\phi^2 + g\bar{\psi}\psi\phi \qquad (3.1)$$

in the standard notations.

We consider a model system consisting of relativistic fermions coupled to oscillators instead of the bosons. The quanta of the oscillator can be imagined to be mesons. Such a simplified system will reduce the complexity of the field theory problem without the loss of the basic

features. Only in this case, the results of the approximate calculations can be tested against the exact solutions.

The model system of fermions coupled to an oscillator through a Yukawa coupling can be represented by the hamiltonian

$$H = H_F + H_{os.} + H_I \tag{3.2a}$$

where

$$H_F = \psi^+ (-i\alpha\cdot\nabla + \beta M)\psi \tag{3.2b}$$

is the hamiltonian for the free fermion with mass M ,

$$H_{os} = \tfrac{1}{2}\pi^2 + \tfrac{1}{2}\mu^2\phi^2 \tag{3.2c}$$

is the hamiltonian for the free oscillator, and

$$H_I = g\,\bar{\psi}\psi\phi \tag{3.2d}$$

is the interaction hamiltonian (with a coupling constant g).

Consider now only one massless fermion with a fixed momentum (energy) k interacting with the oscillator described by H_{os} . When the interaction is not present, the fermion has the energy eigenvalues to be $\pm k$ as shown in figure (1). We will always refer to the state with the lowest energy, i.e., the energy $-k$, as the ground state of the system. Since the absence of a particle in the negative energy orbit is equivalent to the presence of an anti-particle, we shall use a new terminology to refer to these fermions and anti-fermions. We call the system as just 'one-orbit' coupled to an oscillator. In this new terminology, a fermion refers to a particle occupying the positive-

energy orbit. Similarly, in the next chapter, we will call the two-fermion case as the two-orbit case. We remind that the state with the lowest energy will be the ground state of the system.

Let $|o\rangle$ denote the state in which no particle is present (total number of particles is zero). Ψ in (3.2b) corresponds to the following operators:

a which destroys a particle in the positive-energy state,

b which destroys a particle in the negative-evergy state.

The state $b^+|o\rangle$ is the lowest energy state in the absence of the interaction and thus corresponds to the vacuum. The state $a^+|o\rangle$ is the particle state with a positive energy which is the result of a particle-hole excitation. With these definitions, it is obvious that

$$a|o\rangle = 0 \quad , \quad b|o\rangle = 0$$

These creation and destruction operators obey the following usual anticommutation relations.

$$\begin{aligned} \{a, a^+\} &= 1 \quad , \quad \{b, b^+\} = 1 \\ \{a^+, b^+\} &= 0 \quad , \quad \{a, b\} = 0 \\ \{a, b^+\} &= 0 \quad , \quad \{a^+, b\} = 0 \end{aligned} \tag{3.3}$$

With these relations, the hamiltonian for one-orbit coupled to an oscillator, corresponding to (3.2a), can be written as

$$H = K(a^+a - b^+b) + \tfrac{1}{2}\pi^2 + \tfrac{1}{2}\mu^2\phi^2 + g(a^+b + b^+a)\phi \tag{3.4}$$

Here, H is written in a representation in which the free hamiltonians are diagonal, i.e., when α is diagonal. A simple canonical trans-

formation will bring H to the more conventional representation in which β is diagonal. In the next section, a variational calculation is carried out with the hamiltonian in (3.4).

3.2 TIME-DEPENDENT VARIATION

We choose a product of a free orbit wavefunction and a gaussian wavepacket representing the free oscillator as the trial wavefunction. As mentioned in the previous section, when the interaction is absent, the eigenstates of the fermion are the ground state $b^+|0\rangle$ and the particle-hole state $a^+|0\rangle$. When the interaction is present, we must take into account such particle-hole excitation and hence the orbit part of the trial wavefunction is taken to be a combination of $b^+|0\rangle$ and $a^+|0\rangle$ (like a Slater determinant). Thus the trial wavefunction is written as

$$\Psi = N\left[u\, a^+|0\rangle + v\, b^+|0\rangle\right] \exp\left[-\frac{\omega}{2}(\phi-\varphi)^2\right] \qquad (3.5)$$

where N is the normalization constant and u, v, φ and ω are the variation parameters which are treated as time-independent. After finding the ground state energy, Ψ will be made time-dependent so that RPA frequencies can be found.

Using the normalization condition $\int \Psi^* \Psi \, d\tau = 1$, we obtain

$$N = \frac{1}{(u^2+v^2)} \left(\frac{\omega}{\pi}\right)^{1/4} \qquad (3.6)$$

and choose $u^2+v^2 = 1$ (3.7)

The classical hamiltonian is given by

$$\mathcal{H} = \langle \Psi | H | \Psi \rangle$$

$$= k(u^2 - v^2) + \frac{\omega}{4} + \frac{1}{2}\mu^2\left(\varphi^2 + \frac{1}{2\omega}\right) + 2g u v \varphi \qquad (3.8)$$

3.2.1 The Ground State Energy

The minimization of $\mathcal{H}$ is performed by introducing a Lagrange multiplier λ multiplied by (u^2+v^2) as follows.

$$\mathcal{H} - \lambda = k(u^2 - v^2) + \frac{\omega}{4} + \frac{1}{2}\mu^2\left(\varphi^2 + \frac{1}{2\omega}\right) + 2g u v \varphi - \lambda(u^2 + v^2) \qquad (3.9)$$

where the condition (3.7) has been used in the LHS.

The minimization equations are

$$\frac{\partial \mathcal{H}}{\partial u} = 2k u + 2g\varphi v - 2\lambda u = 0 \qquad (3.10a)$$

$$\frac{\partial \mathcal{H}}{\partial v} = -2k v + 2g\varphi u - 2\lambda v = 0 \qquad (3.10b)$$

$$\frac{\partial \mathcal{H}}{\partial \varphi} = \mu^2 \varphi + 2g u v = 0 \qquad (3.10c)$$

$$\frac{\partial \mathcal{H}}{\partial \omega} = -\frac{\mu^2}{4\omega^2} + \frac{1}{4} = 0 \qquad (3.10d)$$

From eq (3.10d), it follows that

$$\omega = \mu \qquad (3.11)$$

To find the other parameters, we combine eqs(3.10a) and (3.10b) to form

$$2k u v = g\varphi(u^2 - v^2) \qquad (3.12)$$

Since $u^2+v^2=1$, eq (3.12) can easily be solved to get

$$u^2 = \left[1 \pm \frac{k}{\sqrt{k^2+g^2\varphi^2}}\right] , \tag{3.13a}$$

$$v^2 = \left[1 \mp \frac{k}{\sqrt{k^2+g^2\varphi^2}}\right] \tag{3.13b}$$

We also obtain

$$\lambda = \pm\sqrt{k^2+g^2\varphi^2} \tag{3.13c}$$

which corresponds to the single particle Fermi energy. With these values, the hamiltonian (eq (3.8)) can be rewritten as

$$\mathcal{H} = \pm\sqrt{k^2+g^2\varphi^2} + \tfrac{1}{2}\mu + \tfrac{1}{2}\mu^2\varphi^2 \tag{3.14}$$

The first term shows that the orbit has now acquired an effetive mass $m^* = g\varphi$. The minimum values of φ, after minimizing $\mathcal{H}$ in eq (3.14) are

(i) $$\varphi = 0 \tag{3.15a}$$

(ii) $$\varphi = -\frac{1}{g}\left(\frac{g^4}{\mu^4} - k^2\right)^{1/2} \tag{3.15b}$$

Using the relations (3.13), the minimum values of u and v can be written as

$$u = \pm\left[\frac{1}{2}\left(1 \pm k\frac{\mu^2}{g^2}\right)\right]^{1/2} , \quad v = \pm\left[\frac{1}{2}\left(1 \mp k\frac{\mu^2}{g^2}\right)\right]^{1/2} \tag{3.15c}$$

In order to know which of these two values is relevant, we have to carry out the second-derivative minimum test. It is found that the two minimum values of φ fall into two different regions as

indicated below.

(i) $\varphi = 0 \quad , \quad \left\{ \begin{matrix} u=0 \ , & v=1 \\ u=1 \ , & v=0 \end{matrix} \right\}$ when $\frac{g^2}{\mu^2} \leq k$

(ii) $\varphi = \frac{1}{g}\left(\frac{g^4}{\mu^4} - k^2\right)^{1/2}$, $u = \pm\left[\frac{1}{2}\left(1 \pm k\frac{\mu^2}{g^2}\right)\right]^{1/2}$

$v = \pm\left[\frac{1}{2}\left(1 \mp k\frac{\mu^2}{g^2}\right)\right]^{1/2}$ when $\frac{g^2}{\mu^2} \geq k$

The ground state energy, evaluated by using eq (3.14), is

(i) $E_o = -k + \frac{1}{2}\mu$ when $\frac{g^2}{\mu^2} \leq k$ (3.16a)

(ii) $E_o = -\frac{1}{2}\frac{g^2}{\mu^2} + \frac{1}{2}\mu - \frac{1}{2}k^2\frac{\mu^2}{g^2}$ when $\frac{g^2}{\mu^2} \geq k$ (3.16b)

It is clear that, in the weak coupling limit $g^2/\mu^2 < k$, the ground state energy is just the sum of the free energy of the orbit and the free energy of the oscillator. In the strong coupling limit $g^2/\mu^2 > k$, the dominant term is $\left(-\frac{1}{2}\frac{g^2}{\mu^2}\right)$ when $k=1$. It is also clear that the negative sign in the first term in eq (3.16) gives the lowest energy. In a later section, we will see how these results can be improved.

3.2.2 Near Equilibrium Dynamics

To investigate the small amplitude motion about the equilibrium ground state, we consider a modified version of the trial wavefunction

given by (3.5). The oscillator part of the wavefunction is taken to be the one similar to (2.14). We start with the new trial wavefunction

$$\Psi = \left(\frac{\omega}{\pi}\right)^{1/4} \left[u\, a^{+}|0\rangle + v\, b^{+}|0\rangle\right] \exp\left[-\frac{\omega}{2}(\phi-\varphi)^2 + iP(\phi-\varphi)\right] \qquad (3.17)$$

where u, v, φ and P are time-dependent and ω is kept independent of time. u and v must also be complex. Following the procedure of Chapter 2, the lagrangian is given by

$$\begin{aligned} \mathcal{L} &= \langle\Psi|(i\,\partial/\partial t)|\Psi\rangle - \mathcal{H} \\ &= i(u^*\dot{u} + v^*\dot{v}) + P\dot{\varphi} - \mathcal{H} \end{aligned} \qquad (3.18)$$

where the classical hamiltonian is given by

$$\begin{aligned} \mathcal{H} &= \langle\Psi|H|\Psi\rangle \\ &= k(u^*u - v^*v) + \tfrac{1}{2}P^2 + \tfrac{1}{2}\mu^2\left(\varphi^2 + \frac{1}{2\omega}\right) + \frac{\omega}{4} \\ &\quad + g(u^*v + v^*u)\varphi \end{aligned} \qquad (3.19)$$

Compare this to eq (3.8).

The normalization condition now becomes

$$u^*u + v^*v = 1 \qquad (3.20)$$

When $\mathcal{H}$ is minimized with respect to the variation parameters, we obtain the same minimization equations as in the time-independent case, i.e., eqs (3.10) and an additional condition that $P=0$. The minimum values of u and v are found to be real and the ground state energy is once again given by eq (3.16).

To start the RPA analysis, we make the following expansion about the equilibrium (ground state).

$$
\begin{aligned}
u &= u_0 + \delta u \quad , & u^* &= u_0^* + \delta u^* \\
v &= v_0 + \delta v \quad , & v^* &= v_0^* + \delta v^* \\
\varphi &= \varphi_0 + \delta\varphi \quad , & P &= P_0 + \delta P
\end{aligned}
\tag{3.21}
$$

These are just the canonical transformations to the new variables δu, δu^*, δv, δv^*, $\delta\varphi$ and δP which are small and time-dependent. When these transformations are inserted in eq (3.19), the hamiltonian becomes

$$
\begin{aligned}
\mathcal{H} = \; & E_0 + \lambda u_0 \delta u^* + \lambda u_0^* \delta u + \lambda v_0 \delta v^* + \lambda v_0^* \delta v \\
& + k\delta u^* \delta u - k\,\delta v^* \delta v + g\varphi_0 \delta u^* \delta v + g\varphi_0 \delta v^* \delta u \\
& + \tfrac{1}{2}\delta P^2 + \tfrac{1}{2}\mu^2 \delta\varphi^2 + g u_0^* \delta v \delta\varphi + g v_0 \delta u^* \delta\varphi \\
& + g v_0^* \delta u \delta\varphi + g u_0 \delta v^* \delta\varphi \\
& + g\,\delta u^* \delta v \delta\varphi + g\,\delta v^* \delta u\, \delta\varphi
\end{aligned}
\tag{3.22}
$$

where the minization equations (3.10) and the fact that u_0 and v_0 are real have been used. This expression, as remarked in Chapter 2, should represent a system of coupled oscillators when the third order terms are neglected. This can be achieved by eliminating the terms linear in δ-variables using the time-dependent normalization condition (3.20). Inserting (3.21) in (3.20), we obtain

$$
u_0 \delta u^* + u_0^* \delta u + v_0 \delta v^* + v_0^* \delta v = -\delta u^* \delta u - \delta v^* \delta v
\tag{3.23}
$$

where the relation $u_0^* u_0 + v_0^* v_0 = 1$ has been used.

With the help of eqs (3.22) and (3.23), the hamiltonian can be rewritten as

$$\mathcal{H} = E_0 + (k-\lambda)\,\delta u^*\delta u - (k+\lambda)\,\delta v^*\delta v + g\varphi_0\,\delta u^*\delta v$$
$$+ g\varphi_0\,\delta v^*\delta u + \tfrac{1}{2}\delta P^2 + \tfrac{1}{2}\mu^2\delta\varphi^2$$
$$+ g u_0^*\,\delta v\delta\varphi + g v_0^*\,\delta u\,\delta\varphi + g u_0\,\delta v^*\,\delta\varphi + g v_0\,\delta v\,\delta\varphi$$

upon the neglect of the third-order terms. The Hamilton's equations of motion are

$$\frac{d}{dt}(\delta P) = -\mu^2\delta\varphi - g v_0\,\delta u^* - g v_0^*\,\delta u - g u_0\,\delta v^* - g u_0^*\,\delta v$$

$$\frac{d}{dt}(\delta\varphi) = \delta P$$

$$i\frac{d}{dt}(\delta u^*) = -(k-\lambda)\,\delta u^* - g\varphi_0\,\delta v^* - g v_0^*\,\delta\varphi \qquad (3.24)$$

$$i\frac{d}{dt}(\delta u) = (k-\lambda)\,\delta u + g\varphi_0\,\delta v + g v_0\,\delta\varphi$$

$$i\frac{d}{dt}(\delta v^*) = (k+\lambda)\,\delta v^* - g\varphi_0\,\delta u^* - g u_0^*\,\delta\varphi$$

$$i\frac{d}{dt}(\delta v) = -(k+\lambda)\,\delta v + g\varphi_0\,\delta u + g u_0\,\delta\varphi$$

These equations of motion are solved, in the normal mode analysis, by assuming a harmonic time dependence of the δ-variables. The eigenfrequencies are

$$\omega_1^2 = 0 \qquad (3.25a)$$

$$\omega_2^2 = \tfrac{1}{2}\left[\mu^2 + 4\left(k^2 + g^2\varphi_0^2\right)\right] \qquad (3.25b)$$
$$\pm \tfrac{1}{2}\left\{\left[\mu^2 - 4\left(k^2+g^2\varphi_0^2\right)\right]^2 - 16\,g^2\left[\mu^2\varphi_0^2 + \sqrt{k^2+g^2\varphi_0^2}\right]\right\}^{1/2}$$

Notice that, when $g = 0$,

$$\omega_2 = \mu, \; 2k$$

The frequency μ corresponds to the first excited state of the free oscillator and $2k$ corresponds to the particle-hole excited state of the free fermion.

The zero frequency ω_1 occurs because of the fact that the symmetry is broken if we interchange u and v .

3.2.3 A Modified Trial Wavefunction

As already noted in Section (3.2.1), the choice of the trial wavefunction Ψ as in (3.5) does not yield any interaction energy in the weak coupling region. The ground state wavefunction may not just be a product of the wavefunctions of the free hamiltonians. This is possibly best remedied by introducing a orbit-oscillator cross term in the trial wavefunction. An appealing form of this cross term is suggested following certain observations noted below.

Consider the hamiltonians H_{os} of the oscillator (3.2c) and H_I of the interaction (3.2d) which form parts of the full hamiltonian H of the entire system.

$$H_{os} + H_I = \tfrac{1}{2}\pi^2 + \tfrac{1}{2}\mu^2\phi^2 + g\,\bar{\Psi}\psi\phi \tag{3.27}$$

This expression can be written as a hamiltonian for an oscillator displaced in space by $\frac{g}{\mu^2}\bar{\Psi}\psi$.

$$H_{os} + H_I = \tfrac{1}{2}\pi^2 + \tfrac{1}{2}\mu^2\left(\phi - \tfrac{g}{\mu^2}\bar{\Psi}\psi\right)^2 - \tfrac{1}{2}\tfrac{g^2}{\mu^2}(\bar{\Psi}\psi)^2 \tag{3.28}$$

If $|n\rangle$ is the nth eigenstate of H_{os}, then the eigenstates of the displaced one (3.28) are given by $e^{-i(\frac{g}{\mu^2})\pi\bar{\Psi}\psi}\,|n\rangle$.

With this observation in mind, we choose a new trial wavefunction as

$$\Psi_N = e^{-i\gamma\pi\bar{\Psi}\psi}\,\Psi \tag{3.29}$$

where Φ is as in (3.5) and γ is an arbitrary variable. The transformation from Φ to Φ_N is unitary since π commutes with ψ and $\bar{\psi}$. It follows that

$$\langle \Phi_N | \Phi_N \rangle = 1$$

In the present example of one orbit coupled to an oscillator, the hamiltonian of which is

$$H = k(a^+a - b^+b) + \tfrac{1}{2}\pi^2 + \tfrac{1}{2}\mu^2\phi^2 + g(a^+b + b^+a)\phi \qquad (3.30)$$

the new trial wavefunction can be taken as

$$\Phi_N = e^{-i\gamma\pi(a^+b + b^+a)}\,\Phi \qquad (3.31)$$

where Φ is given by eq (3.5). For mathematical convenience, which will become clear later, put $\gamma = \alpha/\sqrt{\omega}$. The normalized trial wavefunction now is

$$\Phi_N = e^{-i\frac{\alpha}{\sqrt{\omega}}\pi(a^+b + b^+a)}\left[u a^+|0\rangle + v b^+|0\rangle\right]\exp\left[-\tfrac{\omega}{2}(\phi - \varphi)^2\right] \qquad (3.32)$$

where α is an additional variational parameter available to us.

To reduce the complexity, we will perform only a stationary variational calculation and will be interested in obtaining the ground state energy. The extension to the time-dependent case is quite straightforward. The expectation value of the hamiltonian is

$$\begin{aligned}\mathcal{H} &= \langle \Phi_N | H | \Phi_N \rangle \\ &= \langle \Phi | e^{i\frac{\alpha}{\sqrt{\omega}}\pi(a^+b + b^+a)}\, H\, e^{-i\frac{\alpha}{\sqrt{\omega}}\pi(a^+b + b^+a)} | \Phi \rangle\end{aligned} \qquad (3.33)$$

To evaluate the above integral, the following relation is very helpful.

$$e^{i\lambda S} H e^{-i\lambda S} = H + i\lambda [S, H] + \frac{(i\lambda)^2}{2!} [S, [S, H]] + \cdots\cdots + \frac{(i\lambda)^n}{n!} [S, [S, \cdots; [S, H] \cdots]] + \cdots\cdots \quad (3.34)$$

The expectation value of the term $(a^+a - b^+b)$ in H is calculated as follows. Take $S = (a^+b + b^+a)$ and $\lambda = \frac{\alpha}{\sqrt{\omega}}\pi$. Using the fact that π commutes with a, a^+, b, b^+, perform first the integration in the orbit space to get

$$H_1 = \langle \Psi_N | (a^+a - b^+b) | \Psi_N \rangle$$
$$= (u^2 - v^2) \int \left(\frac{\omega}{\pi}\right)^{1/2} \exp\left[-\frac{\omega}{2}(\phi - \varphi)^2\right] \left(e^{2i\frac{\alpha}{\sqrt{\omega}}\pi}\right) \exp\left[-\frac{\omega}{2}(\phi - \varphi)^2\right] d\phi \quad (3.35)$$

By a Fourier transformation, the integral in (3.35) can be transformed into momentum space and can easily be evaluated to obatain

$$H_1 = (u^2 - v^2)\, e^{-\alpha^2} \quad (3.36)$$

Since π commutes with a, a^+, b, b^+, it is easy to see that

$$H_2 = \tfrac{1}{2} \langle \Psi_N | \pi^2 | \Psi_N \rangle = \tfrac{1}{2} \langle \Psi | \pi^2 | \Psi \rangle = \tfrac{1}{4}\omega \quad (3.37)$$

To evaluate the rest of the integrals in $\mathcal{H}$, consider any function of ϕ, say, $f(\phi)$. Any function $f(\phi - \lambda)$ can be expanded in a Taylor series which becomes exactly equal to the expansion (3.34) since $\pi = i\,\partial/\partial\phi$. Therefore,

$$e^{i\lambda\pi} f(\phi) e^{-i\lambda\pi} = f(\phi - \lambda) \quad (3.38)$$

$$H_3 = \frac{1}{2}\mu^2 \langle \Psi_N | \phi^2 | \Psi_N \rangle$$

$$= \frac{1}{2}\mu^2 \langle \Psi | \left(\phi - \frac{\alpha}{\sqrt{\omega}}(a^+b + b^+a)\right)^2 | \Psi \rangle$$

$$= \frac{1}{2}\mu^2\varphi^2 + \frac{1}{4}\frac{\mu^2}{\omega} + \frac{1}{2}\mu^2\frac{\alpha^2}{\omega} - 2\mu^2\frac{\alpha}{\sqrt{\omega}}uv\varphi \qquad (3.39)$$

$$H_4 = g \langle \Psi_N | (a^+b + b^+a)\phi | \Psi_N \rangle$$

$$= g \langle \Psi | (a^+b + b^+a)\left[\phi - (a^+b + b^+a)\right] | \Psi \rangle$$

$$= 2guv\varphi - g\frac{\alpha}{\sqrt{\omega}} \qquad (3.40)$$

Collecting the various terms from eqs (3.36 - 3.40), the expectation value $\mathcal{H}$ of the hamiltonian is

$$\mathcal{H} = k(u^2 - v^2)e^{-\alpha^2} + \left(\frac{\omega}{4} + \frac{\mu^2}{4\omega}\right) + \frac{1}{2}\mu^2\varphi^2$$
$$+ 2\left(g - \mu^2\frac{\alpha}{\sqrt{\omega}}\right)uv\varphi - \left(g\frac{\alpha}{\sqrt{\omega}} - \mu^2\frac{\alpha^2}{2\omega}\right) \qquad (3.41)$$

Minimization:

Instead of writing the equations minimizing $\mathcal{H}$ with respect to all the parameters at the same time, we proceed, equivalently, stepwise so that we do not miss any interesting features of the intermediate structures of the hamiltonian. As usual, introducing a Lagrange multiplier λ in eq (3.41), we have

$$\mathcal{H}-\lambda = k(u^2-v^2)\,e^{-\alpha^2} + \left(\frac{\omega}{4}+\frac{\mu^2}{4\omega}\right) + \frac{1}{2}\mu^2\varphi^2$$

$$+2\left(g-\mu^2\frac{\alpha}{\sqrt{\omega}}\right)uv\varphi - \left(g\frac{\alpha}{\sqrt{\omega}} - \mu^2\frac{\alpha^2}{2\omega}\right) - \lambda(u^2+v^2) \qquad (3.42)$$

Minimizing with respect to u and v, we obtain

$$\frac{\partial\mathcal{H}}{\partial u} = 2k\,e^{-\alpha^2}u + 2\left(g-\mu^2\frac{\alpha}{\sqrt{\omega}}\right)\varphi\,v - 2\lambda\,u = 0 \qquad (3.43a)$$

$$\frac{\partial\mathcal{H}}{\partial v} = -2k\,e^{-\alpha^2}v + 2\left(g-\mu^2\frac{\alpha}{\sqrt{\omega}}\right)\varphi\,u - 2\lambda\,v = 0 \qquad (3.43b)$$

These two equations can be manipulated to give

$$2k\,e^{-\alpha^2}uv = \left(g-\mu^2\frac{\alpha}{\sqrt{\omega}}\right)\varphi\,(u^2-v^2) \qquad (3.44)$$

$$\lambda = \pm\left[k^2\,e^{-2\alpha^2} + \left(g-\mu^2\frac{\alpha}{\sqrt{\omega}}\right)^2\varphi^2\right]^{1/2} \qquad (3.45)$$

By comparing these equations with (3.12) and (3.13c), we notice that the effect of the unitary transformation (3.32) in the trial wavefunction is to introduce a transformation

$$k \longrightarrow k\,e^{-\alpha^2}$$

$$g \longrightarrow g-\mu^2\frac{\alpha}{\sqrt{\omega}}$$

Eqs (3.44) and (3.45) can be easily solved to get

$$u^2 = \frac{1}{2}\left[1 \pm \frac{k\,e^{-\alpha^2}}{\lambda}\right] \quad , \quad v^2 = \frac{1}{2}\left[1 \mp \frac{k\,e^{-\alpha^2}}{\lambda}\right] \qquad (3.46)$$

Thus, inserting (3.46) in (3.41), $\mathcal{H}$ becomes

$$\mathcal{H} = \pm\left[k^2 e^{-2\alpha^2} + \left(g - \mu^2\frac{\alpha}{\sqrt{\omega}}\right)^2\varphi^2\right]^{1/2} + \left(\frac{\omega}{4} + \frac{\mu^2}{4\omega}\right) + \frac{1}{2}\mu^2\varphi^2 - \left(\frac{g\alpha}{\sqrt{\omega}} - \frac{\mu^2\alpha^2}{2\omega}\right) \tag{3.47}$$

Obviously, the negative sign in the first term gives the lowest energy. We also notice that the orbit has acquired an effective mass $m^* = \left(g - \mu^2\frac{\alpha}{\sqrt{\omega}}\right)\varphi$.

Continuing the minimization process, now with respect to φ , we obtain

$$\frac{\partial \mathcal{H}}{\partial \varphi} = -\frac{\left(g - \mu^2\frac{\alpha}{\sqrt{\omega}}\right)^2\varphi}{\left[k^2 e^{-2\alpha^2} + \left(g - \mu^2\frac{\alpha}{\sqrt{\omega}}\right)^2\varphi^2\right]^{1/2}} + \mu^2\varphi = 0 \tag{3.48}$$

Again, there are two solutions to φ :

(i) $\varphi = 0$ (3.49a)

(ii) $$\varphi = \pm\frac{1}{\left(g - \mu^2\frac{\alpha}{\sqrt{\omega}}\right)}\left[\frac{1}{\mu^4}\left(g - \mu^2\frac{\alpha}{\sqrt{\omega}}\right)^4 - k^2 e^{-2\alpha^2}\right]^{1/2} \tag{3.49b}$$

Exactly in which cases these two solutions are valid is determined by conducting the second-derivative minimum test. Of course, for such a test, the minimum values of α and ω must be found first. Substituting the solutions of φ given by (3.49), we obtain (taking only the negative sign of the first term in (3.47))

Case (i) when $\varphi = 0$:

$$\mathcal{H} = -k e^{-\alpha^2} + \left(\frac{\omega}{4} + \frac{\mu^2}{4\omega}\right) - \left(g\frac{\alpha}{\sqrt{\omega}} - \frac{\mu^2\alpha^2}{2\omega}\right) \tag{3.50a}$$

Case (ii) when $\varphi \neq 0$:

$$\mathcal{H} = -\frac{1}{2}\frac{k^2 e^{-2\alpha^2}\mu^2}{\left(g - \mu^2\frac{\alpha}{\sqrt{\omega}}\right)^2} - \frac{1}{2\mu^2}\left(g - \mu^2\frac{\alpha}{\sqrt{\omega}}\right) \tag{3.50b}$$

$$+\left(\frac{\omega}{4} + \frac{\mu^2}{4\omega}\right) - \left(\frac{g\alpha}{\sqrt{\omega}} - \frac{\mu^2\alpha^2}{2\omega}\right)$$

Compared to eqs (3.16), these equations show the appearance of new terms due to the interaction part of the hamiltonian. We are now left with the last set of variational parameters to be minimized. We discuss the cases $\varphi = 0$ and $\varphi \neq 0$ separately.

Case (i) when $\varphi = 0$:

In this case, $\mathcal{H}$ given by (3.50a) has to be minimized. The minimum value of ω is determined by

$$\frac{\partial \mathcal{H}}{\partial \omega} = \frac{1}{4} - \frac{\mu^2}{4\omega^2} + \frac{1}{2}\frac{g\alpha}{\sqrt{\omega^3}} - \frac{\mu^2\alpha^2}{2\omega^2} = 0 \tag{3.51a}$$

$$\omega^2 + 2g\alpha\sqrt{\omega} - \mu^2(1 + 2\alpha^2) = 0 \tag{3.51b}$$

The minimum value of α is determined by

$$\frac{\partial \mathcal{H}}{\partial \alpha} = 2k\alpha e^{-\alpha^2} + \mu^2\frac{\alpha}{\omega} - \frac{g}{\sqrt{\omega}} = 0 \tag{3.52a}$$

$$2k\alpha e^{-\alpha^2}\omega - g\sqrt{\omega} + \mu^2\alpha = 0 \tag{3.52b}$$

The transcendental equations (3.51b) and (3.52b) can be solved by numerical techniques only. From eq (3.52b), we obtain

$$\sqrt{\omega} = \frac{e^{\alpha^2}}{4k\alpha}\left[g \pm \left(g^2 - 8\mu^2 k\alpha^2 e^{-\alpha^2}\right)^{1/2}\right] \tag{3.53}$$

Substituting this value in eq (3.51b), after some algebra, we get

$$\left(\frac{1}{16}\mu^6\alpha^4 - \frac{1}{16}g^4\right)e^{4\alpha^2} + \left(\frac{1}{4}g^2\mu^2 k\alpha^4 + \frac{1}{2}g^2\mu^2 k\alpha^2\right)e^{3\alpha^2}$$
$$- \frac{1}{2}\mu^2 k^2\alpha^4\left(1+2\alpha^2\right)e^{2\alpha^2} - g^2k^3\alpha^4 e^{\alpha^2}$$
$$+ \mu^2 k^4\alpha^4\left(1+2\alpha^2\right)^2 = 0 \tag{3.54}$$

This is an equation in α^2 and hence when searching for solutions by numerical method one need not consider the negative solutions of α^2. Once the positive solutions of α^2 are found, we retain only the positive root of α to maintain the transformation (3.32) in the trial wave-function unaltered. Even in the positive range, α^2 has many solutions because of the presence of the exponential terms. For each value of α, there corresponds two solutions to $\sqrt{\omega}$ (eq(3.53)). Of course, only the real solutions of $\sqrt{\omega}$ must be retained.

Case (ii) when $\varphi \neq 0$:

In this case, $\mathcal{H}$ given by eq(3.50b) has to be minimized. The minimum value of ω is determined by

$$\frac{\partial \mathcal{H}}{\partial \omega} = \frac{\mu^4 k^2 \alpha e^{-2\alpha^2}}{2\sqrt{\omega^3}\left(g - \frac{\mu^2 \alpha}{\sqrt{\omega}}\right)^3} + \frac{1}{4}\left(1 - \frac{\mu^2}{\omega^2}\right) = 0 \qquad (3.55)$$

$$2\mu^4 k^2 \alpha e^{-2\alpha^2} \omega^2 + (\omega^2 - \mu^2)\left(g\sqrt{\omega} - \mu^2 \alpha\right)^3 = 0 \qquad (3.56)$$

The minimum value of α is determined by

$$\frac{\partial \mathcal{H}}{\partial \alpha} = -\frac{\mu^4 k^2 e^{-2\alpha^2}}{\sqrt{\omega}\left(g - \frac{\mu^2 \alpha}{\sqrt{\omega}}\right)^3} + \frac{2\mu^2 k^2 \alpha e^{-2\alpha^2}}{\left(g - \frac{\mu^2 \alpha}{\sqrt{\omega}}\right)^2} = 0 \qquad (3.57)$$

Therefore, we get

(i) $e^{-2\alpha^2} = 0$ which is an irrelevant solution

and

$$\text{(ii)} \quad -\frac{\mu^2}{\sqrt{\omega}\left(g - \frac{\mu^2 \alpha}{\sqrt{\omega}}\right)} + 2\alpha = 0 \qquad (3.58)$$

$$\sqrt{\omega} = \frac{\mu^2}{2g\alpha}(1 + 2\alpha^2) \qquad (3.59)$$

Inserting eq (3.59) in eq (3.56), after some algebra, we get

$$16\mu^4 k^2 \alpha^4 (1+2\alpha^2)^4 e^{-2\alpha^2} + \mu^6 (1+2\alpha^2)^4 - 16 g^4 \alpha^4 = 0 \qquad (3.60)$$

The structure of eq(3.60) is similar to that of eq (3.54) and the discussion regarding the solutions of eq (3.54) is relevant here also.

The ground state energy of the system is determined by eq (3.50) and, of course, there are two values corresponding to the two solutions of φ . The following systematic procedure must be adopted to ensure that the solution we obtain, indeed, corresponds to the lowest energy.

(1) Find the minimum values of ω and α so that α and ω are positive real for both the cases of $\varphi = 0$ and $\varphi \neq 0$.
(2) If there are several relevant solutions in each case, retain only those which satisfy the second-derivative minimum test.
(3) After the previous step, if there are still more than one solution, find the energy using the expressions appropriate to the two solutions of φ . The lowest of all the values is taken to be the ground state energy.

To know the modifications of results brought about by the new trial wavefunction, let us compare eqs (3.50) with (3.16). The energy corresponding to the solution $\varphi = 0$ now has an additional term depending on the coupling constant. This means that, in eq (3.50a), there is a contribution from the interaction to the ground state energy. Another change that has occurred is in the value of ω which now varies with g . Some numerical results are given in Table (4) and, in the next section, we will compare them to the exact solutions.

3.3 COMPARISON OF APPROXIMATE RESULTS TO THE EXACT CALCULATIONS

3.3.1 Exact Calculations

To find the exact energy eigenvalues of the system, the hamiltonian (3.4), i.e.,

$$H = k\left(a^{+}a - b^{+}b\right) + \tfrac{1}{2}\pi^{2} + \tfrac{1}{2}\mu^{2}\phi^{2} + g\left(a^{+}b + b^{+}a\right)\phi \qquad (3.61)$$

is written in a representation in which the free hamiltonians of the orbit and oscillator are diagonal. Then the entire hamiltonian matrix is diagonalized by numerical methods. Let

$$\Psi = a^{+}|0\rangle\, U(\phi) + b^{+}|0\rangle\, V(\phi) \qquad (3.62)$$

be the eigenfunction of H. $U(\phi)$ and $V(\phi)$ are some functions of which will later be expanded in a suitable basis representation. The eigenvalue equation

$$H\Psi = E\Psi$$

gives

$$\begin{aligned} k\,a^{+}|0\rangle\, U(\phi) - k\,b^{+}|0\rangle\, V(\phi) + \tfrac{1}{2}(\pi^{2}+\mu^{2}\phi^{2})\left[a^{+}|0\rangle U(\phi) + b^{+}|0\rangle V(\phi)\right] \\ + g\,b^{+}|0\rangle\, U(\phi)\,\phi + g\,a^{+}|0\rangle\, V(\phi)\,\phi \\ = E\left[a^{+}|0\rangle\, U(\phi) + b^{+}|0\rangle V(\phi)\right] \end{aligned} \qquad (3.63)$$

Multiplying eq (3.63) on the left first by $\langle 0|a$ and then by $\langle 0|b$, we get the following two equations.

$$k\,U(\phi) + \left(\tfrac{1}{2}\pi^{2} + \tfrac{1}{2}\mu^{2}\phi^{2}\right)U(\phi) + g\phi\, V(\phi) = E\,U(\phi) \qquad (3.64a)$$

$$-k\,V(\phi) + \left(\tfrac{1}{2}\pi^2 + \tfrac{1}{2}\mu^2\phi^2\right) V(\phi) + g\phi\, U(\phi) = E\, V(\phi) \qquad (3.64b)$$

We now expand $U(\phi)$ and $V(\phi)$ in a harmonic oscillator basis (specifically the eigenfunctions of the free oscillator part of the hamiltonian).

$$\text{i.e.,} \qquad U(\phi) = \sum_n C_n |n\rangle \qquad (3.65a)$$

$$V(\phi) = \sum_m d_m |m\rangle \qquad (3.65b)$$

where

$$\left(\tfrac{1}{2}\pi^2 + \tfrac{1}{2}\mu^2\phi^2\right)|n\rangle = \mathcal{E}_n |n\rangle \qquad (3.66)$$

$$\mathcal{E}_n = \left(n + \tfrac{1}{2}\right)\mu$$

Therefore, the eigenvalue equations (3.64) become

$$(k + \mathcal{E}_n)\, C_n + g \sum_m d_m \langle n|\phi|m\rangle = E\, C_n \qquad (3.67a)$$

$$(-k + \mathcal{E}_m)\, d_m + g \sum_n C_n \langle m|\phi|n\rangle = E\, d_m \qquad (3.67b)$$

The coefficients of the C's and d's in the LHS of eq (3.67) are the elements of the matrix representing the hamiltonian of the system. This matrix is diagonalized following the method indicated in Section (2.3.1) and Appendix (B) to obtain the eigenvalues of the hamiltonian.

3.3.2 Comparison of the Approximate Calculations

Numerical calculations were performed for the case when $k = 1.0$ and $\mu = 0.1$. The ground state energy, for various values of the

coupling constant g , were obtained in the variational scheme using both the trial wavefunctions Ψ and Ψ_N . These values are listed in Table (4) along with the exact values.

It is clear that the results with the modified trial wavefunction Ψ_N (Section 3.2.3) are certainly better and closer to the exact values for all values of g . However, for very large values of g the two approximate calculations tend to give almost same values for the ground state energy.

The behaviour of the values of ω and α in the modified trial wavefunction is also noteworthy. From Section (3.2.3), it is easy to get that $\alpha=0$ and $\omega=\mu$ for $g=0$. For smaller values of g , α is non-zero and ω deviates substantially from μ as can be seen from Table (5). At large values of g , α becomes very small and ω tends towards μ . As remarked in Section (3.2.3), α has several solutions. In the numerical calculations, it was found that, for very large values of g , α had two solutions which satisfied the minimum conditions. One of the values is very small and the other value is very large and always the small values of α gave the lowest value for the ground state energy. This fact can be proved analytically also as discussed below.

For very large values of g , it is found that $\varphi \neq 0$ is the correct solution. Therefore, to find α and ω , we have to consider the minimization equations (3.59) and (3.60).

i.e.,

$$\omega = \frac{\mu^2}{2g\alpha}(1+\alpha^2) \tag{3.59}$$

$$16\mu^4\alpha^4 e^{-2\alpha^2}(1+2\alpha^2)^4 + \mu^6(1+2\alpha^2)^4 - 16g^4\alpha^4 = 0 \tag{3.60}$$

Small α :

When α is small, $e^{-2\alpha^2} \approx 1$, $(1+2\alpha^2) \approx 1$

Therefore, eq (3.60) becomes

$$16(\mu^4 - g^4)\alpha^4 + \mu^6 = 0$$

We can neglect μ^4 compared to g^4 in the first term and hence we obtain

$$\alpha = \frac{\mu^{3/2}}{2g} \tag{3.68}$$

and from (3.59)

$$\omega = \frac{\mu^2}{2g}\left(\frac{2g}{\mu^{3/2}} + \frac{\mu^{3/2}}{g}\right) \tag{3.69}$$

Large α :

When α is large, $e^{-2\alpha^2} \approx 0$, $1+2\alpha^2 \approx 2\alpha^2$

Thus, eq (3.60) becomes

$$16\mu^6\alpha^8 - 16g^4\alpha^4 = 0$$

the solution of which is

$$\alpha = g/\mu^{3/2} \tag{3.70}$$

and from (3.59)

$$\omega = \frac{\mu^2}{2g}\left(\frac{\mu^{3/2}}{g} + \frac{2g}{\mu^{3/2}}\right) \tag{3.71}$$

We notice that ω has the same value in both the cases. The ground state energy (eq (3.50b) is

$$E_0 = -\frac{1}{2}\frac{1}{(g^2/\mu^2)}\, e^{-2\alpha^2}(1+2\alpha^2)^2 - \frac{1}{2}\left(\frac{g^2}{\mu^2}\right) + \frac{1}{4}\left(\omega^2+\frac{\mu^2}{\omega^2}\right)$$

For small α ,

$$E_0 = -\frac{1}{2}\frac{1}{(g^2/\mu^2)} - \frac{1}{2}\left(\frac{g^2}{\mu^2}\right) + \frac{1}{4}\left(\omega^2+\frac{\mu^2}{\omega^2}\right) \qquad (3.72a)$$

For large α ,

$$E_0 = -\frac{1}{2}\frac{g^2}{\mu^2} + \frac{1}{4}\left(\omega^2+\frac{\mu^2}{\omega^2}\right) \qquad (3.72b)$$

Thus, we see that the small value of α always gives the lowest value for the ground state energy.

CHAPTER 4

TWO-ORBIT INTERACTION

We now come to the more interesting case of two-orbit interaction treated from a meson field theoretical point of view. It should be remembered that meson, in this work, refers to quanta of an oscillator. The theory and the mathematical techniques developed in the previous chapters are employed, in a straightforward manner, to carry out approximate calculations for the system of two orbits corresponding to two relativistic fermions interacting with an oscillator. We will be interested, specifically, in the role of the meson, the binding energy of the system and how the exchange energy is manifested.

Consider two orbits with fixed energies k_1 and k_2 interacting with an oscillator through a Yukawa type of coupling. It should be remembered that the word orbit is being used to refer to fermions and anti-fermions which can exist in the positive and negative energy levels when the interaction is absent (figure (2)). The ground state corresponds to case when both the negative energy orbits are filled. Now, there is the possibility of such excitations as one-particle-one-hole excitation and two-particle - two-hole excitations.

As in the case of one-orbit, let $|0\rangle$ denote the state in which no particles are present. We define the following creation and destruction operators.

a_1 destroys a particle in the state with positive energy k_1,

b_1 destroys a particle in the state with negative energy $-k_1$.

a_1^+, b_1^+ are the corresponding creation operators.

The operators a_2, b_2 and a_2^+, b_2^+ are defined in the same manner for the states with energy $\pm k_2$.

Naturally, $b_1^+ b_2^+ |0\rangle$ is the ground state and $a_1^+ a_2^+ |0\rangle$ is the two-particle - two-hole excited state. All these definitions refer to the system in the absence of the interaction. The hamiltonian of the system of two orbits interacting through an oscillator can now written as

$$H = k_1 (a_1^+ a_1 - b_1^+ b_1) + k_2 (a_2^+ a_2 - b_2^+ b_2) + \tfrac{1}{2}\pi^2 + \tfrac{1}{2}\mu^2\phi^2 + g(a_1^+ b_1 + b_1^+ a_1 + a_2^+ b_2 + b_2^+ a_2)\,\phi \qquad (4.1)$$

4.1 TIME DEPENDENT VARIATION

To begin with, let us choose a product of the free orbit wavefunction and a gaussian wavepacket as the trial wavefunction. That means we are extending the wavefunction Ψ in (3.5) to include two orbits. The trial wavefunction is

$$\Psi = \left(\frac{\omega}{\pi}\right)^{1/4} \left[(u_1 a_1^+ + v_1 b_1^+)(u_2 a_2^+ + v_2 b_2^+)|0\rangle\right] \times \exp\left[-\frac{\omega}{2}(\phi - \varphi)^2\right] \qquad (4.2)$$

Ψ is normalized when $(u_1^2 + v_1^2)(u_2^2 + v_2^2) = 1$

The choice

$$u_1^2 + v_1^2 = 1 \quad , \quad u_2^2 + v_2^2 = 1 \qquad (4.3)$$

takes care of the number operator to give the correct number of particles.

4.1.1 The Ground State Energy

Let us first carry out a stationary variational calculation with the variation parameters u_1, v_1, u_2, v_2, φ and ω which are assumed to be independent of time. The expectation value of the hamiltonian is

$$\begin{aligned}\mathcal{H} &= \langle \Psi | H | \Psi \rangle \\ &= k_1 (u_1^2 - v_1^2) + k_2 (u_2^2 - v_2^2) + \frac{\omega}{4} + \frac{1}{2}\mu^2(\varphi^2 + \frac{1}{2\omega}) \\ &\quad + 2g (u_1 v_1 + u_2 v_2)\varphi \end{aligned} \tag{4.4}$$

Introducing the Lagrange multipliers λ_1 and λ_2 to minimize $\mathcal{H}$, the hamiltonian becomes

$$\begin{aligned}\mathcal{H} - \lambda_1 - \lambda_2 = {} & k_1 (u_1^2 - v_1^2) + k_2 (u_2^2 - v_2^2) + \left(\frac{\omega}{4} + \frac{\mu^2}{4\omega}\right) \\ & + \frac{1}{2}\mu^2\varphi^2 + 2g(u_1 v_1 + u_2 v_2)\varphi \\ & - \lambda_1 (u_1^2 + v_1^2) - \lambda_2 (u_2^2 + v_2^2) \end{aligned} \tag{4.5}$$

where eq (4.3) has been used.

Minimizing with respect to u_1, v_1, u_2, v_2, we obtain

$$\frac{\partial \mathcal{H}}{\partial u_1} = 2k u_1 + 2g\varphi v_1 - 2\lambda_1 u_1 = 0 \tag{4.6a}$$

$$\frac{\partial \mathcal{H}}{\partial v_1} = -2k v_1 + 2g\varphi u_1 - 2\lambda_1 v_1 = 0 \tag{4.6b}$$

$$\frac{\partial \mathcal{H}}{\partial u_2} = 2k u_2 + 2g\varphi v_2 - 2\lambda_2 u_2 = 0 \tag{4.6c}$$

$$\frac{\partial \mathcal{H}}{\partial v_2} = -2k\, v_2 + 2g\varphi\, u_2 - 2\lambda_2 v_2 = 0 \qquad (4.6d)$$

Combining (4.6a) with (4.6b) and (4.6c) with (4.6d), we get

$$2k_1 u_1 v_1 = g\varphi\,(u_1^2 - v_1^2) \qquad (4.7a)$$

$$2k_2 u_2 v_2 = g\varphi\,(u_2^2 - v_2^2) \qquad (4.7b)$$

Using eq (4.3), these two equations can easily be solved to get

$$u_1^2 = \frac{1}{2}\left[1 \pm \frac{k_1}{\sqrt{k_1^2 + g^2\varphi^2}}\right] \quad , \quad v_1^2 = \frac{1}{2}\left[1 \mp \frac{k_1}{\sqrt{k_1^2 + g^2\varphi^2}}\right] \qquad (4.8a)$$

$$u_2^2 = \frac{1}{2}\left[1 \pm \frac{k_2}{\sqrt{k_2^2 + g^2\varphi^2}}\right] \quad , \quad v_2^2 = \frac{1}{2}\left[1 \mp \frac{k_2}{\sqrt{k_2^2 + g^2\varphi^2}}\right] \qquad (4.8b)$$

Also, we obtain

$$\lambda_1 = \pm\sqrt{k_1^2 + g^2\varphi^2} \quad , \quad \lambda_2 = \pm\sqrt{k_2^2 + g^2\varphi^2} \qquad (4.9)$$

Inserting eqs (4.8) in (4.4), the hamiltonian becomes

$$\mathcal{H} = \pm\sqrt{k_1^2 + g^2\varphi^2} \pm \sqrt{k_2^2 + g^2\varphi^2} + \frac{1}{4}\left(\omega + \frac{\mu^2}{\omega}\right) + \frac{1}{2}\mu^2\varphi^2 \qquad (4.10)$$

Notice the appearance of the effective mass of the orbits with single particle energy λ_1 and λ_2. Only the negative signs of λ_1 and λ_2 in (4.10) give the minimum energy.

Minimizing $\mathcal{H}$ in (4.10) with respect to φ and ω, we obtain

$$\frac{\partial \mathcal{H}}{\partial \varphi} = \mu^2 \varphi - \frac{g^2 \varphi}{\sqrt{k_1^2 + g^2\varphi^2}} - \frac{g^2 \varphi}{\sqrt{k_2^2 + g^2\varphi^2}} = 0 \tag{4.11}$$

$$\frac{\partial \mathcal{H}}{\partial \omega} = \frac{1}{4} - \frac{\mu^2}{4\omega^2} = 0 \tag{4.12}$$

Eq (4.12) immediately gives

$$\omega = \mu \tag{4.13}$$

From eq (4.11), it is clear that φ has two solutions:

(i) $\varphi = 0$ (4.14a)

(ii) a solution of

$$\frac{g^2}{\mu^2}\left[\frac{1}{\sqrt{k_1^2 + g^2\varphi^2}} + \frac{1}{\sqrt{k_2^2 + g^2\varphi^2}}\right] = 1 \tag{4.14b}$$

The second derivative minimum tests for these extremum values show that the minimum values of φ are as follows.

(i) $\varphi = 0$ when $\frac{g^2}{\mu^2} < \frac{k_1 k_2}{k_1 + k_2}$

(ii) $\varphi \neq 0$ (solution of eq (4.14b)) when $\frac{g^2}{\mu^2} > \frac{k_1 k_2}{k_1 + k_2}$

With the use of eqs (4.13) and (4.10), the ground state energy is given by

$$E_0 = -\sqrt{k_1^2 + g^2\varphi^2} - \sqrt{k_2^2 + g^2\varphi^2} + \frac{1}{2}\mu + \frac{1}{2}\mu^2\varphi^2 \tag{4.15}$$

Corresponding to the two solutions of φ, the ground state energy is

$$E_0 = -k_1 - k_2 + \frac{1}{2}\mu \qquad \text{when} \quad \frac{g^2}{\mu^2} < \frac{k_1 k_2}{k_1 + k_2} \tag{4.16a}$$

$$E_0 = -\sqrt{k_1^2 + g^2\varphi_0^2} - \sqrt{k_2^2 + g^2\varphi_0^2} + \frac{1}{2}\mu + \frac{1}{2}\mu^2\varphi_0^2$$

$$\text{when} \quad \frac{g^2}{\mu^2} > \frac{k_1 k_2}{k_1 + k_2} \tag{4.16b}$$

A Special Case: When $k_1 = k_2$

When $k_1 = k_2 \equiv k$, eq (4.14b) can be easily solved to obtain the minimum value of φ as

$$\varphi^2 = \frac{1}{g^2}\left(4\frac{g^4}{\mu^4} - k^2\right) \tag{4.17}$$

Thus, the ground state energy is

$$E_0 = \begin{cases} -2k + \frac{1}{2}\mu & \text{when} \quad \frac{g^2}{\mu^2} < \frac{k}{2} \\ -2\frac{g^2}{\mu^2} + \frac{1}{2}\mu - \frac{1}{2}k^2\frac{\mu^2}{g^2} & \text{when} \quad \frac{g^2}{\mu^2} > \frac{k}{2} \end{cases} \tag{4.18}$$

4.1.2 Near Equilibrium Dynamics

By treating the variation parameters u_1 , v_1 , u_2 , v_2 and φ as time-dependent, the small oscillations around the ground state are studied as usual. When φ is time-dependent, we must start with the following trial wavefunction.

$$\Psi = \left(\frac{\omega}{\pi}\right)^{1/4}\left[(u_1 a_1^+ + v_1 b_1^+)(u_2 a_2^+ + v_2 b_2^+)|0\rangle\right]$$

$$\times \exp\left[-\frac{\omega}{2}(\phi - \varphi)^2 + iP(\phi - \varphi)\right] \tag{4.19}$$

With u_1, v_1, u_2 and v_2 being complex, the langrangian is

$$\mathcal{L} = \langle \Phi | i \frac{\partial}{\partial t} | \Phi \rangle - \mathcal{H}$$

$$= i\left(u_1^* \dot{u}_1 + v_1^* \dot{v}_1\right) + i\left(u_2^* \dot{u}_2 + v_2^* \dot{v}_2\right) + P\dot{\varphi} - \mathcal{H} \qquad (4.20)$$

where

$$\mathcal{H} = \langle \Phi | H | \Phi \rangle$$

$$= k_1\left(u_1^* u_1 - v_1^* v_1\right) + k_2\left(u_2^* u_2 - v_2^* v_2\right)$$

$$+ \frac{1}{4}\left(\omega + \frac{\mu^2}{\omega}\right) + \frac{1}{2}\mu^2\varphi^2 + \frac{1}{2}P^2$$

$$+ g\left[\left(u_1^* v_1 + v_1^* u_1\right) + \left(u_2^* v_2 + v_2^* u_2\right)\right]\varphi \qquad (4.21)$$

is the classical hamiltonian. The methods of the previous section will help us to find the minimum values of the variation parameters and the ground state energy. The pattern of the results is similar to the one-orbit case (Chapter 3). It is found that u_1, v_1, u_2, v_2 are real when $\mathcal{H}$ is minimized and hence the ground state energy is as given in the stationary variational case.

By expanding the variation parameters about the equilibrium values, the RPA frequencies can be found. The calculations have to be performed following exactly the same method used in the one-orbit case (Section 3.2.2). The only difference in this case is that there are two additional parameters u_2 and v_2. Instead of repeating the already familiar method of Section (3.2.2), we merely give the final result.

The RPA frequencies are

(i) $$\omega_1 = 0 \tag{4.22}$$

(ii) solutions of

$$(\omega_2^2-\mu^2)(\omega_2^2-4\lambda_1^2)(\omega_2^2-4\lambda_2^2)$$
$$+2g^2\left[\omega_2^4-2(\lambda_1^2+\lambda_2^2)(\omega_2^2-4g^2\varphi^2)-4\omega^2g^2\varphi^2\right]=0 \tag{4.23}$$

where

$$\lambda_1^2 = k_1^2+g^2\varphi^2 \quad , \quad \lambda_2^2 = k_2^2+g^2\varphi^2$$

When $g=0$, we get

$$\omega_1 = 0$$
$$\omega_2 = \mu\,,\ 2k_1\,,\ 2k_2$$

As in the case of one-orbit, Ψ in (4.2) is not a proper choice. This inference is drawn by examining the ground state energy given by eq (4.16). For the weak coupling, there is no contribution to total energy from the interaction. Moreover, we have not gained any information about the exchange effect of the interaction between the two fermions.

4.1.3 Variation with the Modified Trial Wavefunction

In order to improve the results of the last section, we follow the example of the one-orbit case and try a new wavefunction of the type given in (3.29).

$$\Phi_N = e^{-i\gamma\pi\,\bar{\Psi}\Psi}\,\Phi \tag{4.24}$$

In the present case,

$$\bar{\Psi}\Psi = a_1^+ b_1 + b_1^+ a_1 + a_2^+ b_2 + b_2^+ a_2 \tag{4.25}$$

As we shall see later, this transformation introduces the important exchange effect which could obviously be not present in the one-orbit case. The new trial wavefunction is

$$\begin{aligned}\Phi_N = {} & e^{-i\frac{\alpha}{\sqrt{\omega}}\pi\left[(a_1^+ b_1 + b_1^+ a_1) + (a_2^+ b_2 + b_2^+ a_2)\right]} \\ & \times\left[(u_1 a_1^+ + u_2 b_1^+)(u_2 a_2^+ + v_2 b_2^+)|0\rangle\right] \\ & \times\left(\frac{\omega}{\pi}\right)^{1/4} \exp\left[-\frac{\omega}{2}(\phi-\varphi)^2\right]\end{aligned} \tag{4.26}$$

We just carry out a stationary variational calculation here. The expectation value of the hamiltonian (4.1) is

$$\begin{aligned}\mathcal{H} &= \langle\Phi_N|\,H\,|\Phi_N\rangle \\ &= \langle\Phi|\,e^{i\frac{\alpha}{\sqrt{\omega}}\pi\bar{\Psi}\Psi}\,H\,e^{-i\frac{\alpha}{\sqrt{\omega}}\pi\bar{\Psi}\Psi}\,|\Phi\rangle\end{aligned} \tag{4.27}$$

where Φ is given by eq (4.2).

The integrals in eq (4.27) can be evaluated by following the methods used in Section (3.2.3). Thus, we obtain

$$H_1 = \langle \Psi_N | k_1 (a_1^\dagger a_1 - b_1^\dagger b_1) | \Psi_N \rangle$$
$$= k_1 (u_1^2 - v_1^2) e^{-\alpha^2} \qquad (4.28a)$$

$$H_2 = \langle \Psi_N | k_2 (a_2^\dagger a_2 - b_2^\dagger b_2) | \Psi_N \rangle$$
$$= k_2 (u_2^2 - v_2^2) e^{-\alpha^2} \qquad (4.28b)$$

$$H_3 = \langle \Psi_N | \tfrac{1}{2} \pi^2 | \Psi_N \rangle$$
$$= \frac{1}{4} \omega \qquad (4.28c)$$

Before evaluating the expectation value of $\frac{1}{2}\mu^2\phi^2$, consider the following.

$$e^{i\frac{\alpha}{\sqrt{\omega}}\pi\bar{\Psi}\Psi} \left(\tfrac{1}{2}\mu^2\phi^2\right) e^{-i\frac{\alpha}{\sqrt{\omega}}\pi\bar{\Psi}\Psi}$$
$$= \tfrac{1}{2}\mu^2 \left(\phi - \frac{\alpha}{\sqrt{\omega}}\bar{\Psi}\Psi\right)^2$$
$$= \tfrac{1}{2}\mu^2 \left\{ \phi - \frac{\alpha}{\sqrt{\omega}} \left[(a_1^\dagger b_1 + b_1^\dagger a_1) + (a_2^\dagger b_2 + b_2^\dagger a_2) \right] \right\}^2 \qquad (4.28d)$$

We now get a cross term between $(a_1^\dagger b_1 + b_1^\dagger a_1)$ and $(a_2^\dagger b_2 + b_2^\dagger a_2)$ which appears only because we are considering more than one orbit. Similar effect is introduced in the interaction term also.

$$H_4 = \langle \Psi_N | \tfrac{1}{2}\mu^2\phi^2 | \Psi_N \rangle$$
$$= \tfrac{1}{2}\mu^2 \left[\varphi^2 + \frac{\alpha^2}{\omega} (2 + 8 u_1 v_1 u_2 v_2) - 4(u_1 v_1 + u_2 v_2)\varphi + \frac{1}{2\omega} \right]$$
$$(4.28e)$$

$$H_5 = \langle \Psi_N | \, g(a_1^\dagger b_1 + b_1^\dagger a_1 + a_2^\dagger b_2 + b_2^\dagger a_2)\,\phi \, | \Psi_N \rangle$$

$$= 2g(u_1 v_1 + u_2 v_2)\varphi - \frac{g\alpha}{\sqrt{\omega}}(2 + 8\, u_1 v_1 u_2 v_2) \qquad (4.28f)$$

Collecting all the terms in (4.28), the expectation value of the hamiltonian becomes

$$\mathcal{H} = k_1 (u_1^2 - v_1^2)\, e^{-\alpha^2} + k_2 (u_2^2 - v_2^2)\, e^{-\alpha^2}$$

$$+ \frac{1}{4}\left(\omega + \frac{\mu^2}{\omega}\right) + \frac{1}{2}\mu^2 \varphi^2$$

$$+ \left(\frac{1}{2}\mu^2 \frac{\alpha^2}{\omega} - \frac{g\alpha}{\sqrt{\omega}}\right)(2 + 8\, u_1 v_1 u_2 v_2) + 2\left(g - \mu^2 \frac{\alpha}{\sqrt{\omega}}\right)(u_1 v_1 + u_2 v_2)\varphi \qquad (4.29)$$

For convenience, we put $2\left(\mu^2 \frac{\alpha^2}{\omega} - \frac{g\alpha}{\sqrt{\omega}}\right) \equiv A$, $\left(g - \mu^2 \frac{\alpha}{\sqrt{\omega}}\right) \equiv G$

The term $4A u_1 v_1 u_2 v_2$ in the hamiltonian can be interpreted as an equivalent of Hartree-Fock exchange term. Let us minimize $\mathcal{H}$ first with respect to u's and v's (after introducing the usual Lagrange multipliers λ_1 and λ_2).

$$\frac{\partial \mathcal{H}}{\partial u_1} = 2k_1 e^{-\alpha^2} u_1 + 2G\varphi v_1 + 4A\, v_1 u_2 v_2 - 2\lambda_1 u_1 = 0 \qquad (4.30a)$$

$$\frac{\partial \mathcal{H}}{\partial v_1} = -2k_1 e^{-\alpha^2} v_1 + 2G\varphi u_1 + 4A\, u_1 u_2 v_2 - 2\lambda_1 v_1 = 0 \qquad (4.30b)$$

$$\frac{\partial \mathcal{H}}{\partial u_2} = 2k_2 e^{-\alpha^2} u_2 + 2G\varphi v_2 + 4A\, u_1 v_1 v_2 - 2\lambda_2 u_2 = 0 \qquad (4.30c)$$

$$\frac{\partial \mathcal{H}}{\partial u_2} = -2k_2 e^{-\alpha^2} u_2 + 2G\varphi u_2 + 4A u_1 v_1 u_2 - 2\lambda_2 u_2 = 0 \qquad (4.30d)$$

Though these equations cannot be solved without resorting to numerical methods, it is useful to bring them to some simplified form. Thus, from eq (4.30), we get

$$u_1^2 = \frac{1}{2}\left\{1 \pm \frac{E_1}{\left[E_1^2 + (G\varphi + 2A u_2 v_2)^2\right]^{1/2}}\right\} \qquad (4.31a)$$

$$u_2^2 = \frac{1}{2}\left\{1 \pm \frac{E_2}{\left[E_2^2 + (G\varphi + 2A u_1 v_1)^2\right]^{1/2}}\right\} \qquad (4.31b)$$

where we have put $k_1 e^{-\alpha^2} \equiv E_1$, $k_2 e^{-\alpha^2} \equiv E_2$

Inserting eq (4.31) in (4.29), the hamiltonian becomes (after some algebra)

$$\mathcal{H} = \pm\left[E_1^2 + (G\varphi + 2A u_2 v_2)^2\right]^{1/2} \pm \left[E_2^2 + (G\varphi + 2A u_1 v_1)^2\right]^{1/2}$$
$$+ \frac{1}{4}\left(\omega + \frac{\mu^2}{\omega}\right) + \frac{1}{2}\mu^2\varphi^2 + A\left(1 - 4u_1 v_1 u_2 v_2\right) \qquad (4.32)$$

Thus, in the hamiltonian, we have the single particle energy for each orbit, the energy of the meson, and the interaction energy which now includes an exchange-type term.

Continuing the minimization process, we find

$$\frac{\partial \mathcal{H}}{\partial \varphi} = \mu^2 \varphi + 2G(u_1 v_1 + u_2 v_2) = 0 \tag{4.33a}$$

$$\frac{\partial \mathcal{H}}{\partial \omega} = \left(\frac{1}{4} - \frac{\mu^2}{4\omega^2}\right) + \left(\frac{g\alpha}{2\sqrt{\omega^3}} - \frac{\mu^2\alpha^2}{2\omega^2}\right)(2 + 8u_1 v_1 u_2 v_2)$$

$$+ \frac{\mu^2\alpha}{\sqrt{\omega^3}}(u_1 v_1 + u_2 v_2)\varphi = 0 \tag{4.33b}$$

$$\frac{\partial \mathcal{H}}{\partial \alpha} = -2k_1(u_1^2 - v_1^2)\alpha e^{-\alpha^2} - 2k_2(u_2^2 - v_2^2)\alpha e^{-\alpha^2}$$

$$+ \left(\frac{\mu^2\alpha}{\omega} - \frac{g}{\sqrt{\omega}}\right)(2 + 8u_1 v_1 u_2 v_2) - \frac{2\mu^2}{\sqrt{\omega}}(u_1 v_1 + u_2 v_2)\varphi = 0 \tag{4.33c}$$

In order to find the ground state energy, the seven simultaneous equations (4.30, 4.33) must be solved. This can be done only by numerical method which depends very sensitively on the initial values of the variational parameters supplied for the iteration process.

Let us consider a special case when $k_1 = k_2 = 1.0$.

In this case $u_1 = u_2$ and $v_1 = v_2$

Let $u_1 = u_2 \equiv u$ and $v_1 = v_2 \equiv v$

From eqs (4.30), we obtain

$$2uv\, e^{-\alpha^2} - G\varphi(u^2 - v^2) - 2Auv(u^2 - v^2) = 0 \tag{4.34}$$

and from eq (4.30a), we have

$$\mu^2 \varphi + 4Guv = 0 \tag{4.35}$$

In eqs (4.34) and (4.35), φ can be eliminated to get

$$uv = 0 \qquad \left\{ \begin{matrix} u=0, & v=1 \\ u=1, & v=0 \end{matrix} \right\} \tag{4.36}$$

$$e^{-\alpha^2} + \frac{2G^2}{\mu^2}(u^2 - v^2) - A(u^2 - v^2) = 0 \tag{4.37}$$

The solution to eq (4.37) is

$$u^2 = \frac{1}{2}\left[1 - \frac{e^{-\alpha^2}}{\left(2\frac{G^2}{\mu^2} - A\right)}\right] \quad , v^2 = \frac{1}{2}\left[1 + \frac{e^{-\alpha^2}}{\left(2\frac{G^2}{\mu^2} - A\right)}\right]$$

In (4.36), only the solution ($u=0$, $v=1$) corresponds to the ground state energy.

The corresponding solutions of φ are

$$\text{(i)} \quad \varphi = 0 \tag{4.38a}$$

$$\text{(ii)} \quad \varphi = -\frac{2G}{\mu^2}\left[1 - \frac{e^{-2\alpha^2}}{\left(2\frac{G^2}{\mu^2} - A\right)^2}\right] \tag{4.38b}$$

In each of these two cases, α and ω have to be found separately from eq (4.33).

<u>case (i) when φ =0</u>.

We have to solve

$$\frac{1}{4}\left(1 - \frac{\mu^2}{\omega^2}\right) + 2\left(g\frac{\alpha}{2\sqrt{\omega}} - \frac{\mu^2\alpha^2}{2\omega^2}\right) = 0 \tag{4.39a}$$

$$-2\alpha e^{-\alpha^2} + \left(\frac{\mu^2\alpha}{\omega} - \frac{g}{\sqrt{\omega}}\right) = 0 \tag{4.39b}$$

The ground state energy is

$$E_0 = -2e^{-2\alpha^2} + \frac{\omega}{4} + \frac{\mu^2}{4\omega} + 2\left(\frac{\mu^2\alpha^2}{2\omega} - \frac{g\alpha}{\sqrt{\omega}}\right) \qquad (4.39c)$$

<u>case (ii) when $\langle\varphi\rangle \neq 0$</u>.

We have to solve

$$\frac{1}{4}\left(1 - \frac{\mu^2}{\omega^2}\right) + \frac{\alpha}{\omega}\,\frac{G e^{-2\alpha^2}}{\left(2\frac{G^2}{\mu^2} - A\right)^2} = 0 \qquad (4.40a)$$

$$2\alpha + \frac{G\mu^2}{\sqrt{\omega}\left(-\mu^2 A + 2G^2\right)} = 0 \qquad (4.40b)$$

The ground state energy is

$$E_0 = 2(u^2 - v^2)e^{-\alpha^2} + \left(\frac{\omega}{4} + \frac{\mu^2}{4\omega}\right) + A(1 + 4u^2v^2) - 8G^2\frac{u^2v^2}{\mu^2} \qquad (4.40c)$$

The eqs (4.39) and (4.40) are solved by the standard iteration process based on Gauss elimination method (see Appendix (A)). Care must be taken to supply appropriate initial values to the variables. In the next section, we will list the ground state energy for various values of the coupling constant g and compare them to the exact values and the values obtained by using $\mathcal{H}$.

4.2 COMPARISON OF APPROXIMATE RESULTS TO THE EXACT CALCULATIONS

The exact values of the energy eigenvalues can be calculated by the method described in Section (3.3.1). In this section, we compare exact ground state energy to the approximate ones for various values of g . Also, we calculate the interaction potential energy in the second order perturbation theory and compare it to the binding energy calculated by the exact and the variational methods.

4.2.1 The Ground State Energy

For $k_1 = k_2 = 1$ and $\mu = 0.1$, the ground state energy was calculated by the variational method using the two trial wavefunctions Ψ_1 and Ψ_N and are listed in Table (6) along with the exact values. Because of the limitation of the computer storage, the exact values could not be obtained for very large values of g . Again, we find that the calculations with Ψ_N give more accurate results. However, as g moves towards larger values, both the wavefunctions give almost the same results. The parameter α appearing in the wavefunction Ψ_N tends towards zero as g becomes very high. In this limit, ω approaches the value of μ .

4.2.2 The Interaction Potential Energy

Using the ground state energies of the one-orbit and the two-orbit systems, the binding energy of the two-orbit system can be calculated in the exact and the variational methods. Let the ground state energy of the two-orbit system be denoted by E_V . Figures (3)

show the various possible configurations in the two-orbit case. To calculate the binding energy of the two-orbit, we have to find the interaction energy required to bring together two one-orbit systems to form a two-orbit system. As shown in figure (3e), the one-orbit system is equivalent to one-hole configuration of the two-orbit case. If we take all the energies with respect to the ground state energy of the two-orbit (figure(3a)), we have to consider the two-hole configuration (figure (3f)) to find the binding energy.

Let $E_{1\text{-}H}$ be the one-hole energy and $E_{2\text{-}H}$ the two-hole energy. If E_1 is the energy of the ground state of one-orbit (chapter 3), then

$$E_{1-H} = E_1 - E_V$$

$$E_{2-H} = \tfrac{1}{2}\mu - E_V$$

The binding energy E_B is

$$E_B = E_{2-H} - 2(E_{1-H}) \tag{4.41}$$

We now calculate the interaction potential energy by the perturbation method. Consider the hamiltonian of the two-orbit given by

$$H = H_F + H_{OS} + H_I$$

$$H_F = k_1(a_1^+ a_1 - b_1^+ b_1) + k_2(a_2^+ a_2 - b_2^+ b_2)$$

$$H_{OS} = \tfrac{1}{2}\pi^2 + \tfrac{1}{2}\mu^2\phi^2$$

$$H_I = g(a_1^+ b_1 + b_1^+ a_1 + a_2^+ b_2 + b_2^+ a_2)\phi$$

Treating H_I as the perturbation, the unperturbed eigenstates and the energy eigenvalues are as given below.

Ground State: $|N_0\rangle$

Eigenstate: $b_1^+ b_2^+ |0\rangle \Psi_0$ Energy: $-k_1 - k_2 + \frac{1}{2}\mu$

where Ψ_0 is the ground state of the unperturbed oscillator.

Excited States: $|N_n\rangle$

Let Ψ_n, $n = 1, 2, \cdots$ denote the excited states of the unperturbed oscillator with energy $\varepsilon_n = (n + 1/2)\mu$

Eigenstates:	Energy: E_{N_n}	
$a_1^+ b_2^+ \|0\rangle \Psi_n$	$k_1 - k_2 + \varepsilon_n$	
$a_2^+ b_1^+ \|0\rangle \Psi_n$	$-k_1 + k_2 + \varepsilon_n$	
$a_1^+ a_2^+ \|0\rangle \Psi_n$	$k_1 + k_2 + \varepsilon_n$	$n = 1, 2, 3, \cdots\cdots$

The eigenstates listed above form the complete set of the unperturbed hamiltonian of the two-orbit.

In the first order perturbation, there is no contribution for the interaction energy becasue of the presence of the linear power of ϕ. However, in the second order,

$$E_I = \sum_n \frac{|\langle N_0 | H_I | N_n \rangle|^2}{E_{N_0} - E_{N_n}}$$

$$E_I = -\frac{g^2}{\mu} \frac{(k_1 + k_2 + \mu)}{(2k_1 + \mu)(2k_2 + \mu)} \qquad (4.42)$$

Table (8) shows the interaction potential energy calculated by all the methods mentioned above for various values of g . We notice that the variational calculation with Ψ_N gives quite close results when compared to the exact case. The perturbation results do not match well with both the exact and the variational calculations expecially for large values of g .

CHAPTER 5

SUMMARY

In this work, we have explored ways to solve the problem of two-nucleon interaction from a meson field theoretical point of view. This was achieved by applying a time-dependent variational method to a system of two fermions interacting with an oscillator.

We first developed the calculational schemes for quantum mechanical non-linear systems in the two many-body approximation techniques by working the example of an anharmonic oscillator. By choosing a gaussian wavepacket as the trial wavefunction, the energy of the ground state and the excited states were found in the time-dependent variational method. These approximate solutions were found to match well with the exact values. The frequencies of the small oscillations (RPA) about the equilibrium ground state correspond to the first two excited states. We also showed that the equations-of-motion method of Kerman and Klein can be used as a practical tool to study quantum mechanical non-linear systems. The rapid convergence of the values of the matrix elements and the energy eigenvalues justified the assumptions regarding the magnitudes of the matrix elements. We also found that the first-order Kerman-Klein calculations gave results identical to those of the time-dependent variation. These two approximation techniques can easily be extended to two-dimensional systems such as the coupled anharmonic oscillators. In the TDV, we then have to take

a product of two gaussian wavepackets as the trial wavefunction. Similarly, in the Kerman-Klein method, we can find the energies by designating the eigenstates by two quantum numbers for the two oscillaotrs.

The application of the time-dependent variational method to the system of one orbit coupled to an oscillator is quite straightforward as discussed in Chapter 3. The trial wavefunction Ψ is just a product of the wavefunctions of the free hamiltonians. The energy values, when compared to the exact values, showed the need of a better wavefunction. The modified wavefunction consisted of a unitary transformation on the old trial wavefunction and gave better results. This was natural since the modified wavefunction Ψ_N had a fermion-oscillator cross term as it should be. The ground state energy values with Ψ_N are very close to the exact ones. Also the frequency of the quanta of the oscillator (mesons) varies with the coupling constant g and hence it is a manifestation of the dynamics of the meson involved. However, at very large values of g , the new trial wavefunction Ψ_N tends towards the old one i.e., Ψ, a product of the wavefunctions of the free hamiltonians.

In the case of the two-orbit system coupled to an oscillator, we could extend the calculational scheme of the one-orbit system to include two orbits. The results were similar in pattern to those of the one-orbit system. However, in the two-orbit system, the variational calculations with the modified wavefunction Ψ_N clearly indicated the

appearance of the exchange interaction term. The frequency of the 'meson' which varies with the value of the coupling constant demonstrates the involvement of the dynamics of the meson. The binding energy calculated by the variational method agrees with the exact ones (with the limited number of values we could obtain). However, the perturbation results are substantially away from the variational results. This indicates the need for higher order perturbation calculations.

The method of the Kerman-Klein calculations for the example of the anharmonic oscillator is quite general. It can be extended to the two-orbit system by designating the eigenstates by the quantum numbers corresponding to the fermion state and oscillator state. We noticed that, in the case of the anharmonic oscillator, the TDV and the first-order Kerman-Klein calculations gave identical results. For the two-orbit system, it will not be hard to obtain results identical to those of the TDV method with the trial wavefunction Φ . Thus, by working with higher states ('multi-meson' states) we can improve the first-order Kerman-Klein calculations in a systematic and self-consistent manner. It will be interesting to compare such results to the TDV calculations with the modified trial wavefunction Φ_N.

Thus we have shown ways to apply the variational method to the two-body interaction of the nucleons from a meson field theoretical point of view. The possible extension of this work lies in introducing

boson field instead of the oscillator and studying the full field theoretical problem. After that, one can introduce more fermions and study the properties of the many-particle systems.

APPENDIX

A. Solution of a Set of Simultaneous Non-linear Equations

Here we briefly describe the numerical method to solve the set of non-linear equations encountered in the Kerman-Klein calculations. Let

$$f_i(z_1, \cdots, z_n) = 0 \qquad i = 1, \cdots, n \qquad \text{(A.1)}$$

be the given set of non-linear equations to be solved. These equations are supposed to contain at least one coupling parameter, say, λ. Let us suppose that for some value $\lambda = \lambda_0$ or in certain approximation limit, the approximate solutions $(z_1^0, \cdots, z_n^0)$ are known. Then we have

$$f_i(z_1^0, \cdots, z_n^0) = -c_i \qquad \text{(A.2)}$$

From (A.1) and (A.2), we obtain

$$\sum_j \left(\frac{\partial f_i}{\partial z_j^0}\right) \delta z_j^0 = \sum_j D_{ij}\, \delta z_j^0 \cong c_i \qquad j = 1, \cdots, n \qquad \text{(A.3)}$$

where $\delta z_j^0 = z_j - z_j^0$.

These corrections δz_j^0 can be found by the standard Gauss elimination process. Then

$$z_j^1 = z_j^0 + \delta z_j^0$$

will be the initial values for the next order of approximation. This iteration process is continued till convergence is achieved. One must

be cautious to choose proper initial values z_j^0 and the increment δz_j^0 for the iteration process.

This program can also be used to solved the non-linear equations of the variational calculations of Sections (3.2.3) and (4.1.3).

B. Diagonalization of a symmetric matrix

This brief discussion is about finding the energy eigenvalues of a symmetric real matrix of the kind that appears in the exact calculations of all the systems we considered.

The method due to Jacobi consists of finding the eigenvalues of a real symmetric matrix by a similarity transformation. For any symmetric matrix A, an orthogonal matrix S can be found with the property:

$$S^T A S = D$$

The elements D_{ik} of D have the form

$$D_{ik} = \epsilon_i \delta_{ik}$$

where ϵ_i are the eigenvalues of the matrix.

The fundamental approach of Jacobi method is to annihilate, in turn, the off-diagonal elements of A by 'elementary' orthogonal transformations. For a particular off-diagonal element of A, namely A_{pq}, the transformation is

$$R_{pp} = \cos\theta \qquad R_{pq} = \sin\theta$$
$$R_{qp} = -\sin\theta \qquad R_{qq} = \cos\theta$$

where θ is taken to be a convenient function of the off-diagonal elements. Then the transformation $B = R^T A R$ is carried out. This process is carried out, in turn, for every off-diagonal term. This process is called one cycle. The iteration process is continued in cycles with a new threshold for the off-diagonal elements till the desired accuracy is achieved. For details of this procedure, see reference [6].

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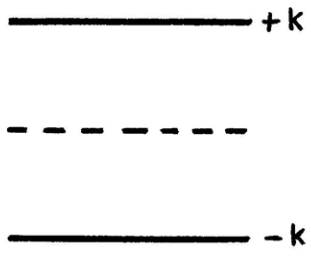


Figure 1: One-orbit

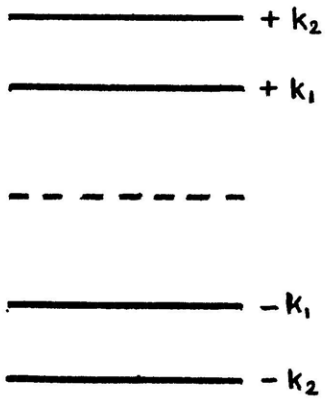
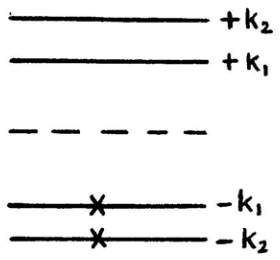
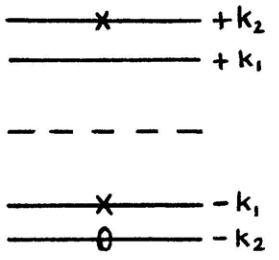


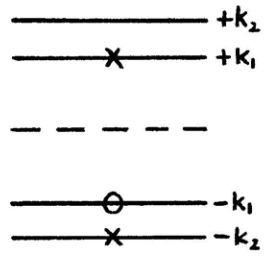
Figure 2: Two-orbit



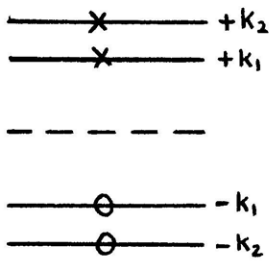
(a) Vacuum



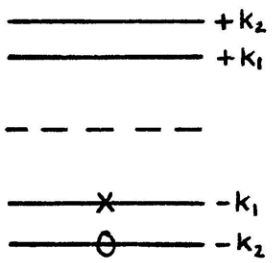
(b) One-Particle
One-Hole
Excitation



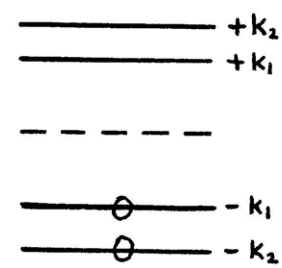
(c) One-Particle
One-Hole
Excitation



(d) Two-Particle
Two-Hole
Excitation



(e) One-Hole
(Equivalent to
One-Orbit)



(f) Two-Hole
(no particle)

X --Particle
O --Hole

Figure 3: Two-Orbit

Matrix Element	First Order	Second Order	Third Order
$\langle 0\|\phi\|1\rangle$	0.59108	0.59534	0.59534
$\langle 1\|\phi\|2\rangle$	0.83591	0.77109	0.77099

Table 1: Anharmonic Oscillator:
Matrix Elements for $\lambda = 1.0$

λ	Exact	TDV	Kerman-Klein Method		
			First Order	Second Order	Third Order
0.1	0.517364	0.517520	0.517520	0.517365	0.517365
1.0	0.620925	0.624016	0.624016	0.620932	0.620927
10.0	1.009134	1.02352	1.02352	1.00921	1.00917

Table 2: Ground State Energy of the Anharmonic Oscillator

λ	Exact	TDV	Kerman-Klein Method		
			First Order	Second Order	Third Order
0.1	1.583603	1.585443	1.585443	1.583614	1.583613
1.0	2.025944	2.055143	2.055143	2.026069	2.025966
10.0	3.506699	3.624767	3.624767	3.507371	3.506741

Table 3a: First Excited State Energy of the Anharmonic Oscillator

	Exact	TDV	Kerman-Klein Method		
			First Order	Second Order	Third Order
0.1	2.708621	2.524061	2.653367	2.708543	2.708631
1.0	3.698415	3.831162	3.486271	3.696452	3.698444
10.0	6.733807	6.98515	6.226008	6.725769	6.733833

Table 3b: Second Excited State Energy of the Anharmonic Oscillator

g	$\frac{g^2}{\mu^2}$	Exact	Variation	
			Using Ψ	Using Ψ_N
0.03162	0.1	-0.95244	-0.95	-0.952436
0.07071	0.5	-0.96365	-0.95	-0.963652
0.1	1.0	-0.9864	-0.95	-0.98439
0.12247	1.5	-1.04884	-1.0333	-1.04721
0.14142	2.0		-1.19998	-1.207021
0.2236	5.0		-2.54985	-2.55088
0.3162	10.0		-4.99913	-4.99938
0.5	25.0		-12.47	-12.47004

Table 4: One-orbit coupled to an Oscillator
Ground State Energy (k =1.0, μ =0.1)

$\frac{q^2}{\mu^2}$	α	ω
0.1	0.04796	0.09544
0.5	0.12308	0.07451
1.0	0.16876	0.05894
1.5	0.23	0.04132
2.0	0.16327	0.06937
5.0	0.0722	0.0979
10.0	0.0504	0.0995
25.0	0.0317	0.09992

Table 5: One-orbit
Minimum values of α, ω
($\mu = 0.1$)

g	$\frac{g^2}{\mu^2}$	Exact	Variation	
			Using Ψ	Using Ψ_N
0.03162	0.1	-1.955009	-1.95	-1.95499
0.07071	0.5	-1.98716	-1.95	-1.98376
0.1	1.0	-2.45666	-2.45	-2.45478
0.14142	2.0		-4.19993	-4.20152
0.2236	5.0		-10.0494	-10.04965

Table 6: Two-orbit
Ground State Energy ($K_1 = K_2 = 1.0$, $\mu = 0.1$)

$\frac{g^2}{\mu^2}$	α	ω
0.0	0.0	0.1
0.1	0.05	0.09055
0.5	0.156	0.04276
1.0	0.085	0.0864
2.0	0.057	0.0968
5.0	0.035	0.0995
100.0	0.008	0.099998

Table 7: Two-orbit
Minimum values of α, ω
($\mu = 0.1$)

$\frac{g^2}{\mu^2}$	Exact	Variation		Perturbation
		Using Ψ	Using Ψ_N	
0.1	-0.00013	0.0	-0.00012	-0.00476
0.5	-0.00986	0.0	-0.00646	-0.02381
1.0	-0.43386	-0.5	-0.436	-0.04762
2.0		-1.74997	-1.73748	-0.09524
5.0		-4.9443	-4.89789	-0.23808

Table 8: Binding Energy of the Two-orbit System
($k_1 = k_2 = 1.0$, $\mu = 0.1$)