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A STUDY OF THE RELATIONSHIP BETWEEN THE SEMI-CLASSICAL AND THE GENERATOR COORDINATE METHODS.

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ABSTRACT

Using a very simple type of wave-packet which are obtained by letting unitary displacement operators having as generators canonical operators $\hat{Q}$ and $\hat{P}$ in the many-body Hilbert space act on a reference state, we investigate the relationship between the semi-classical and the generator coordinate methods. The semi-classical method is based on the time-dependent variational principle whereas in the generator coordinate method the wave-packets are taken as generator states. To establish the equivalence of the two-methods, we examine in detail, using tools developed in previous works, the concept of redundancy of the wave-packet and the importance of the zero-point energy effects. We make a numerical application to the case of the Goldhaber-Teller mode in ^{4}He.

[Nuclear structure - Relationship between the semi-classical and the generator coordinate methods. Redundancy and zero-point energy effects. Numerical application to the Goldhaber-Teller mode in ^{4}He.]

I) INTRODUCTION

The objective of a microscopic theory of collective motion is to reduce the many body problem to a description in terms of only a small number of degrees of freedom. In the idealized case one supposes that there exists an invariant subspace of the many body Hilbert space, the collective subspace, in which the collective and intrinsic degrees of freedom are decoupled. The base states in this subspace are product type wave-functions where the intrinsic degrees of freedom are constrained to be always in one intrinsic state only. The dynamics in the collective subspace is determined by the collective hamiltonian which is equal to the expectation value of the many body hamiltonian in this intrinsic state. One way to perform the explicit separation of the collective degree of freedom is, in the case of a cononical collective degree of freedom, by the introduction of a canonical transformation in the many body Hilbert space from the microscopic degrees of freedom to collective and intrinsic ones. This canonical transformation allow us to write the many body hamiltonian as a sum of a collective hamiltonian $\hat{H}_C$ (which depends on the collective degree of freedom only), an intrinsic hamiltonian, and a coupling term between the intrinsic and collective degrees of freedom. In the idealized case, this last term does not couple the collective to the non-collective states. However in practice the difficulties associated to the explicit use of the canonical transformation lead many authors to present theories which try to find $\hat{H}_C$ in an indirect way by means of a collective path[1]. The collective path is a set of slater determinants labeled by two parameters, $|pq>$, in the case of a dynamical collective path and by one parameter $|q>$, $|q> = |p=0,q>$, in the case of a static collective path. The dependence of the wave-packets on p and q are constructed so as to reflect the distortion of the system during the collective motion and they are, in general, equal to the expectation value on the wave-packet $|pq>$ of dynamical variables defined in the many-body Hilbert space,

$$q = \langle qp|\hat{Q}|qp\rangle$$
$$p = \langle qp|\hat{P}|qp\rangle \qquad \text{(I.1)}$$

and these dynamical variables satisfy the weakly canonical commutation relation

$$\langle pq|\,[\hat{Q},\hat{P}]\,|pq\rangle = i \qquad \text{(I.2)}$$

It is important to point out that the dependence of $|pq\rangle$ on p describes the velocity dependence of the wave-packet and it is not introduced in the sense of describing an additional degree of freedom[1]. Thus, the parameter p is thaught to be associated to a degree of freedom canonically conjugate to the one associated with the parameter q. One uses different prescriptions to determine the collective path which ranges from self-consistent methods to educated guesses based on phenomenological considerations.

The differences between the theories considered in this paper stems from the way that they use the collective path.

In the generator coordinate method (GCM)[3], as used in practice, we select a subspace of the many-body Hilbert space which is spanned by the states which are constructed as a linear superposition of the states along the static collective path $|q\rangle$

$$|f\rangle = \int dq\; f(q)\,|\,q\,\rangle \qquad \text{(I.3)}$$

The only unknown in eq. I.3 is the weight function f(q) which is determined by the variational principle

$$\delta E = \frac{\delta\langle f|H|f\rangle}{\langle f|f\rangle}$$

resulting in the Griffin-Hill-Wheeler (GHW) integral equation for f(q)

$$\int(\langle q|\hat{H}|q'\rangle - E\langle q|q'\rangle)\; f\;(q')\; dq' \;= 0 \qquad \text{(I.4)}$$

There are many ways to transform the GHW equation, eq. I.4, into a Schroedinger type equation in a "collective" coordinate (however, in general, this Schroedinger type equation has a "velocity" dependent potential and a "mass-parameter" which depends on the coordinate). This Schroedinger type equation defines the collective hamiltonian $\hat{H}_C^{GCM}$ of the generator coordinate method.

On the other hand, the semi-classical method[4] uses the dynamical collective path $|pq\rangle$. One finds the time-evolution of the wave-packets through the use of the quantum variational principle

$$\delta I = \delta \int_{t_1}^{t_2} (i\langle pq|\overrightarrow{\partial}_t|pq\rangle - \langle pq|\hat{H}|pq\rangle)dt = 0 \qquad (I.5)$$

with fixed end point variations. As long as the wave-packets fulfill the relation

$$i\langle pq|\partial_p^{\leftarrow}\partial_q^{\rightarrow} - \partial_q^{\leftarrow}\partial_p^{\rightarrow}|pq\rangle = 1$$

the variational principle I.5 leads to the classical hamilton eqs.

$$\dot{p} = -\partial H^{CL}(p,q)/\partial_q \qquad \dot{q} = \partial H^{CL}(p,q)/\partial_p \qquad (I.6)$$

where the classical hamiltonian $H^{CL}(p,q)$ is equal to

$$H^{CL}(p,q) = \langle pq|H|pq\rangle \qquad (I.7)$$

In the semi-classical method we are not interested in the time-evolution of the wave-packets. Indeed in this method one uses the wave-packets $|pq\rangle$ as probes to extract the classical limit of the quantum collective hamiltonian. Thus in the semi-classical method we identify the classical hamiltonian $H^{CL}(p,q)$ with the classical limit of the quantum collective hamiltonian $\hat{H}_C$ [2]. The quantum collective hamiltonian is reconstructed by a requantization procedure.

These two methods are conceptually and practically different and when it is discussed in the literature its advantages and disadvantages the point of view usually adopted is that with respect to the dynamics the semi-classical method is superior to the GCM since it uses a dynamical path as opposed to the GCM which, in general, uses a static collective path[1]. An example which is always presented in support of this point of view is the case of translation of the nucleus as a whole where the mass parameter calculated according to the semi-classical method has the correct value, whereas the value given by the GCM is in general incorrect. The disadvantage of the semi-classical method is that since one always reaches a "classical" stage it incorporates in a wrong way the effects associated with the zero-point motion of the wave-packet $|pq\rangle$. However these effects are handled in a correct way in a purely quantum method as the generator coordinate method. Therefore a generalization of the GCM which incorporates the advantages of both methods, as used in practice, is to use as generator states the states along the collective path, $|pq\rangle$. In the literature the GCM which uses dynamical wave-packets as generator states is called dynamical GCM, DGCM, as opposed to the ones which uses static wave-packets called static GCM, SGCM[1].

In general the DGCM is an inprovement both with respect to the SGCM and to the semi-classical method. However in reference 1 it is investigated under what conditions the description of the dynamics according to three methods agree. In this work they come out with two basic requirements in order to make the three methods equivalent:

a) the dynamical wave-packets $|pq\rangle$ should be redundant i.e., the collective subspace associated by the GCM to the static, $|q\rangle$, and dynamical, $|pq\rangle$, wave packets are identical.

b) the dynamical effects of the zero point energy are negligible.

The idea behind requirement a) is the observation that

the parameter p is introduced to describe a dynamical variable canonically conjugate to the one associated with the parameter q. Therefore both wave-packets are thought to describe the distortion of the system along one canonical degree of freedom. This implies that the subspaces associated with the DGCM and SGCM should be a Hilbert space spanned by this degree of freedom and thus identical. Once this requirement is satisfied the condition b) is nothing more than the requirement that the dynamical wave-packet is able to extract the classical limit of the quantum collective Hamiltonian of the GCM. Differently from what was done in reference 1, the aim of our paper is to investigate these questions using a very simple type of dynamical wave packet, which is obtained by letting unitary displacement operators having as generators canonical operators in the many-body Hilbert space, act in a reference state

$$|pq\rangle = e^{-iq\hat{P}} \; e^{ip\hat{Q}} |0\rangle \qquad [\hat{Q},\hat{P}] = i \tag{I.8}$$

This, we think, will illuminate many aspects of the relationship between the semi-classical and the generator coordinate methods and will shed new light on the understanding of this relationship in the case of more complex types of wave-packets[1].

The semi-classical method is presented in chapter II. The generator coordinate method is presented in chapter III, and we show, using the techniques developed in references 8,9 and 10, how we can handle the overcompleteness of the dynamical wave-packets $|pq\rangle$ in DGCM. Also we show how we can define the collective hamiltonian and collective operators. In this chapter the relationship between the subspaces associated with the static and dynamical wave-packets is also discussed. In chapter IV we compare the methods and we make a numerical application to the Goldhaber-Teller mode in ^{4}He which can be described by a wave-packet of the type shown in eq. I.8. In chapter V we present our concluding remarks.

II) THE SEMI-CLASSICAL METHOD

As was pointed out by many authors[4,5,6] the evolution in time of quantum many-body systems can be determined by a variational principle analogous to the hamilton principle of classical mechanics.

The lagrangian, which is a functional of $|\psi(t)>$ and its hermitian conjugate is equal to

$$L(\psi,\psi^*) = i<\psi(t)|\partial_t^{\rightarrow}|\psi(t)> - <\psi(t)|\hat{H}|\psi(t)> \qquad (II.1)$$

and the equations of motion are found by requiring stationarity of the action with respect to fixed end points variations of $|\psi(t)>$ and $|\psi(t)>^*$,

$$\delta I = \delta \int_{t_1}^{t_2} (i<\psi(t)|\dot{\psi}(t)> - <\psi(t)|\hat{H}|\psi(t)>)dt = 0 \qquad (II.2)$$

subject to the conditions

$$|\delta\psi(t_1)> = |\delta\psi(t_2)> = 0$$

As an example, if we impose that $|\psi(t)>$ varies only in the space of Slater determinants eq. II.2 leads to the TDHF equations[5,6] which in the small amplitude approximation is equal to the RPA.

What is called the semi-classical method in the literature[4] and in our paper amounts to consider restricted parametrizations of $|\psi(t)>$ in terms of (in the case of one canonical collective degree of freedom) dynamical wave-packets $|\psi(p(t),q(t))>$. The dependence of the wave-packet on q(t) is supposed to describe the distortion of the system during the collective motion and the dependence on p(t) describes the "velocity" dependence of the dynamical wave-packet. These dynamical wave-packets can be chosen in various ways which ranges from self-consistent methods (like TDHF and CHF) to educated guesses as to the nature of the collective motion under

consideration.

One determines the evolution in time of the parameters q(t) and p(t) through the use of the variational principle II.2 which leads to the classical hamilton equations

$$\dot{p} = - \partial H^{CL}(p,q)/\partial q \qquad \dot{q} = \partial H^{CL}(p,q)/\partial p$$

where the classical hamiltonian is

$$H^{CL}(p,q) = \langle pq|\hat{H}|pq\rangle \tag{II.3}$$

provided one has

$$i \langle pq| \partial^{\leftarrow}_{p} \partial^{\rightarrow}_{q} - \partial^{\leftarrow}_{q} \partial^{\rightarrow}_{p} |pq\rangle = 1 \tag{II.4}$$

In our paper we consider wave-packets parametrized as in eq. I.8

$$|pq\rangle = e^{-iq\hat{P}} e^{ip\hat{Q}} |0\rangle \tag{II.5}$$

where $\hat{Q}$ and $\hat{P}$ are canonical collective variables in the many-body Hilbert space.

The parameters q and p in eq. II.5 are equal to the expectation value of $\hat{Q}$ and $\hat{P}$ on the dynamical wave-packets $|pq\rangle$.

$$p = \langle pq|\hat{P}|pq\rangle$$
$$q = \langle pq|\hat{Q}|pq\rangle$$

where we used the property that the reference state $|0\rangle$ satisfies the eqs.,

$$\langle 0|\hat{Q}|0\rangle = \langle 0|\hat{P}|0\rangle = 0$$

Given the wave-packets II.5, it is easily seen that eq. II.4 holds

since it becomes

$$\langle pq|\left[i\hat{P},\hat{Q}\right]|pq\rangle = 1$$

The hamilton eqs. can be rewritten in this case as

$$\dot{q}(t) = \langle pq|\left[-i\hat{Q},\hat{H}\right]|pq\rangle$$
$$\dot{p}(t) = \langle pq|\left[-i\hat{P},\hat{H}\right]|pq\rangle$$

In practical applications one is interested in cases where the collective motion is slow. This allow us to expand the classical hamiltonian $H^{CL}(p,q)$, eq. II.3, in a power series in p. Owing to the time reversal properties of $\hat{Q}$ and $\hat{P}$ and the reference state $|0\rangle$ in the expansion one has only even powers of p and it is equal to

$$H^{CL}(p,q) = \frac{p^2}{2M^{CL}(q)} + V^{CL}(q) + O(p^4) \qquad \text{(II.6)}$$

In eq. II.6 $M^{CL}(q)$ and $V^{CL}(p)$ are the classical mass parameter and potential respectively and they are qual to

$$V^{CL}(q) = \langle q|\hat{H}|q\rangle$$
$$M^{CL}(q)^{-1} = \partial p^2 \langle pq|H|pq\rangle\big|_{p=0} = \langle q|\left[\hat{Q},\left[\hat{H},\hat{Q}\right]\right]|q\rangle$$

As discussed in ref. 2, in the semi-classical method we are not interested in the time-evolution of the parameters p(t) and q(t). In this method the wave-packets $|p(t),q(t)\rangle$ are used as a probe to extract the classical limit of the quantum collective hamiltonian $\hat{H}_C(\hat{P},\hat{Q})$. Thus the fundamental hypothesis of the semi-classical method is that the hamiltonian $H^{CL}(p,q)$ is equal to the classical limit of the quantum collective hamiltonian $\hat{H}_C(\hat{Q},\hat{P})$.

The validity of this hypothesis depends strongly on the properties of the wave-packets $|pq\rangle$ as will become clear later on in this paper. Indeed, besides other effects, the dispersion of $\hat{Q}$ and $\hat{P}$

gives rise to an intrinsic energy, the zero point energy of the wave packet, which is always present in the hamiltonian $H^{CL}(p,q)$. Therefore the identification of $H^{CL}(p,q)$ with the classical limit of $\hat{H}_C(\hat{P},\hat{Q})$ is valid only when this zero point energy is, unless by an unimportant constant factor, negligible. Once this identification is made, to derive the quantum collective hamiltonian in the semi-classical method, one is faced with the problem of quantizing the classical hamiltonian $H^{CL}(p,q)$, which in the limit of slow motion is given by eq. II.6. This step introduces additional difficulties which stems from the dependence of the mass parameter with the coordinate. This property leads to the use of different orderings in the canonical quantization of q and p all of them having the same classical limit. This question is clearly discussed in reference seven where it is pointed out that the question of which ordering to use is intimately connected to the zero point energy corrections and so we defer a discussion of this point to chapter IV. Here we are going to use a prescription suggested in ref. 2 in which the quantum collective hamiltonian in the semi-classical method reads

$$\hat{H}_C^{SC}(\hat{P},\hat{Q}) = \frac{1}{4}\left(\hat{P}^2 \frac{1}{2\hat{M}^{CL}(\hat{Q})} + \frac{1}{2\hat{M}^{CL}(\hat{Q})}\hat{P}^2 + 2\,\hat{P}\frac{1}{2\hat{M}^{CL}(\hat{Q})}\hat{P}\right) + \hat{V}^{CL}(\hat{Q}) \qquad \text{(II.7)}$$

This ordering will be seen later on to be identical to the one given by a proper quantization of the motion along the collective path using GCM.

III) THE GENERATOR COORDINATE METHOD

In the previous chapter we presented a brief discussion of the semi-classical method based on the time dependent variational principle (TDVP), eq. II.2. As shown there, at one point of this method one reaches a classical stage. This stems from the non-linear character of the variational space of the wave-packets $|pq\rangle$. Indeed, if we impose that $|\psi(t)\rangle$ varies in a subspace of the many-body Hilbert space the TDVP is equivalent to quantum mechanics restricted to this subspace. Therefore to have a theory built upon the TDVP which satisfies the linear character of quantum mechanics (the principle of superposition) one should take as the variational space of $|\psi(t)\rangle$ a linear space. A theory of this kind is the GCM introduced by Griffin-Hill-Wheeler[3].

In the GCM one considers a subspace of the many-body Hilbert space spanned by the states which can be constructed as a linear superposition of the generator states $|\alpha\rangle$

$$|f\rangle = \int f(\alpha)\ |\alpha\rangle\ d\alpha \qquad \text{(III.1)}$$

The only unknown in eq. III.1 is the weight-function $f(\alpha)$ which is determined by the TDVP (in the stationary limit) resulting in the GHW integral equation

$$\int (\langle\alpha|\hat{H}|\alpha'\rangle - E\langle\alpha|\alpha'\rangle)\ f(\alpha')\ d\alpha' = 0 \qquad \text{(III.2)}$$

In references 8 and 9 it is shown that we can always associate to the GHW "ansatz" eq. III.1 a projection operator defined in the many-body Hilbert space. Therefore the dynamics in the GCM scheme is equivalent to the many-body dynamics restricted to this subspace, the GCM collective subspace S, and we can identify the GCM collective hamiltonian with the projection of the many-body hamiltonian onto S.

$$\hat{H}_C^{GCM} = \hat{S}\,\hat{H}\,\hat{S}$$

where $\hat{S}$ is the projection operator on S.

In this chapter, using tools developed earlier[8,9,10], we are going to investigate the properties of the GCM collective subspace associated with the one-parameter (static) and two-conjugate parameters (dynamical) family of generator states $|q\rangle$ and $|pq\rangle$ respectively. We are also going to show how we can define, a posteriori collective dynamical variables and how we can express the collective hamiltonian $\hat{H}_C^{GCM}$ in terms of these variables. All the details of what follows can be found in reference 10.

III-A) A Representation In The GCM Collective Subspace Static and Dynamical Wave-Packets as Generator States.

The static and dynamical wave-packets are respectively equal to

$$\begin{aligned} |q\rangle &= e^{-iq\hat{P}}\,|0\rangle \\ |pq\rangle &= e^{-iq\hat{P}}\,e^{ip\hat{Q}}\,|0\rangle \\ [\hat{Q},\hat{P}] &= i \end{aligned} \qquad \text{(III.3)}$$

The reference state $|0\rangle$ is the vacuum of a boson constructed in terms of the operators $\hat{Q}$ and $\hat{P}$,

$$\begin{aligned} \hat{B}\,|0\rangle &= 0 \\ \hat{B} &= \frac{1}{\sqrt{2}}\left(\frac{\hat{Q}}{b_o} + i\,\hat{P}\,b_o\right) \\ b_o^2 &= 2\,\langle 0|\hat{Q}^2|0\rangle \end{aligned} \qquad \text{(III.4)}$$

Using eqs. III.4 we can easily show that the wave-packets satisfy the relation

$$(-i\partial_p + i\, b_o^2 (i\partial_q - p))\,|pq\rangle = 0 \qquad \text{(III.5a)}$$

which can be rewritten as

$$((\hat{Q}-\hat{q}) + ib_o^2\,(\hat{P}-p))\,|pq\rangle = 0 \qquad \text{(III.5b)}$$

To determine the natural representation in the GCM collective subspace consider first the static wave packet. Using eqs. III.4 the overlap kernel $\langle q|q'\rangle$ is easily seen to be equal to

$$\langle q|q'\rangle = e^{-(q-q')^2/4b_o^2}$$

The eigenfunctions and eigenvalues of the overlap kernel are determined by the equation

$$\int_{-\infty}^{+\infty} \langle q|q'\rangle\, \phi_k(q')\, dq' = 2\pi\lambda(k)\, \phi_k(q)$$

and they are equal to

$$\phi_m(q) = \frac{1}{\sqrt{2\pi}}\, e^{ikq}$$

$$\lambda(k) = b_o/\sqrt{\pi}\; e^{-k^2 b_o^2} \qquad \text{(III.6)}$$

According to reference 10 the natural representation in the collective subspace S, associated to the SGCM is given by

$$|k\rangle_1 = \frac{1}{\sqrt{2\pi\lambda(k)}} \int |q\rangle \phi_k(q)\, dq = \frac{\hat{\pi}_k^{PY}\,|0\rangle}{\sqrt{\langle 0|\hat{\pi}_k^{PY}|0\rangle}} \qquad \text{(III.7)}$$

where $\hat{\pi}_k^{PY}$ is the Peierls-Yoccoz projection operator associated with the operator $\hat{P}$

$$\hat{\pi}^{PY}_{k} = \frac{1}{2\pi} \int dq \; e^{ikq} \; e^{-iq\hat{P}} \qquad \text{(III.8)}$$

Thus, the orthonormal states $|k\rangle_1$ are seen to be equal to the normalized Peierls-Yoccoz projection of the reference state $|0\rangle$ associated with the operator $\hat{P}$, and the projection operator onto S, can be written as

$$\hat{S}_1 = \int dk \; |k\rangle_1 \; {}_1\langle k| \qquad \text{(III.9)}$$

On the other hand, the overlap kernel $\langle pq|p'q'\rangle$ is easily seen to be equal to (using eqs. III.4)

$$\langle pq|p'q'\rangle = e^{i(q-q')\frac{(p+p')}{2}} \; e^{-\frac{(q-q')^2}{4b_o^2}} \; e^{-\frac{(p-p')^2 b_o^2}{4}} \qquad \text{(III.10)}$$

The eigenfunctions and eigenvalues of this overlap kernel are determined by the equation

$$\int \langle pq|p'p'\rangle \; \phi_{n,k}(p',q')dp'dq' = 2\pi\lambda_n(k) \; \phi_{n,k}(p,q)$$

and they are equal to

$$\phi_{n;k}(p,q) = \frac{e^{iqk}}{\sqrt{2\pi}} \; \phi_n(p-k)$$

and the eigenvalues are independent of k. The eigenfunctions $\phi_n(p)$ and the eigenvalues λ_n are eigenfunctions and eigenvalues of the Hilbert Schmidt kernel

$$\tilde{N}(p,p') = \langle 0| \; e^{-ip\hat{Q}} \delta(\hat{P}) \; e^{ip'Q} \; |0\rangle$$

$$= \frac{1}{2\pi} \int dq \langle pq|p'0\rangle \qquad \text{(III.11)}$$

In our case III.11 is equal to

$$\tilde{N}(p,p') = \left(\frac{b_o}{\sqrt{\pi}}\right)^{1/2} e^{-p^2 b_o^2/2} \left(\frac{b_o}{\sqrt{\pi}}\right)^{1/2} e^{-p'^2 b_o^2/2} \tag{III.12}$$

which shows that it is separable and equal to the product of two Fourier transforms of the ground state of a harmonic oscillator. Therefore its eigenfunctions and eigenvalues are easily seen to be equal to

$$\phi_n(p) = \phi_n^{h_o}(p)$$

$$\lambda_n = \delta_{n,o}$$

As is thoroughly discussed in references 8 and 9 the existence of zero eigenvalues of the overlap kernel implies that the generator states are not linearly independent. The linear dependence can be expressed as

$$|pq\rangle = \int dp'dq' \; |p'q'\rangle \, R(p'q';pq) \tag{III.13}$$

where the kernel $R(p'q',pq)$ is the projection operator onto the orthogonal complement of the null space of $\hat{N}$

$$R(p'q';pq) = \int dk \; \phi_{o;k}(p',q') \; \phi^*_{o;k}(p,q) = \frac{1}{2\pi} \langle p'q'|pq\rangle \tag{III.14}$$

Following reference 10 the natural representation in the subspace S_2 associated with the DGCM is given by

$$|k\rangle_2 = \frac{1}{2\pi} \int |pq\rangle \phi_{0;k}(p,q) \; dpdq = \hat{\pi}^{PT}|0\rangle \tag{III.15}$$

where $\hat{\pi}^{PT}$ is the so-called Peierls-Thouless double projection operator associated with the operator $\hat{P}$

$$\hat{\pi}^{PT} = \int dpdq \ \frac{e^{iqk}}{2\pi} \ \phi_o^{h_o}(p-k) \ e^{-iq\hat{P}} \ e^{ip\hat{Q}} \qquad \text{(III.16)}$$

Thus the orthonormal states $|k\rangle_2$ are seen to be equal to the so-called Peierls-Thouless double projection of the reference state $|0\rangle$ associated with the operator $\hat{P}$ and the projection operator in $\hat{S}_2$ is given by

$$\hat{S}_2 = \int dk \ |k\rangle_{2\,2}\langle k|$$

III-B) Relationship Between The Subspaces

In section III-A we have shown how we can quantize the collective motion along the static path and the dynamical path using GCM. However, in general, the subspaces associated with these two paths are different[1,10]. In other words, the two subspaces carry different quantum degress of freedom. However, as has been pointed out before , when one uses the dynamical wave-packet $|pq\rangle$ in the semi-classical method one thinks of $|pq\rangle$ as describing the distortion of the system along one canonical degree of freedom only. Therefore when comparing the two theories, one of the requirements that one has to impose, as was done in reference 1, is that the subspaces associated with the static and dynamical paths should be identical. The dynamical wave-packets which satisfy these requeriments are called redundant.

In general it is very difficult to establish the neessary and sufficient conditions that a dynamical wave-packet should satisfy in order to be redundant. In the case of wave-packets generated as in eq. I.8 this has been done in ref. 10 with the conclusion

that the requirement is that the reduced kernel, eq. III.11, should have only one eigenvector with non-zero eigenvalue. Besides in ref. 1 a sufficient condition is discussed, called local-redundancy which leads to a redundant dynamical wave-packet. In our case the requirement of local redundancy demands that eq. III.5 holds. All this leads us to the conclusion that the dynamical wave-packet considered in this paper is redundant and the proof of this fact runs as follows.

As the generators states $|q\rangle$ and $|pq\rangle$ are vectors defined in the collective subspaces S_1 and S_2 respectively, one can find its components along the base $|k\rangle_1$ and $|k\rangle_2$. To do so one uses eqs. III.7 and III.15 and one finds

$$|pq\rangle = \int dk \; e^{-ikq} \; \phi_o^{h.o}(p-k) \; |k\rangle_2$$
$$|q\rangle = \int dk \; \sqrt{\lambda(k)} \; e^{-ikq} \; |k\rangle_1 \qquad \text{(III.17)}$$

Since $|q\rangle = |p=0,q\rangle$ one has

$$|q\rangle = \int dk \; e^{-ikq} \; \phi_o^{h.o}(k) \; |k\rangle_2 .$$

Using the above eq. in eq. III.7 one has

$$|k\rangle_1 = |k\rangle_2$$

which proves the identity of the two subspaces.

To have a better understanding on this matter, consider a canonical transformation from the particle degrees of freedom to collective, $\hat{Q}$ and $\hat{P}$, and intrinsic degrees of freedom. Together with this transformation we introduce a product representation of the many-body Hilbert space,

$$|Q,\xi\rangle = |Q\rangle \otimes |\xi\rangle$$

where the states $|Q\rangle$ span a space of one degree of freedom, the collective space, and $|\xi\rangle, |\xi\rangle = |\xi_1, \xi_2, \ldots \xi_{N-1}\rangle$, one of (N-1) degrees of freedom, the intrinsice space. The wave-function associated by

the $|Q\xi\rangle$ representation to the base states $|k\rangle_1$ and to the wave-packets $|q\rangle$ and $|pq\rangle$ are respectively

$$\langle Q\xi|\, k\rangle_1 = \frac{e^{ikQ}}{\sqrt{2\pi}}\ \chi_o(\xi) \tag{III.18}$$

$$\langle Q\xi|q\rangle = \left(\frac{1}{\sqrt{\pi}\, b_o}\right)^{1/2}\ e^{-(Q-q)^2/2b_o^2}\ \chi_o(\xi)$$

$$\langle Q\xi|qp\rangle = \left(\frac{1}{\sqrt{\pi} b_o}\right)^{1/2}\ e^{ip(Q-q)}\ e^{-(Q-q)^2/2b_o^2}\ \chi_o(\xi)$$

This shows that in the collective subspace $S_1 (S_1=S_2)$ the collective and intrinsic degrees of freedom are kinematically decoupled and both wave packets are given by the product of a wave-packet in the collective variable and a wave-function which depends only on the intrinsic variables. The difference between the wave-packets is the velocity dependence of $|pq\rangle$ which is introduced by the phase in eq. III.18. Thus the redundancy is seen to be a consequence of the fact that a family of static gaussian wave-packets form a complete set in the collective space (that has only one degree of freedom) whereas the dynamical gaussian wave-packet form an overcomplete set.

This overcompleteness is responsible for the linear dependence of $|pq\rangle$ (see eq. III.13) which leads to the existence of eigenvectors of the overlap kernel with zero eigenvalue.

III-C) Collective Operators And Collective Hamiltonians

Once one has the natural representation in S_1 the collective operators can be found[10]:

$$\hat{P}_{S_1}|k\rangle_1 = k|k\rangle_1$$

$$\hat{Q}_{S_1}|k\rangle_1 = -i\partial/\partial_k |k\rangle_1 \qquad \text{(III.19)}$$

Since $|k\rangle_1$ is equal to the Peierls-Yoccoz projection of the reference state $|\phi\rangle$ associated with the operator $\hat{P}$ one has, by construction

$$\hat{P}|k\rangle_1 = k|k\rangle_1 \qquad \text{(III.20)}$$

Also we can easily show using ups III.5 and III.7 that

$$\hat{Q}|k\rangle_1 = -i\partial/\partial_k |k\rangle_1 \qquad \text{(III.21)}$$

Thus, the canonical collective operators in the GCM collective subspace are equal to the projection onto this subspace of the canonical operators in the full many-body Hilbert space

$$\hat{Q}_{S_1} = \hat{Q}S_1 = \hat{S}_1\hat{Q}$$

$$\hat{P}_{S_1} = \hat{P}\hat{S}_1 = \hat{S}_1\hat{P}$$

The natural representation $|k\rangle_1$ is the specific representation obtained by the diagonalization of the overlap kernel and eqs. III.19 - III.21 shows that it diagonalizes the operator $\hat{P}$. However once we found this "momentum" representation by unitary transformations in S_1, we can find a representation which diagonalizes any hermitian operator defined in S_1. In particular we can find a "coordinate" representation given by the Fourier transform of the momentum representation

$$|X\rangle_1 = \frac{1}{\sqrt{2\pi}} \int e^{-ikX} |k\rangle_1$$

$$= \frac{\hat{\pi}^{PY}_X |0\rangle}{\langle 0|\hat{\pi}^{PY}_X|0\rangle} \qquad \text{(III.22)}$$

where $\hat{\pi}_X^{PY}$ is the Peierls-Yoccoz projection operator associated with the operator $\hat{Q}$

$$\hat{\pi}_X^{PY} = \frac{1}{2\pi} \int e^{-ixp} e^{ip\hat{Q}} dp$$

which diagonalizes the operator $\hat{Q}$

$$\begin{aligned} \hat{Q}|X\rangle_1 &= X|X\rangle_1 \\ \hat{P}|X\rangle_1 &= i\partial/\partial_X|X\rangle_1 \end{aligned} \qquad \text{(III.23)}$$

As discussed before the GCM collective hamiltonian is defined as the projection of the many-body hamiltonian onto the GCM collective subspace

$$\hat{H}_C^{GMC} = \hat{S}_1 \hat{H} \hat{S}_1 \qquad \text{(III.24)}$$

Using the "coordinate" representation III.22, the dynamical equation in S_1 can be written as a wave-equation in the "coordinate" representation

$$\int h(x,x')\ \phi(x',t)\ dx' = ih\partial\phi(x,t)/\partial t$$

where

$$h(x,x') = {}_1\langle x|\hat{H}|x'\rangle_1$$

and $\phi(x,t)$ is the collective wave-function $\phi(x,t) = {}_1\langle x|\phi(t)$. Also we can express the GCM collective hamiltonian in terms of the collective variables $\hat{Q}_{S_1}$, $\hat{P}_{S_1}$ [10],

$$\hat{S}_1 \hat{H} \hat{S}_1 = \hat{S}_1 \left(\sum_{m=0}^{\infty} \frac{1}{2^m} : \hat{P}^m \hat{H}^{(m)}(\hat{Q}) : \right) \hat{S}_1$$

where the normal order is defined as

$$: \hat{P}^m \hat{H}^{(m)}(\hat{Q}) : = \{\hat{P},\{\hat{P},\ldots\{\hat{P},\hat{H}^{(m)}(\hat{Q})\}\ \ldots\}\}$$

m anti-commutators

$$\hat{H}^{(m)}(X) = \int d\xi \frac{(-i\xi)^m}{m!} \ {}_1\langle x + \xi/2|\hat{H}|x - \xi/2\rangle_1$$

$$= \int d\xi \frac{(-i)^m}{m!} \ {}_1\langle x + \xi/2|\left[\hat{Q},\left[\hat{Q},\ldots\left[\hat{H},\hat{Q}\right]\ \ldots\right]\right]|x-\xi/2\rangle_1$$

m - commutators

(III.25)

We see that this ordering is identical to the one given by eq. II.7, if we stop at second order in a expansion in powers of $\hat{P}$. Other useful expressions of $\hat{H}^{(m)}(x)$ are

$$\hat{H}^{(m)}(x) = \int dk \frac{e^{ikx}}{m!} \frac{d^m}{dK^m} \langle K+k/2|\hat{H}|K-k/2\rangle_1 \Big|_{K=0}$$

$$= \int dk \frac{e^{ikx}}{m!} \frac{d^m}{dK^m} \frac{1}{2\pi} \int \frac{d_q d_{q'} \phi_k^*(\frac{q+q'}{2}) \langle q|\hat{H}|q'\rangle \phi_K^*(q-q')}{\sqrt{\lambda(K+k/2)\lambda(K-k/2)}} \Big|_{K=0}$$

(III.26)

In general the reduced energy kernel is a function which depends slowly on the difference of the generator coordinates. Therefore we can expand the reduced energy kernel as a power series expansion on the difference of the generator coordinates

$$h(q,q') = \sum_{n=0}^{\infty} \frac{h_{2n}}{2n!} \left(\frac{q+q'}{2}\right)(q-q')^{2n} \qquad \text{(III.27)}$$

where $h(q,q')$ is simmetric in q and q' due to the time-reversal properties of $\hat{Q}$. Using this expansion in eq. III.26 one has[11]

$$\hat{H}^{(2m)}(X) = (-1)^m \frac{(2b_o)^{2m}}{(2m)!} \frac{1}{2\pi} \int dk \ e^{ikx} \ e^{k^2 b_o^2/4}$$

$$\sum_{n=m}^{\infty} \frac{b_o^{2n}}{(n-m)!} \int dQ \ h_{2n}(\hat{Q}) e^{-iQk}$$

IV) COMPARISON BETWEEN THE SEMI-CLASSICAL AND THE GENERATOR COORDINATE METHOD. APPLICATION TO THE GOLDHABER-TELLER MODE IN ^4He

The classical hamiltonian $H^{CL}(p,q)$ is equal to (see eq. II.3)

$$H^{CL}(p,q) = \langle pq | \hat{H} | pq \rangle \tag{IV.1}$$

and since the wave-packets $|pq\rangle$ are states defined in the GCM collective subspace S_1 one has

$$\begin{aligned} H^{CL}(p,q) &= \langle pq | \hat{S}_1 \hat{H} \hat{S}_1 | pq \rangle \\ &= \langle pq | \hat{H}_C^{GCM} | pq \rangle \end{aligned} \tag{IV.2}$$

Also the use of the product representation III.17 shows that the GCM quantum collective hamiltonian is the trace on the intrinsic variables of $\hat{H}|\chi_o\rangle\langle\chi_o|$

$$\hat{H}_C^{GCM} = \mathrm{tr}_\xi \hat{H} |\chi_o\rangle\langle\chi_o| \tag{IV.3}$$

The eq. IV.2 shows that the "classical" hamiltonian $\hat{H}^{CL}(p,q)$ is equal to the expectation value of the quantum collective hamiltonian $\hat{H}_C^{GCM}$ on the wave-packet $|pq\rangle$. We would like to point out that this property is very general since it depends only on the fact that the dynamical wave-packet belongs to the GCM collective subspace S_1. Thus we can state that the description of the dynamics according to the two methods is equivalent when the "classical" hamiltonian $H^{CL}(p,q)$ is the classical limit of the GCM quantum collective hamiltonian $\hat{H}_C^{GCM}(\hat{P},\hat{Q})$. The difference between the "classical" hamiltonian $H^{CL}(p,q)$ and the "classical" limit of the quantum collective hamiltonian $\hat{H}_C^{GCM}(\hat{P},\hat{Q})$ is the zero-point energy of the wave-packet

$|pq\rangle$[1,7]

$$H^{CL}(p,q) = H_C^{GCM}(\langle\hat{P}\rangle,\langle\hat{Q}\rangle) + E_{ZP}(p,q) \qquad \text{(IV.4)}$$

Once one has established that the dynamical wave-packet $|pq\rangle$ is redundant, we can say that the two theories are equivalent when the dynamical effects of the zero-point energy are negligible. In what follows we are going to analyse these effects in a specific example, the Goldhaber-Teller mode in ^4He.

IV-4) The Goldhaber-Teller Model Of The Giant Dipole Ressonance

According to the Goldhaber-Teller model of the giant dipole ressonance the dipole vibration is described as a rigid displacement of the protons against the neutrons. In the dynamical case we also have a relative momentum between protons and neutrons. This picture of the dipole vibration can be described by the dynamical wave-packet[10,12]

$$|pq\rangle = e^{-iq\hat{P}}\, e^{ip\hat{Q}}\, |0\rangle \qquad \text{(IV.5)}$$

In eq. IV.5 the operators $\hat{Q}$ and $\hat{P}$ are respectively the z-component of the relative coordinate and momentum between protons and neutrons

$$\hat{Q} = \hat{R}_Z - \hat{R}_N$$

$$\hat{P} = \frac{N}{A}\hat{P}_Z - \frac{Z}{A}\hat{P}_N$$

$\hat{R}_Z, \hat{P}_Z, \hat{R}_N, \hat{P}_N$ are the z-component of the center of mass coordinate and the center of mass momentum of the protons and the neutrons respectively. In the case of self-conjugate nuclei (N=Z) $\hat{Q}$ and $\hat{P}$ are equal to

$$\hat{Q} = \frac{2}{A} \sum_i \hat{x}_3(i)\, T_3(i)$$

$$\hat{P} = \frac{1}{2} \sum_i \hat{p}_3(i)\, T_3(i)$$

where $\hat{x}(i)$ and $\hat{p}(i)$ are the coordinate and momentum operators of nucleon i and $\hat{T}_3(i)$ is the z-component of the isospin operator. The reference state $|0\rangle$ is the ground state of the nucleus or an approximation of it.

The operators $\hat{Q}$ and $\hat{P}$ are canonical

$$[\hat{Q}, \hat{P}] = i \tag{IV.6}$$

and the parameters q and p are equal to the expectation value of $\hat{Q}$ and $\hat{P}$ on the wave-packet $|pq\rangle$

$$\begin{aligned} \langle pq|\hat{Q}|pq\rangle &= q \\ \langle pq|\hat{P}|pq\rangle &= p \end{aligned} \tag{IV.7}$$

where we assumed

$$\langle 0|\hat{P}|0\rangle = \langle 0|\hat{Q}|0\rangle$$

In our application to dipole oscillation in ^4He we approximate the reference state $|0\rangle$ by a slater determinant of harmonic oscillator wave-functions. In this case it is easily seen that

$$(\hat{Q} + i\hat{P}b_o^2)\ |0\rangle = 0 \tag{IV.8}$$

where b_o is the size-parameter of the oscillator of the relative motion of the protons against the neutrons

$$b_o = \sqrt{\frac{\hbar}{\mu w_o}} = \sqrt{\frac{4}{A}}\ a_o$$

where μ is the reduced mass, $\mu = \frac{Am}{4}$ and a_o is the size parameter of the oscillator well, $a_o = \sqrt{\frac{\hbar}{mw}}$. The discussion up to now indicates that the dynamical wave-packet $|pq\rangle$ satisfies all the requirements

imposed on the previous sections. Thus the last ingredient necessary to perform a numerical calculation is the many-body hamiltonian which we assume to be of the Skyrme type[12,13],

$$H = \sum_i t(i) + \frac{1}{2}\sum_{i,j} V_{ij} + \frac{1}{3!}\sum_{i,j,k} V_{ijk} \qquad \text{(IV.9)}$$

where the two-body force is[13]

$$\begin{aligned} V_{ij} = {} & t_o(1+x_o P_\sigma)\,\delta(\hat{\underset{\sim}{r}}(i)-\hat{\underset{\sim}{r}}(j)) + \\ & + \frac{1}{2}\left[t_1 \left(\left(\frac{\hat{\underset{\sim}{p}}(i)-\hat{\underset{\sim}{p}}(j)}{2}\right)^2 \delta(\hat{\underset{\sim}{r}}(i)-\hat{\underset{\sim}{r}}(j)) + \right.\right. \\ & + \delta(\hat{\underset{\sim}{r}}(i) - \hat{\underset{\sim}{r}}(j)) \left(\frac{\hat{\underset{\sim}{p}}(i)-\hat{\underset{\sim}{p}}(j)}{2}\right)^2 + \\ & \left.\left. + 2\, t_2 \frac{\left(\hat{\underset{\sim}{p}}(i) - \hat{\underset{\sim}{p}}(j)\right)}{2} \delta(\hat{\underset{\sim}{r}}(i)-\hat{\underset{\sim}{r}}(j)) \left(\frac{\hat{\underset{\sim}{p}}(i)-\hat{\underset{\sim}{p}}(j)}{2}\right) \right] \right. \\ & + \hat{V}_{SO_{ij}} \end{aligned} \qquad \text{(IV.10)}$$

where $\hat{P}_\sigma$ is the spin exchange operator and $\hat{V}_{SO_{ij}}$ is the spin orbit force.

The three-body force is parametrized as[12,13]

$$V_{ijk} = t_3\, \delta(\hat{\underset{\sim}{r}}(i)-\hat{\underset{\sim}{r}}(j))\, \delta(\hat{\underset{\sim}{r}}(i)-\hat{\underset{\sim}{r}}(k)) \qquad \text{(IV.11)}$$

IV-B) The Semi-Classical Hamiltonian

The semi-classical hamiltonian eq. II.3 is given by

$$H^{CL}(p,q) = \langle q|H|q\rangle + \sum_{n=0}^{\infty} \frac{p^{2n}}{(2n)!}(-1)^n \qquad \text{(IV.12)}$$

$$\langle q| \underbrace{[\hat{Q},[\hat{Q}\ldots[\hat{Q},\hat{H}]\ldots]]}_{\text{2n Brackets}} |q\rangle$$

where $|q\rangle$ is equal to

$$|q\rangle = e^{-iq\hat{P}} |0\rangle \qquad \text{(IV.13)}$$

In the specific case of the Skyrme force one has [12,14]

$$\left[\hat{Q},\left[\hat{Q},\hat{H}\right]\right] = \frac{1}{\mu} + \frac{1}{2} \sum_{i,j} \frac{4(t_1+t_2)}{A^2} \delta(\hat{\underline{r}}(i)-\hat{\underline{r}}(j))(1-T_3(i)T_3(j)) \qquad \text{(IV.14)}$$

which shows that

$$\left[\hat{Q},\left[\hat{Q},\left[\hat{Q},\hat{H}\right]\right]\right] = 0 \qquad \text{(IV.15)}$$

Therefore the expansion stops at second order and the semi-classical hamiltonian can be exactly written as

$$H^{CL}(p,q) = \frac{p^2}{2M_{CL}(q)} + V_{CL}(q) \qquad \text{(IV.16)}$$

where the semi-classical potential and mass-parameter are respectively equal to

$$V_{CL}(q) = \langle q|\hat{H}|q\rangle$$

$$B_{CL}(q) = M_{CL}^{-1}(q) = \langle q|\left[\hat{Q},\left[\hat{H},\hat{Q}\right]\right]|q\rangle \qquad \text{(IV.17)}$$

The inverse of the semi-classical mass-parameter can be written as

$$B_{CL}(q) = \frac{1+\varepsilon(q)}{\mu}$$

where $\varepsilon(q)$ is the enhancement factor of the energy weighted dipole sum rule

$$\varepsilon(q) = \frac{2\mu}{\hbar^2} \frac{1}{2} \langle q|\left[\hat{Q},\left[\hat{V},\hat{Q}\right]\right]|q\rangle$$

IV-C) The GCM Quantum Collective Hamiltonian

The quantum collective hamiltonian is given by eq. III.25 and as a consequence of eq. IV.15 it reduces to

$$\hat{H}_C^{GCM} = \hat{S}(H^{(0)}(\hat{Q}) + \frac{1}{4}\{\hat{P},\{\hat{P},H^{(2)}(\hat{Q})\}\})\hat{S}$$

where the quantum collective potential and mass parameter are equal to

$$\hat{V}(Q) = \hat{H}^{(0)}(\hat{Q})$$

$$\hat{B}(Q) = M(Q)^{-1} = \frac{\hat{H}^{(2)}(Q)}{2} \qquad \text{(IV.18)}$$

In our example the reduced energy kernel is exactly given by[12]

$$h(q,q') = V_{CL}(\bar{q}) - \frac{\hbar^2}{8b_o^4 M_{CL}(\bar{q})}\tilde{q} \qquad \text{(IV.19)}$$

where

$$\bar{q} = (q+q')/2$$

$$\tilde{q} = q-q'$$

Thus $\hat{V}(\hat{Q})$ and $\hat{B}(\hat{Q})$ can be written as

$$\hat{V}(Q) = \frac{1}{2\pi}\int dK\, e^{iKQ}\, e^{K^2 b_o^2/4} \int d\bar{q}\,(V_{CL}(q) - \frac{\hbar^2 \Delta P^2}{2M_{CL}(\bar{q})})\, e^{-i\bar{q}K}$$

$$\hat{B}(Q) = \frac{1}{2\pi}\int dK\, e^{iKQ}\, e^{K^2 b_o^2/4} \int d\bar{q}\, B_{CL}(\bar{q})\, e^{-i\bar{q}K} \qquad \text{(IV.20)}$$

where

$$\Delta P^2 = \langle 0|P^2|0\rangle = \frac{1}{2b_o^2}$$

We can also invert these equations to express the semi-classical potential and mass-parameter as

$$B_{CL}(q) = \tilde{B}(q)$$

$$V_{CL}(q) = \tilde{V}(q) + \frac{\hbar^2 \Delta P^2}{2} B_{CL}(q) \qquad \text{(IV-21)}$$

where $\tilde{B}(Q)$ and $\tilde{V}(Q)$ are the expectation values of the quantum inverse mass-parameter and potential on the wave-packet $|q\rangle$

$$\tilde{B}(q) = \int B(x) \left| \langle x|q\rangle \right|^2 dx$$

$$\tilde{V}(q) = \int V(x) \left| \langle x|q\rangle \right|^2 dx \qquad \text{(IV.22)}$$

Of course, we could also derive these equations by taking the expectation value of $\hat{H}_C^{GCM}$ on the wave-packet $|pq\rangle$ as shown in eq. IV.2.

Thus the zero-point energy in our example is given by

$$E_{ZP}(p,q) = \frac{p^2}{2} (\tilde{B}(q)-B(q)) + \tilde{V}(q)-V(q) +$$

$$+ \frac{\Delta P^2}{2} \tilde{B}(q) \qquad \text{(IV.23)}$$

Usually the effects of the zero point energy are investigated in the static limit $(p=0)$[7]. Also one separates it into two pieces, the potential zero point energy

$$E_{PZP}(q) = \tilde{V}(q)-V(q) \qquad \text{(IV.24)}$$

which depends only on the potential and a kinetic zero-point energy

$$E_{KZP}(q) = \frac{\hbar^2 \Delta P^2}{2} \tilde{B}(q) \qquad \text{(IV.25)}$$

which depends on the kinetic energy.

IV-D) Qualitative Discussion

According to what has been shown so far, the zero-point energy corrections depend on the properties of the wave-packet $|pq\rangle$ and the GCM inverse mass-parameter and potential.

To shed light on this point, we consider the case where the quantum inverse mass-parameter does not depend on the coordinate,

$$B(x) = B_o .$$

Therefore it follows that the semi-classical inverse mass-parameter is also independent of the coordinate and so the kinetic zero-point energy is a constant in this case.

Therefore we can always find a wave-packet so that the dynamical effect of $E_{ZP}(q)$ is negligible. Indeed we can decrease the width of the wave-packet $|q\rangle$ until one has $\tilde{V}(q) \simeq V(q)$. However the uncertainty principle states that when ΔQ^2 is small ΔP^2 becomes large and so the kinetic zero point energy increases; but since it is a constant, it does not have any effect on the dynamics. However when $\tilde{B}(x)$ depends on the coordinate this is not guaranteed a priori since, as before, we can make the potential zero point energy small but the kinetic zero-point energy, which now depends on the coordinate increases when we decrease the width of the wave-packet. Another example which has been investigated in the literature[15] is the case when it is valid to consider an expansion of the reduced energy kernel as a power series in q and q',

$$h(q,q') = h_o + \frac{1}{2}(h_{20}q^2 + h_{20}q'^2 + 2h_{11}qq') + \ldots .$$

where

$$h_{02} = -\langle 0|\hat{H}\hat{P}^2|0\rangle + E_0\langle 0|\hat{P}^2|0\rangle$$

$$h_{20} = -\langle 0|\hat{P}^2\hat{H}|0\rangle + E_0\langle 0|\hat{P}^2|0\rangle$$

$$= h_{02}$$

$$h_{11} = \langle 0|\hat{P}\hat{H}\hat{P}|0\rangle - E_0\langle 0|\hat{P}^2|0\rangle$$

In this case the quantum collective hamiltonian is, using eqs. III. 25 and III.26

$$\hat{H}_C^{GCM} = \hat{S}_1(E_0 + \frac{\hat{P}^2}{2M_0} + \frac{1}{2}K_M\hat{Q}^2 + E_{ZP})\hat{S}_1$$

where

$$B_0 = M_0^{-1} = \langle 0|[\hat{Q},[\hat{H},\hat{Q}]]|0\rangle$$

$$K_M = \langle 0|[\hat{P},[\hat{H},\hat{P}]]|0\rangle$$

$$E_{ZP} = \langle 0|\frac{\hat{P}^2}{2M_0} + \frac{1}{2}K_M\hat{Q}^2|0\rangle$$

The semi-classical hamiltonian in this case becomes

$$H^{CL}(p,q) = E_0 + \frac{p^2}{2M_0} + \frac{1}{2}K_M q^2$$

which differs from the GCM quantum collective hamiltonian by the constant zero point energy which does not have any effect on the dynamics.

IV-E) The Effect Of The Zero-Point Energy On The Goldhaber-Teller Mode In ^4He

All the details of the calculations can be found in references 14 and 16. In the case of ^4He we can find analytic expressions for all the quantities of interest which was the procedure

adopted in this paper.

Before discussing the numerical results we would like to make two comments

a) The center of mass motion is exactly factorized in the wave-packet $|pq\rangle$ so there is no spurious center of mass motion.

b) The spin-orbit force does not contribute to the inverse mass-parameters and potentials since the density of protons and neutrons on the wave-packet $|pq\rangle$ is a scalar in spin space (there is no vector part in the density).

In figure 1 we have a graph of the classical and quantum mass parameter as a function of the coordinate. This graph indicates that the mass parameters varies slowly with x and in the limit of x going to infinite it reduces to the reduced mass. This is an expected result since when the neutron-proton clouds are well separated the neutron-proton interaction vanishes and so does the enhancement factor. In figure two we have a graph of the classical and quantum potentials. We can see that they differ considerably, the main effect being that the quantum potential is softer. In figure 3 we plot the zero-point energy as a function of x and we see that it depends strongly on $\dot{x}$. Figures 4 and 5 which are plots of the kinetic zero point energy and potential zero point energy show that the x dependence of the zero point energy comes almost exclusively from the potential zero point energy. Indeed fig.4 shows that, in our case, the kinetic zero point energy is almost a constant which is a consequence of the almost independence of the classical mass parameter on the coordinate. On the other hand, the strong dependence of the potential zero point energy on x is a consequence of the fact that we are using as a probe a very wide wave-packet ($\Delta Q^2 = a_0^2/2$) compared to a characteristic dimension in which the quantum potential changes apreciably ($\sim a_0$). Figure 5 also shows that the potential zero point energy goes to zero for large x since the quantum potential goes to a constant value and so the potential zero point energy vanishes. Therefore for large x the only difference between

the classical and quantum potential comes from the kinetic zero point energy.

To discuss in more detail the effect of the zero point energy on the dynamics one should solve the Schroedinger equation for the semi-classical and quantum collective hamiltonians. However this, as an extension of the work to O^{16} and Ca^{40} will be the subject of a separate publication.

V) CONCLUDING REMARKS

In this paper we have investigated the relationship between the semi-classical and the generator coordinate methods, using dynamical wave-packets parametrized as

$$
\begin{aligned}
&|pq\rangle = e^{-iq\hat{P}}\, e^{ip\hat{Q}}\, |0\rangle \\
&[\hat{Q},\hat{P}] = i \\
&(\hat{Q}+i\hat{P}b_o^2)\,|0\rangle = 0
\end{aligned}
\qquad \text{(V.1)}
$$

In reference 1 it is proposed that the two theories are equivalent once two requirements are satisfied: a) the wave-packet $|pq\rangle$ is redundant, where redundancy means that the subspaces associated by the GCM to the dynamical, $|pq\rangle$ and static, $|q\rangle = |p=0,q\rangle$ wave-packets, taken as generator states, are identical; b) the effects of the zero-point motion of the wave-packet $|pq\rangle$ is negligible. The requirement a) is based on the observation that the dependence of $|pq\rangle$ on the parameters p and q is thought to describe the distortion of the system along one canonical degree of freedom. Once the wave-packet is redundant requirement b) means that $|pq\rangle$ is able to extract the classical limit of the GCM quantum collective hamiltonian.

Using tools developed earlier[8,9,10] we show that the wave-packet $|pq\rangle$ parametrized as in V.1 is redundant which in our case is a consequence of the global decoupling between the intrinsic and collective degrees of freedom. Once the wave-packet is redundant we show that the semi-classical hamiltonian is equal to the expectation value of the quantum collective hamiltonian in the wave-packet $|pq\rangle$. So, the two theories are identical from the point of view of the dynamics if $|pq\rangle$ is able to extract the classical limit of the GCM quantum collective hamiltonian. This last property depends essentially on the type of wave-packet which is used and it reduces to the analyses of the effects of the zero-point energy of $|pq\rangle$. This problem is investigated numerically for the Goldhaber-Teller mode in

^{4}He where it is shown that the effects of zero-point motionis apreciable. In our example this comes almost exclusively from the potential zero-point energy and, of course, this depends on the type of mode that is considered. As this point we would like to remark that the conditions under which the wave-packet $|pq\rangle$ is able to extract the classical limit of the GCM quantum collective hamiltonian are in general different from the conditions under which the Ehrenfest theorem holds. This stems from the fact $|pq\rangle$ is a parametrized (constrained) wave-packet and not a time-dependent solution of the Schroedinger equation in the GCM collective subspace. So, one can in certain circunstances, parametrize $|pq\rangle$ so as to be able to extract the classical limit of $\hat{H}_C^{GCM}$ even though the dynamics given by $\hat{H}_C^{GCM}$ is not semi-classical.

There are many-examples where the study of the effects of the zero-point motion in microscope theories of collective motion is important[17] as the case of fission, especially in light nuclei.

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FIGURE CAPTIONS

FIG. 1 - Plot of the classical mass parameter (full line) and quantum mass parameter (dotted - dashed line) in units of the nuclear mass as a function of the "coordinate" x. The size parameter of the oscillator well, a_o, is equal to 1.57 fermis.

FIG. 2 - Plot of the classical potential (full-line) and quantum potential (dotted-dashed line) as a function of the "coordinate" x.

FIG. 3 - Plot of the zero-point energy as a function of the "coordinate" x.

FIG. 4 - Plot of the kinetic zero point energy as a function of the "coordinate" x .

FIG. 5 - Plot of the potential zero-point energy as a function of the "coordinate" x.

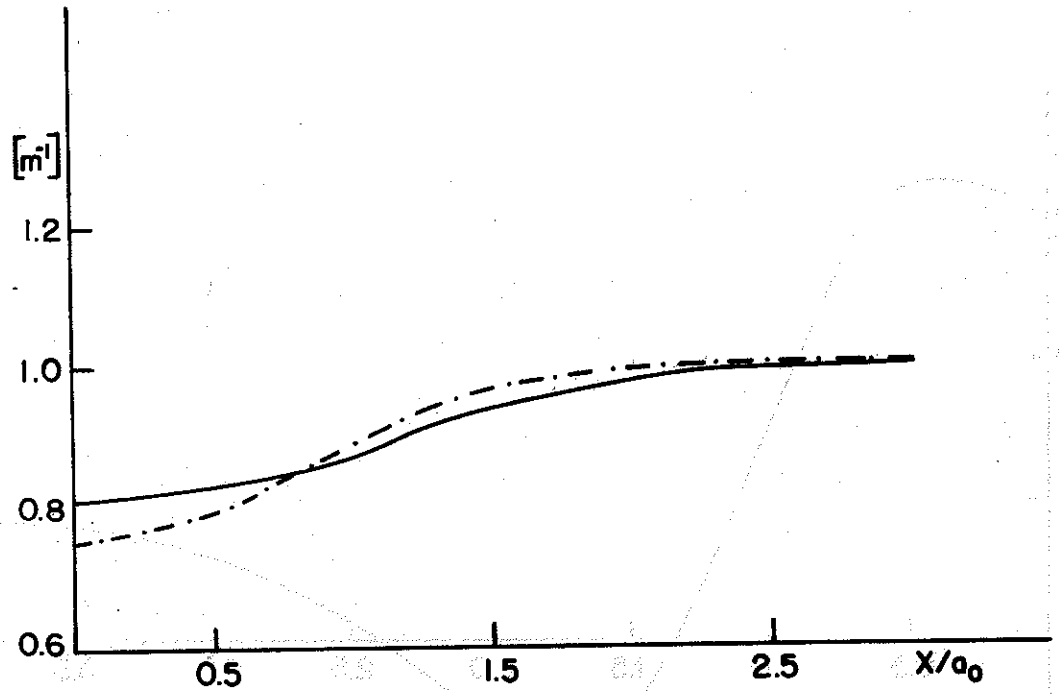
[m⁻¹]
1.2
1.0
0.8
0.6
0.5
1.5
2.5
X/a₀

Fig. 1

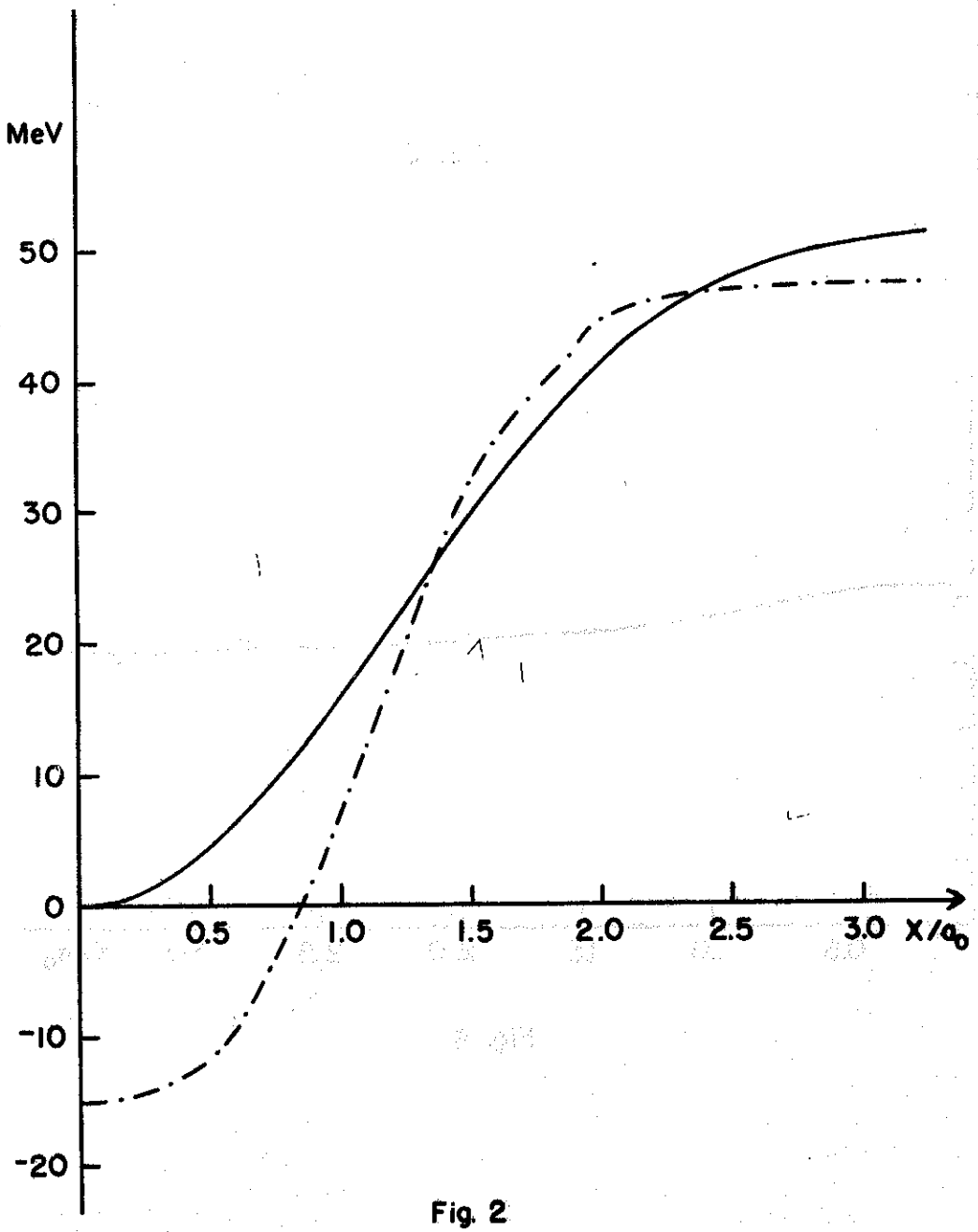
MeV
50
40
30
20
10
0
-10
-20
0.5
1.0
1.5
2.0
2.5
3.0
X/a₀

Fig. 2

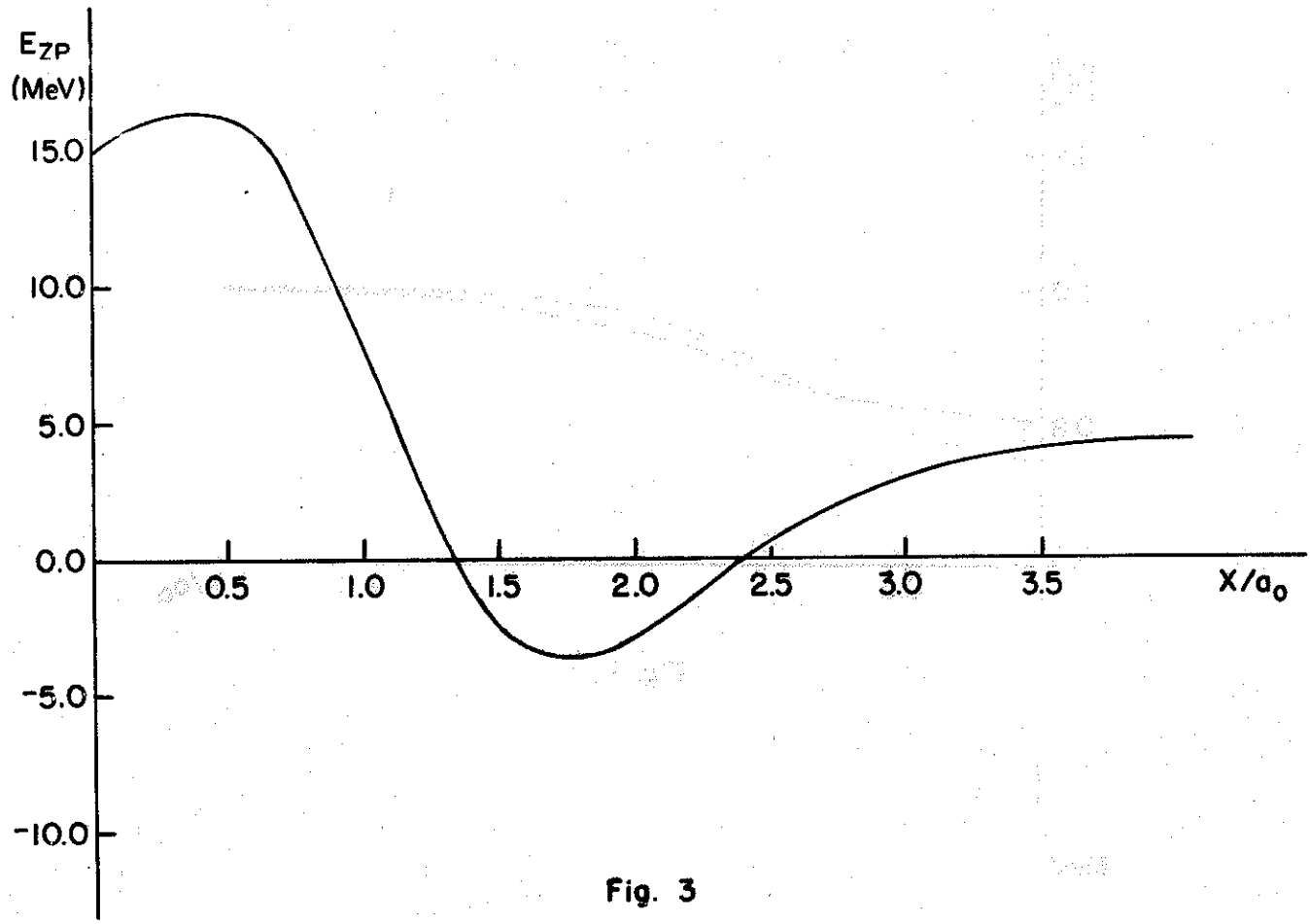
E_{ZP}
(MeV)
15.0
10.0
5.0
0.0
-5.0
-10.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
X/a_0

Fig. 3

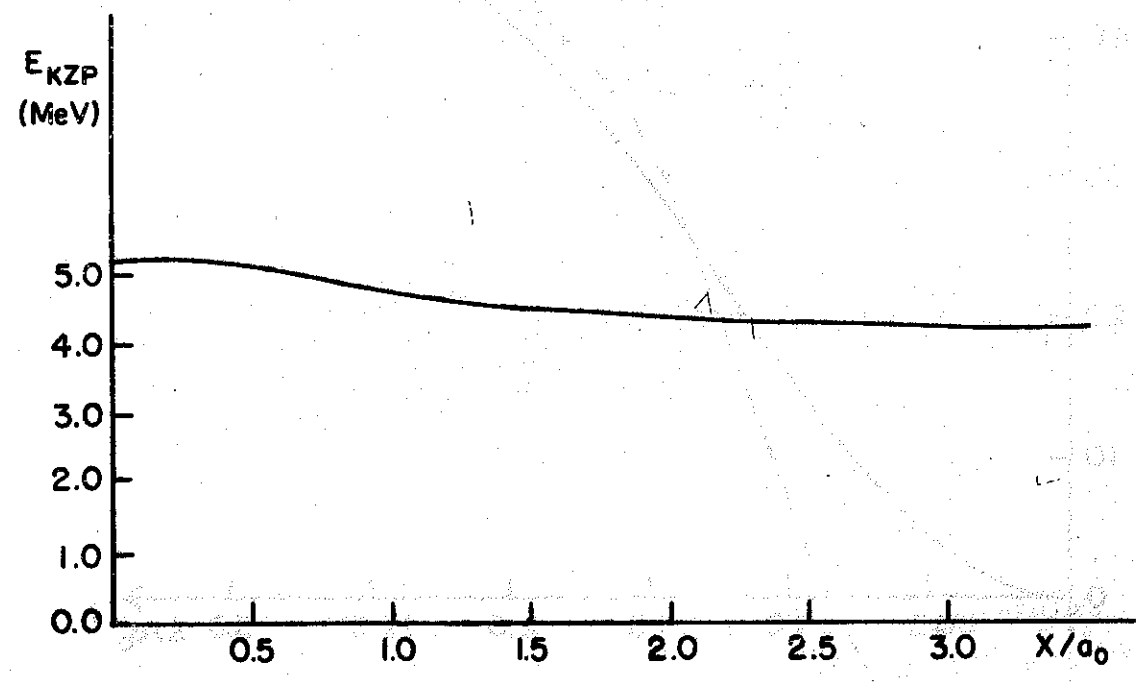
E_{KZP}
(MeV)
5.0
4.0
3.0
2.0
1.0
0.0
0.5
1.0
1.5
2.0
2.5
3.0
X/a_0

Fig. 4

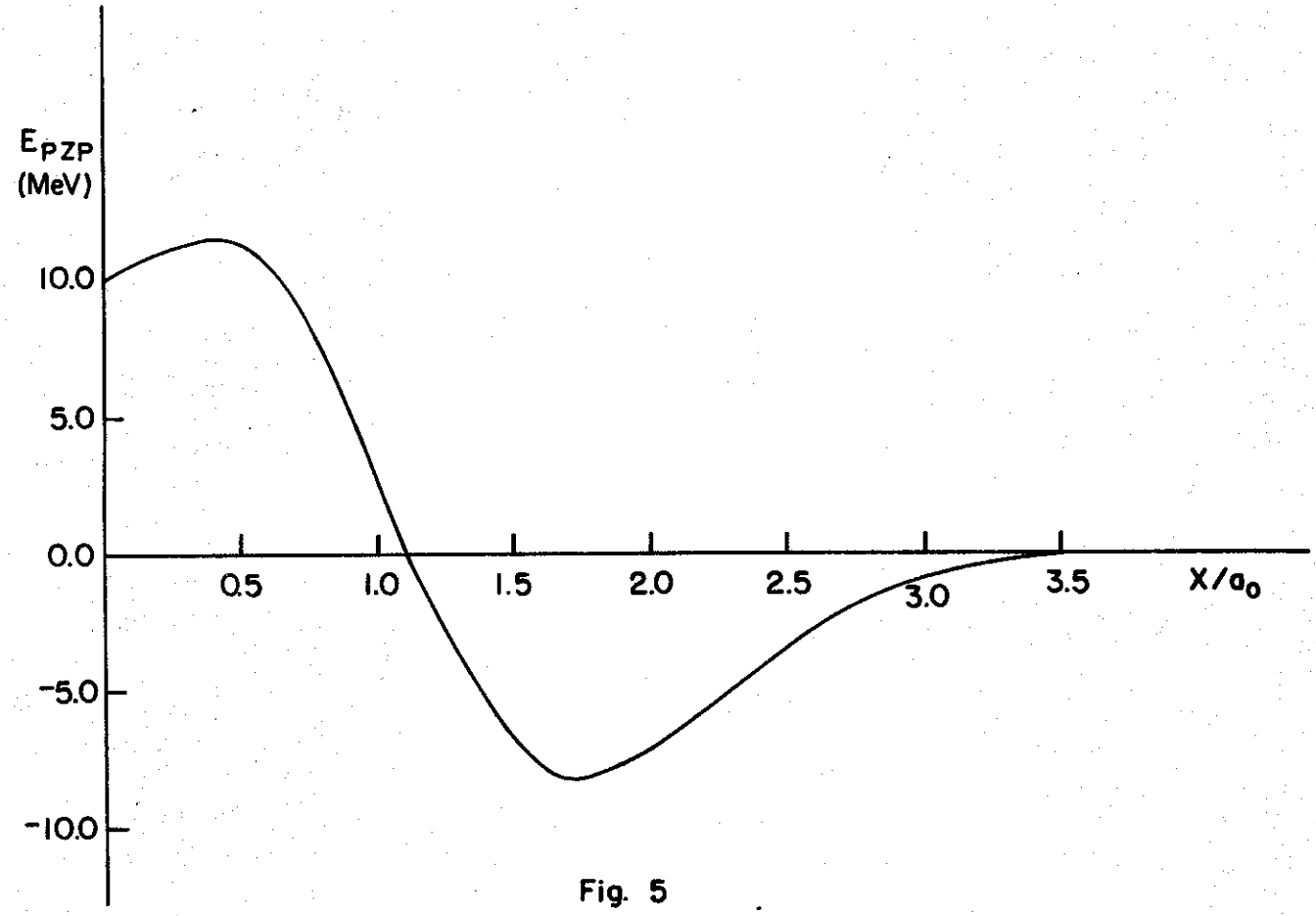

Fig. 5