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SEMICLASSICAL QUANTIZATION OF THE SHELL MODEL *

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Abstract: The classical limit of the nuclear shell model is shown to be a many-dimensional hamiltonian system in which the coordinates and momenta are the coherent-state parameters of the original quantum system. Several methods for semiclassical quantization of this system are discussed, including surfaces of section and the Birkhoff-Gustavson transformation to action-angle variables. Application to a schematic three-level shell model indicates some of the new problems involved in requantizing multi-dimensional systems which are not present in one-dimensional examples. These include difficulties in finding periodic orbits and the onset of stochasticity.

1. Introduction

Several recent studies have suggested that functional-integral representations of the many-body propagator are of potential use in nuclear physics problems, particularly when evaluated in the stationary-phase (semiclassical) approximation. Indeed, the realization that the latter is closely related to the phenomenologically successful time-dependent Hartree-Fock (TDHF) approximation offers hope of ultimately achieving tractable descriptions of a variety of nuclear observables. Among these are bound-state energies [1,2]), the nuclear partition function, spontaneous and induced fission lifetimes [3,4]), and elements of the many-body S-matrix [5]).

This paper is concerned with semiclassical approximations to the eigenvalues of nuclear hamiltonians, specifically shell-model hamiltonians. Functional integral treatments imply that these can be obtained by considering the "classical" periodic TDHF trajectories for a given hamiltonian and then "requantizing" them, naively in analogy with the familiar Sommerfeld-Wilson quantization integral [6]). One can also obtain this same prescription by requiring that the TDHF equations preserve the gauge-invariance of the original Schrödinger equation [7]). To date, semiclassical methods have been applied with good results to a schematic two-level shell model [1,7,8]), and to certain interacting boson hamiltonians [9]). For these cases, in which the non-trivial classical TDHF equations are one-dimensional, there is a readily identifiable constant of the motion (the total energy) and requantization is fairly straightforward and

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unambiguous. However, in the more general case of a non-integrable (multi-dimensional) system, even the quantization prescription is in dispute.

Our primary goal in this paper is to explore the conceptual and practical aspects of semiclassical quantization procedures in somewhat more realistic systems, those in which the non-trivial classical TDHF equations are of dimension two or greater. For small amplitude (low energy) excitations, there is no problem since the classical description reduces to the readily integrable one of a set of uncoupled harmonic normal modes and the familiar RPA limit is recovered. However, there is good reason to expect qualitative changes at higher energies where the classical mechanics need no longer be integrable and, in fact, the periodic trajectories are even difficult to find, let alone quantize.

A considerable literature already exists concerning the semiclassical quantization of non-integrable systems [10,11]), largely in connection with problems of intramolecular dynamics. This has developed concurrently with the growing emphasis in classical mechanics on the topological and global structure of trajectories rather than on their microscopic detail. Hence, much of the material we present here amounts to a restatement of these ideas in a language appropriate to nuclear physics and their application to nuclear problems. This alone seems to be a worthwhile goal as many basic points remain in dispute and the field continues to be an active area of current research. It is particularly intriguing to ask how such classical concepts as strange attractors or stochasticity are manifest in the quantum spectrum [12]). Conversely, it may be that a classical description can offer novel insights into level densities, collectivity, doorway states and giant resonances.

We have chosen to analyze in detail a simple nuclear hamiltonian which gives non-integrable classical behavior, a schematic three-level shell model, for which the classical dynamics is two-dimensional. In sect. 2, we review the use of coherent states to obtain the classical hamiltonian corresponding to an arbitrary shell-model hamiltonian. Sect. 3 contains a description and discussion of several quantization methods. In sect. 4, we present our results for the SU(3) model. Finally, sect. 5 contains a summary and our conclusions.

2. Semiclassical description of the shell model

We use the formalism of Blaizot and Orland [18]), in which a shell-model coherent state is parametrized by a set of c-numbers z_{ph}, with p and h particle and hole orbitals; z_{ph} can be thought of as an $n_p \times n_h$ matrix, where n_p and n_h are the numbers of particle and hole orbitals. The coherent states are generated by a Thouless transformation,

$$|z\rangle = \exp\left(\sum_{ph} z^*_{ph} a^+_p a_h\right)|0\rangle, \tag{2.1}$$

of the fermion vacuum state of all hole orbitals filled, $|0\rangle$. They allow a completeness relation of the form

$$\int \prod_{ph} \frac{dz_{ph} dz_{ph}^*}{2\pi i} |z\rangle \mu(z, z^*) \langle z| = 1. \tag{2.2}$$

$$\mu(z, z^*) = [\det(1 + z^+ z)]^{-(n_p + n_h - 1)}. \tag{2.3}$$

The wave function of the system, $|\Psi\rangle$, is then described by the analytic function $\psi(z)$, by giving its projection on the coherent state $|z\rangle$:

$$\psi(z) = \langle z|\Psi\rangle, \tag{2.4}$$

so that

$$|\Psi\rangle = \int \prod_{ph} \frac{dz_{ph} dz_{ph}^*}{2\pi i} |z\rangle \mu(z, z^*) \psi(z). \tag{2.5}$$

The fact that the measure $\mu(z, z^*)$ is not unity essentially means that the coherent states (2.1) are not orthonormal and hence that the variables z_{ph}, z_{ph}^* are not canonical in the corresponding classical system. We therefore transform to the canonical variables [13]:

$$\beta_{ph} = \sum_{h'} z_{ph'} [(1 + z^+ z)^{-\frac{1}{2}}]_{h'h}. \tag{2.6}$$

The completeness relation in terms of the β_{ph} variables now has unit measure:

$$\int \prod_{ph} \frac{d\beta_{ph} d\beta_{ph}^*}{2\pi i} |\beta\rangle \langle\beta| = 1. \tag{2.7}$$

The expectation value of a given hamiltonian can be calculated from the density matrix elements

$$\begin{aligned} \rho_{\alpha\beta} &\equiv \langle\beta|\alpha_\beta^+ a_\alpha|\beta\rangle, \\ \rho_{ph} &= [\beta(1 - \beta^+\beta)^{\frac{1}{2}}]_{ph}, \qquad \rho_{hp} = \rho_{ph}^*, \\ \rho_{pp'} &= (\beta\beta^+)_{pp'}, \\ \rho_{hh'} &= \delta_{hh'} - (\beta^+\beta)_{hh'}. \end{aligned} \tag{2.8}$$

The eigenvalue problem we seek to solve is

$$H(a_\alpha^+, a_\beta)|\Psi\rangle = E|\Psi\rangle. \tag{2.9}$$

Using the property of coherent states,

$$\frac{\partial}{\partial z^*_{\mathrm{ph}_i}}|z\rangle = z_{\mathrm{ph}}|z\rangle, \tag{2.10}$$

we obtain a Schrödinger equation equivalent to the original problem,

$$H\left(\beta_{\mathrm{ph}}, -i\hbar\frac{\partial}{\partial\beta_{\mathrm{ph}}}\right)\psi(\beta_{\mathrm{ph}}) = E\psi(\beta_{\mathrm{ph}}). \tag{2.11}$$

The boundary conditions on ψ are somewhat uncertain, since the β are restricted to lie in a hypersphere by virtue of (2.6). The semiclassical limit of this Schrödinger equation can be obtained by the WKB ansatz and the methods of subsect. 3.1, giving a classical hamiltonian $H(\beta_{\mathrm{ph}}, \beta^*_{\mathrm{ph}})$ with Hamilton's equations,

$$\begin{aligned} i\dot{\beta}_{\mathrm{ph}} &= \partial H/\partial\beta^*_{\mathrm{ph}}, \\ -i\dot{\beta}^*_{\mathrm{ph}} &= \partial H/\partial\beta_{\mathrm{ph}}. \end{aligned} \tag{2.12}$$

This classical hamiltonian is then just the expectation value of the shell-model hamiltonian calculated with the density matrix (2.8), and (2.12) are the familiar TDHF equations.

The solution to the original problem (2.9) can also be expressed as a path-integral for the propagator,

$$\begin{aligned} K(\beta, \beta', T) &= \int D[\beta, \beta^*] \exp\left(iS[\beta, \beta^*]/\hbar\right), \\ S[\beta, \beta^*] &= \int_0^T \mathrm{d}t\{\mathrm{Tr}(i\beta^+\beta - \langle\beta|H|\beta\rangle)\}. \end{aligned} \tag{2.13}$$

The stationary phase approximation to this path integral, $\delta S = 0$, is identical to the TDHF variational principle and also yields the equations of motion (2.12).

3. Quantization

Given a classical hamiltonian, there are essentially two methods for finding semiclassical approximations to the quantum energy levels. The first of these is Einstein-Brillouin-Keller quantization [14-16]), while the second is that based on periodic trajectores [2, 10, 13, 17]). We treat each in turn, specializing to a two-dimensional system, and then give a partial reconciliation [18]). An "analytic" algorithm, the Birkhoff-Gustavson transformation [19]), is also discussed.

3.1. EBK QUANTIZATION [14])

We start with a Schrödinger equation, such as eq. (2.10), written in terms of "coordinate" and "momentum" operators, $\boldsymbol{q}$ and $\boldsymbol{p} = -i\hbar\partial/\partial\boldsymbol{q}$:

$$H(\boldsymbol{q}, \boldsymbol{p})\psi(\boldsymbol{q}) = E\psi(\boldsymbol{q}), \tag{3.1}$$

where ψ is a stationary state and E is its energy, and make a WKB-like ansatz,

$$\psi(\boldsymbol{q}) = A(\boldsymbol{q})\exp\left(\frac{iS(\boldsymbol{q})}{\hbar}\right), \tag{3.2}$$

with A and S real. To zeroth and first order in $\hbar$, respectively, one finds

$$H\left(\boldsymbol{q}, \frac{\partial S}{\partial \boldsymbol{q}}\right) = E, \tag{3.3}$$

$$\frac{\partial}{\partial \boldsymbol{q}}(\boldsymbol{v}A^2) = 0, \tag{3.4}$$

where

$$\boldsymbol{v} = \frac{\partial}{\partial \boldsymbol{p}} H(\boldsymbol{q}, \boldsymbol{p}).$$

Eq. (3.3) is the Hamilton-Jacobi equation of classical mechanics [20]), and (3.4) is the Liouville equation, allowing the interpretation of A^2 as the classical phase-space density. Defining $\boldsymbol{p} = \partial S/\partial \boldsymbol{q}$, a variable instead of an operator, (3.3) can be solved by the method of characteristics to obtain Hamilton's equations,

$$\dot{\boldsymbol{q}} = \partial H/\partial \boldsymbol{p},$$

$$\dot{\boldsymbol{p}} = -\partial H/\partial \boldsymbol{q},$$

$$S = \int \boldsymbol{p}\cdot\dot{\boldsymbol{q}}\,\mathrm{d}t. \tag{3.5}$$

Solving these equations may not produce a single-valued or even multivalued function $S(\boldsymbol{q})$; the trajectory may generate an arbitrarily large number of $\boldsymbol{p}$ values for an arbitrarily small neighborhood about a given $\boldsymbol{q}$. In that case the system is said to be stochastic. If however, the classical variables are finitely multivalued (a finite number of $\boldsymbol{p}$-values for each $\boldsymbol{q}$-value), the system is said to be quasiperiodic and we may replace the WKB ansatz (3.2) by $\sum_{\text{branches}} A\exp(iS/\hbar)$. We then demand single-valuedness of the semiclassical wave function; i.e. that the difference ΔS between any sheet and itself be a

multiple of $2\pi\hbar$. Furthermore, the semiclassical wave function should match correctly to an Airy function [21]) at the edges of the classically allowed region, giving the Maslov correction [16,22]) to the quantization condition,

$$\int_{\gamma_i} \nabla S \cdot \mathrm{d}s = \int_{\gamma_i} \boldsymbol{p} \cdot \mathrm{d}\boldsymbol{q} = 2\pi\hbar(n_i + \tfrac{1}{4}\alpha_i), \tag{3.6}$$

with n_i an integer, γ_i a circuit in phase-space lying on the manifold consisting of the sheets $\boldsymbol{p}(\boldsymbol{q})$ and α_i the number of times the circuit γ_i touches the edges of the classically allowed region. This manifold is analogous to the Riemann sheet of complex analysis and has the topology of a torus, as is clear from the "hairy coconut" theorem: the hamiltonian velocity forms a combable tangent vector field which is nowhere zero, so the topology cannot be spherical. We thus have two independent circuits and hence two quantum numbers.

These considerations are the basic ideas underlying the EBK method for calculating semiclassically the energy levels of a system whose classical variables are finitely multivalued functions of $\boldsymbol{q}$. One additional ingredient is the KAM theorem [23]), which

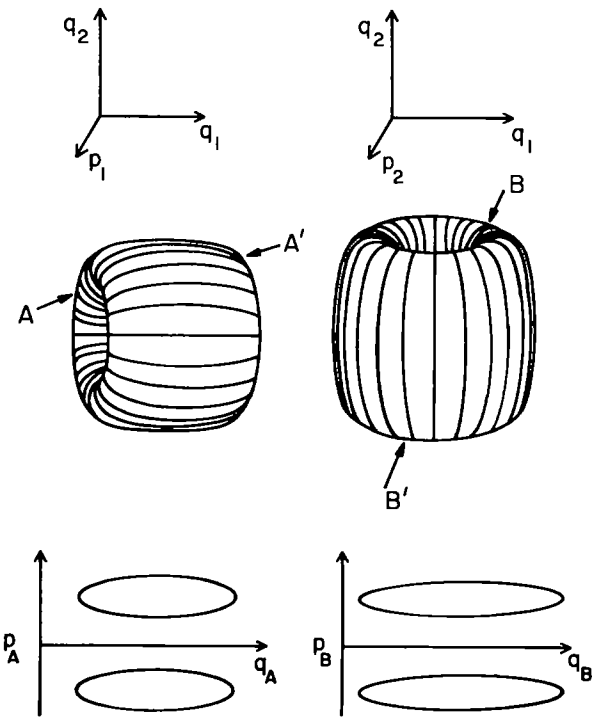


Fig. 1. Schematic illustration of a four-dimensional invariant torus when projected in three-dimensional space. One dimension can be omitted because of energy conservation. Two of the four possible coordinate triplets are shown, with surfaces of section.

states that if a bounded system is sufficiently close to being separable, then it has this property, so that the trajectories do lie on such invariant tori or, in other words, they are quasiperiodic. For a system with two degrees of freedom (two coordinates and two momenta), the energy shell has dimensionality three, a quasiperiodic trajectory has dimensionality two, and a periodic trajectory is undimensional. Separability is determined by the excitation energy of the system. When this energy is zero, the system is static at the Hartree-Fock minimum; for very small excitations, the system exhibits uncoupled RPA modes; for higher energies, these modes might couple non-linearly, and the system may no longer be separable. We therefore expect to be able to requantize the system when the excitation energy is "sufficiently small" in the sense of KAM.

One practical way to evaluate the EBK quantization integrals around topologically independent circuits is by examining a planar section of the trajectory manifold [Poincaré map [24])]. A point is marked on this plane each time the trajectory pierces it. If the trajectory is quasiperiodic, the eventual figure traced out is a smooth curve; if it is stochastic, the result is a "splatter". By rotating the coordinates $q_1, q_2, p_1, p_2 \rightarrow q_A, q_B, p_A, p_B$ so that the section plane is defined by $q_A =$ constant, then $\int \boldsymbol{p} \cdot \dot{\boldsymbol{q}}$ around that circuit is just the area of the circuit in (q_B, p_B) space. The surfaces of section must have reflection symmetry about the q-axis, since time-reversal takes $(\boldsymbol{q}, \boldsymbol{p}) \rightarrow (\boldsymbol{q}, -\boldsymbol{p})$, and this transformation cannot affect the global shape of the manifold if H is time-reversal invariant. The energy shell has two natural projections, (q_1, q_2, p_1) or (q_1, q_2, p_2) as in fig. 1; the torus and section are also shown for each of these projections.

3.2. QUANTIZATION BY PERIODIC TRAJECTORIES [1, 2, 10, 13, 17])

The path integral route to quantization consists of writing the propagator as a Feynman path integral,

$$K(\boldsymbol{q}, \boldsymbol{q}'; T) = \int D[\boldsymbol{q}(t), \boldsymbol{p}(t)] \exp\left(iS[\boldsymbol{q}(t), \boldsymbol{p}(t)]/\hbar\right),$$

$$S[\boldsymbol{q}(t), \boldsymbol{p}(t)] = \int_0^T (\boldsymbol{p} \cdot \dot{\boldsymbol{q}} - H) \mathrm{d}t. \tag{3.7}$$

This is also the form of the shell-model propagator given in eqs. (2.13). The quantization, by first-order stationary phase, consists of finding all periodic classical trajectories such that

$$W \equiv ET + S = \int_0^T \boldsymbol{p} \cdot \mathrm{d}\boldsymbol{q} = 2\pi\hbar(n + \tfrac{1}{2}), \tag{3.8}$$

where E, T, S are the energy, period and action, respectively, of the circuit. For simplicity, the following is restricted to the case of a system with two degrees of freedom, which has a four-dimensional phase space. The second-order stationary phase approxi-

mation involves the stability angle ν of the trajectory, giving the quantization condition

$$(m+\tfrac{1}{2})\nu + \int \boldsymbol{p}\cdot \mathrm{d}\boldsymbol{q} = 2\pi\hbar(n+\tfrac{1}{2}), \tag{3.9}$$

where ν is the non-zero eigenvalue of the stability matrix of the path; it measures the frequency of small oscillations about the periodic trajectory and the integers m and n thus form a complete set of quantum numbers. The classical energy of this trajectory is an approximation to the quantum eigenenergy. Quantization by periodic trajectories is therefore seen to be a blend of Sommerfeld-Wilson quantization along the path and an harmonic approximation transverse to the path.

3.3. DISCUSSION

At first sight, EBK and periodic trajectory quantization are completely different. However, Berry and Tabor [18]) have shown that the two are in a sense equivalent, in the quasiperiodic part of the classical phase-space. They are equivalent in that a stationary phase approximation to the EBK method produces a sum over periodic trajectories, which can also be obtained from the path integral formulation. In the quasiperiodic regime, the trajectory has (non-analytic) constants of the motion, the actions obtained by integration along a circuit on the invariant torus, as in subsect. 3.1. These together with the corresponding angle variables are canonical [25]) and are a good coordinate system since the hamiltonian is a function only of the actions. Setting these actions to $2\pi\hbar(n+\frac{1}{2})$ gives the semiclassical energy levels. Berry and Tabor wrote the density of states as a sum of delta-functions at these values, used Poisson's formula to transform each delta-function to an integral, and invoked the SPA for each integral. The result is a sum over an integer-valued lattice, each point of the lattice representing a periodic trajectory whose frequencies have the same ratio as the ratio of the lattice coordinates.

The same sum over periodic trajectories can be obtained from the quantum expression $\mathrm{Tr}\,\delta(E-H)$ for the density of states. Expressed as a path integral in the action-angle coordinates, the trace becomes a trivial integration over angles. This reveals the basic flaw in the analysis of Gutzwiller *et al.* [17]) who find the stationary paths to their SPA for the trace to be periodic trajectories. However, Helleman and Bountis [26]) have shown that periodic trajectories are dense in the phase-space, so that this SPA is not justified. Furthermore, there is natural topology to the periodic trajectories (the integer lattice of Berry and Tabor) which the quantization by periodic trajectories ignores.

On a practical level, Noid and Marcus [27]) tried direct quantization by periodic trajectories, as in (3.8), of a Henon-Heiles hamiltonian

$$H = \tfrac{1}{2}(p_1^2+q_1^2+p_2^2+q_2^2)+q_1^2q_2-\tfrac{1}{3}q_2^3. \tag{3.10}$$

They found periodic trajectories by simply adjusting the initial conditions until the surfaces of section became sets of points instead of curves. Numerous spurious energy levels were found in addition to the expected levels.

Helleman and Bountis [26]) used a slightly more systematic approach to the search for periodic trajectories of a similar system and found families of them filling phase-space. Unfortunately they did not go on to quantize the system. Their method consists of writing q_1, q_2 as a Fourier series. The action, which is the time-integral of the lagrangian, is thus an explicit function of these Fourier coefficients. Hamilton's principle states that this action is stationary with respect to the Fourier coefficients at a classical trajectory. Naively, Newton's method can be used to solve these equations. However, there is a problem in that the second-derivative matrix, which must be invertible for Newton's method to work, has a zero eigenvalue at the classical trajectory, corresponding to time translation along the periodic trajectory. Helleman and Bountis add extra constraints to Newton's method to remove this degeneracy, but these must be carefully tuned to the hamiltonian considered and are not easily generalized. In addition, matters are further obscured if momentum is not proportional to velocity, since the lagrangian must be constructed from the hamiltonian, which is only implicitly defined as a function of the coordinates and velocities.

3.4. THE BIRKHOFF-GUSTAVSON TRANSFORMATION [19])

An analytic method of semiclassical quantization is a Taylor series expansion about the harmonic oscillator (RPA) modes known as the Birkhoff-Gustavson (BG) transformation. Without loss of generality the classical hamiltonian can be written

$$H(\boldsymbol{q}, \boldsymbol{p}) = \sum_k \tfrac{1}{2}\omega_k(q_k^2 + p_k^2) + H^{(3)}(\boldsymbol{q}, \boldsymbol{p}) + H^{(4)}(\boldsymbol{q}, \boldsymbol{p}) + \ldots, \tag{3.11}$$

where $H^{(s)}(\boldsymbol{q}, \boldsymbol{p})$ is a homogeneous polynomial of degree s. The method attempts to make a canonical transformation to new variables $\boldsymbol{Q}, \boldsymbol{P}$, such that the hamiltonian H is a function only of the variables $Q_k^2 + P_k^2$, which are thus automatically action variables. The transformation is iterated for successive values of s, reducing cubic, quartic, etc., terms in H to the above form. The algebra is straightforward, but extremely tedious.

The BG procedure provides a full set of action variables only if the RPA frequencies ω_k are non-resonant; i.e., if there is not set of integers $\{j_k\}$ with $\sum_k j_k\omega_k = 0$. If r linearly independent such resonance conditions exist in a system of n degrees of freedom, the transformation provides $n-r$ action variables, leaving an r-dimensional problem to be quantized by other means.

The power series for energy as a function of the actions diverges everywhere [28]). This divergence is caused by resonances arbitrarily close to any set of frequences ω_k. However, the usual methods [29]) of summing a divergent series can be applied, for example by taking the sum of the series as far as the term of minimum magnitude.

We tested the BG procedure in a three-dimensional system, using the Henon-Heiles-type hamiltonian of Noid, Koszykowski and Marcus [30]):

$$H = \tfrac{1}{2}\sum_{k=1}^{3}(p_k^2 + \omega_k^2 q_k^2) + 0.1(q_1 q_2^2 - 0.1q_1^3 + q_2 q_3^2 + 0.1q_3^3). \tag{3.12}$$

They used $\omega_1 = 0.7$, $\omega_2 = 1.3$, $\omega_3 = 1$, which are resonant ($\omega_1 + \omega_2 - 2\omega_3 = 0$) and calculated energy levels with an extension of the surface of section method. This is computationally laborious since it essentially involves finding points where the three-dimensional trajectory touches a line (not just where a two-dimensional trajectory crosses a line, as in subsect. 3.1). We implemented the BG method on a computer to fourth order in the actions and algebraic expressions with some 20 000 terms were generated. Problems with rounding error were encountered in subtracting large, almost equal terms. To avoid the resonance, we averaged the series over the neighboring values

TABLE 1

Comparison of energy levels for the 3-dimensional Henon-Heiles potential

State	Exact	Noid *et al.* [ref. [30])]	This work (BG)	RPA (harmonic)
(0, 0, 0)	1.494	1.493	1.496	1.500
(1, 0, 0)	2.184	2.185	2.195	2.200
(0, 0, 1)	2.485	2.486	2.488	2.500
(0, 1, 0)	2.771	2.771	2.782	2.800
(2, 0, 0)	2.872	2.873	2.890	2.900
(1, 0, 1)	3.177	3.177	3.187	3.200

States are labelled by the three quantum numbers (n_1, n_2, n_3).

of $\omega_3 = 0.98, 0.99, 1.01, 1.02$ with the same ω_1, ω_2; for these values, the divergence in the Taylor series is at a higher order than that which we kept. These semiclassical results are compared with the exact energies in table 1. The agreement seems reasonable.

4. The SU(3) model

The SU(3) model [31]) is an exactly soluble three-level schematic shell model. It is a generalization of the familiar two-level SU(2) Lipkin-Meshkov-Glick model, whose semiclassical realization is one-dimensional [1,7,8]). However, the dimensionality of the semiclassical limit of the SU(3) model is two, so that the usual WKB quantization is inapplicable. It therefore forms a non-trivial test of the methods of sect. 3.

The model is defined by N distinguishable particles labelled by an index n which can occupy three single-particle levels, $k = 0, 1, 2$, with energies ε_k. Furthermore, there is a two-body interaction, which moves pairs of particles between these levels. The hamiltonian is

$$H = \sum_k \varepsilon_k \left(\sum_n a_{nk}^+ a_{nk} \right) + \frac{1}{2} \sum_{k,l} V_{kl} \left(\sum_n a_{nk}^+ a_{nl} \right)^2, \tag{4.1}$$

where $V_{ij} = V_{ji}$, $V_{ii} = 0$. To obtain the complete spectrum of the model, we need consider for each N only the band of states which are totally symmetric under interchange of any two particles. For simplicity, we have chosen the parameters $\varepsilon_0 = -\varepsilon$, $\varepsilon_1 = 0$, $\varepsilon_2 = \varepsilon$, $V_{ij} = V(1-\delta_{ij})$, with $V > 0$.

The exact eigenstates of the model can be obtained by diagonalization H in a basis which has definite occupation numbers in each level. The number of such states (partitions of N into three integers) is of order $\frac{1}{2}N^2$, so the matrix size soon becomes quite large. Since H only connects states with even differences in occupation numbers, the calculation can be reduced to four diagonalizations, each of dimensionality $\approx \frac{1}{8}N^2$.

The coherent state representation of a totally symmetric wave function for the SU(3) system is

$$|\Psi\rangle = \int \mathrm{D}z_1 \mathrm{D}z_2 \exp\left(z_1^* \sum_n a_{n1}^+ a_{n0} + z_2^* \sum_n a_{n2}^+ a_{n0}\right)|0\rangle\, \psi(z_1, z_2), \tag{4.2}$$

where the vacuum is the state with all particles in the lower orbital, and with $\mathrm{D}z$ the same measure as in (2.2). The z are independent of N because we consider only totally symmetric states. Using the methods of sect. 2 to take the classical limit, we obtain

$$\begin{aligned} H(\beta, \beta^*) = {} & N\varepsilon(-1+|\beta_1|^2+2|\beta_2|^2) \\ & +\tfrac{1}{2}VN(N-1)[(1-|\beta_1|^2-|\beta_2|^2)(\beta_1^2+\beta_1^{*2}+\beta_2^2+\beta_2^{*2}) \\ & +\beta_1^{*2}\beta_2+\beta_1^2\beta_2^{*2})]. \end{aligned} \tag{4.3}$$

A more convenient set of variables can be obtained from the real and imaginary parts of β:

$$\beta\sqrt{2} = q + ip,$$

$$\beta^*\sqrt{2} = q - ip,$$

so that

$$\begin{aligned} \frac{H(q,p)}{N\varepsilon} = {} & -1+\tfrac{1}{2}q_1^2(1-\chi)+\tfrac{1}{2}q_2^2(2-\chi)+\tfrac{1}{2}p_1^2(1+\chi)+\tfrac{1}{2}p_2^2(2+\chi) \\ & +\tfrac{1}{4}\chi[(q_1^2+q_2^2)^2-(p_1^2+p_2^2)-(q_1^2-p_1^2)(q_2^2-p_2^2)-4q_1q_2p_1p_2], \end{aligned} \tag{4.4}$$

where $\chi = (N-1)V/\varepsilon$ is the dimensionless strength of the interaction. In the classical

limit, the time evolution of the system is independent of the particle number N at fixed χ, so that N appears only in the quantization condition

$$\int_{\gamma_i} \boldsymbol{p} \cdot \mathrm{d}\boldsymbol{q} = \frac{2\pi\hbar}{N}(n_i + \tfrac{1}{4}\alpha_i). \tag{4.5}$$

We identify $\boldsymbol{q}$ as the coordinate and $\boldsymbol{p}$ as the momentum because of the behavior of the coherent-state wave function under time-reversal, *viz*, $\beta \to \beta^*, \boldsymbol{q} \to \boldsymbol{q}, \boldsymbol{p} \to -\boldsymbol{p}$. Further support for this identification is the fact that $p_1 = p_2 = 0$ implies $\dot{q}_1 = \dot{q}_2 = 0$.

In fig. 2 are contour plots of the "static" hamiltonian $H(\boldsymbol{q}, \boldsymbol{p} = 0)/N\varepsilon$. This "potential energy" exhibits one minimum for $0 \leqq \chi < 1$, two minima for $1 < \chi < 3$, and four minima for $\chi > 3$. The minimum value of this potential is the Hartree-Fock ground-state energy of the system. The locations of the minima and the HF energies are

$$\begin{aligned}
&q_1 = 0, && q_2 = 0, && E = -1, && \chi < 1,\\
&q_1 = 1 - \frac{1}{\chi}, && q_2 = 0, && E = -1 - \frac{(\chi-1)^2}{4\chi}, && 1 < \chi < 3,\\
&q_1^2 = \tfrac{2}{3}, && q_2^2 = \frac{2\chi-6}{3\chi}, && E = -\frac{\chi}{3} - \frac{1}{\chi}, && \chi > 3.
\end{aligned} \tag{4.6}$$

The frequencies ω_1, ω_2 of small oscillations about the minimum are N times the RPA frequencies. The low-lying energy levels are then given by the RPA as

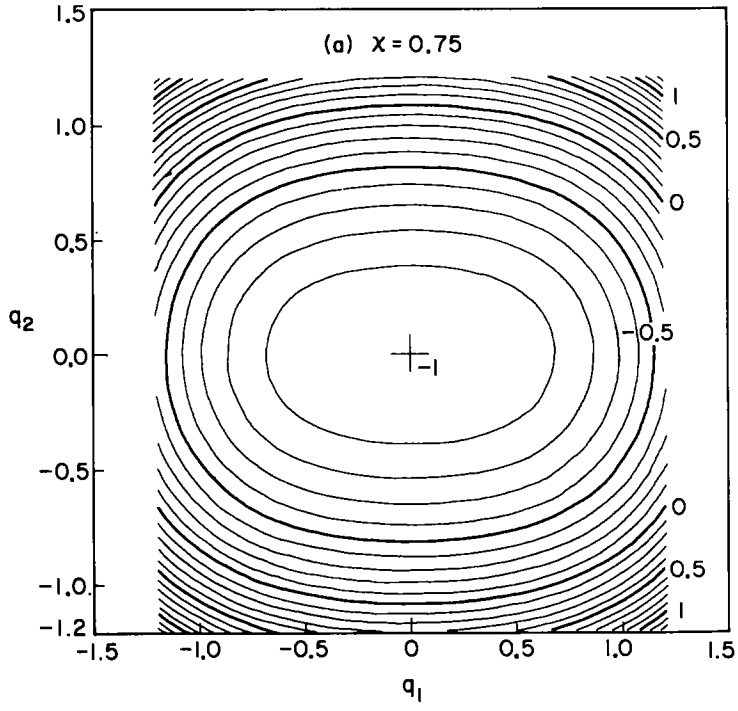
$$E = E_{\mathrm{HF}} + \sum_{i=1}^{2} \frac{\hbar\omega_i}{N}(n_i + \tfrac{1}{2}), \qquad n_i = 0, 1, 2, \ldots. \tag{4.7}$$

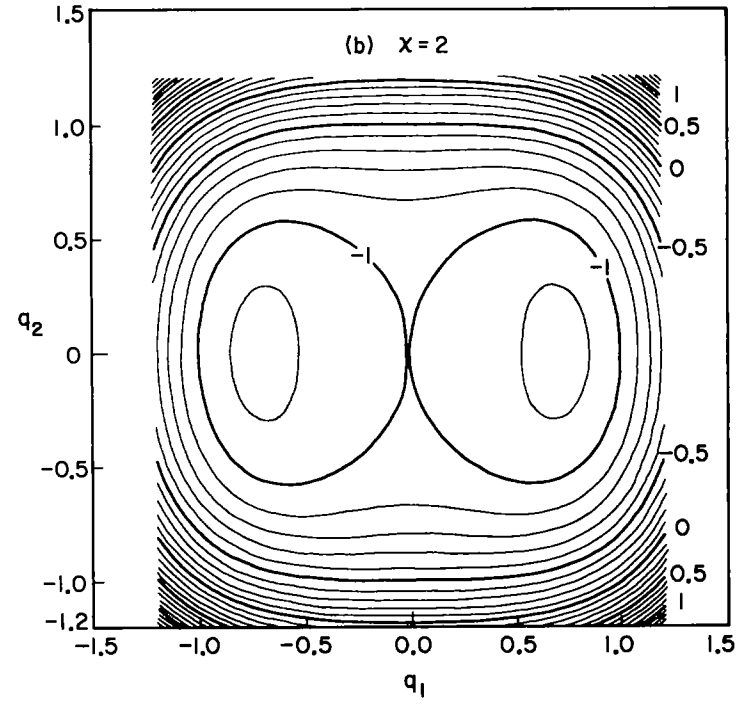
These frequencies are,

$$\omega = \begin{cases} \sqrt{1-\chi^2}, \quad \sqrt{4-\chi^2}, & \chi < 1 \\ \sqrt{2(\chi^2-1)}, \tfrac{1}{2}\sqrt{3(\chi+1)(\chi-3)}, & 1 < \chi < 3 \\ \left[\dfrac{4}{3}(\chi^2 - 3 \pm \sqrt{3\chi^2+9})\right]^{\frac{1}{2}}, & \chi > 3. \end{cases} \tag{4.8}$$

For $1 < \chi < 3$ and $\chi > 3$ at sufficiently low energies, the classically allowed region is split into two or four identical separate regions, respectively. The energies at which these regions coalesce are the energies of the saddle points of the "potential energy"

$$\begin{aligned}
&E = -1, && && 1 < \chi < 3,\\
&E = -1 - \frac{(\chi-1)^2}{4\chi}, && E = -1 - \frac{(\chi-2)^2}{4\chi}, && \chi > 3.
\end{aligned} \tag{4.9}$$


(a) X = 0.75
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.2
q_2
-1.5
-1.0
-0.5
0
0.5
1.0
1.5
q_1
1
0.5
0
-0.5
-1
0
0.5
1


(b) X = 2
1.5
1.0
0.5
0
-0.5
-1.0
-1.2
q_2
-1.5
-1.0
-0.5
0.0
0.5
1.0
1.5
q_1
1
0.5
0
-0.5
-1
-1
-0.5
0
0.5
1

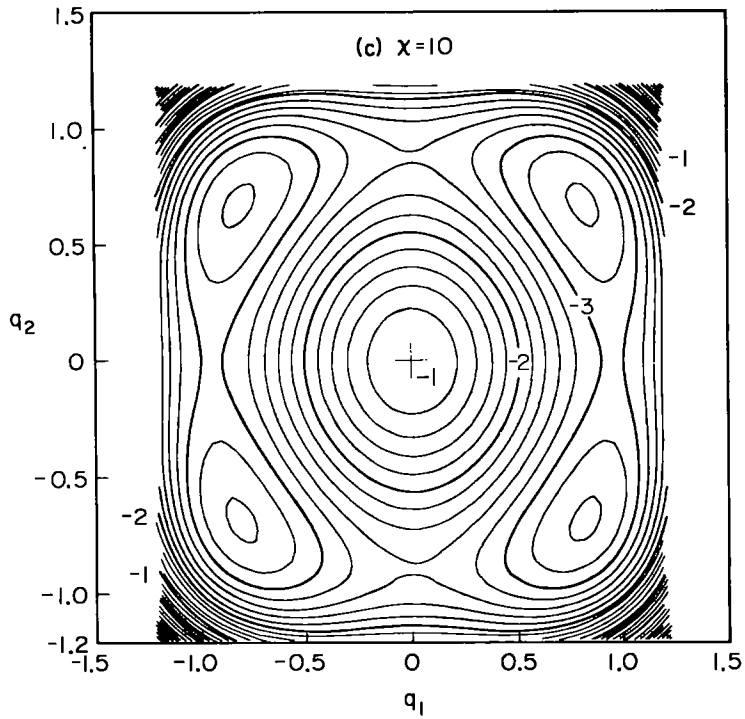
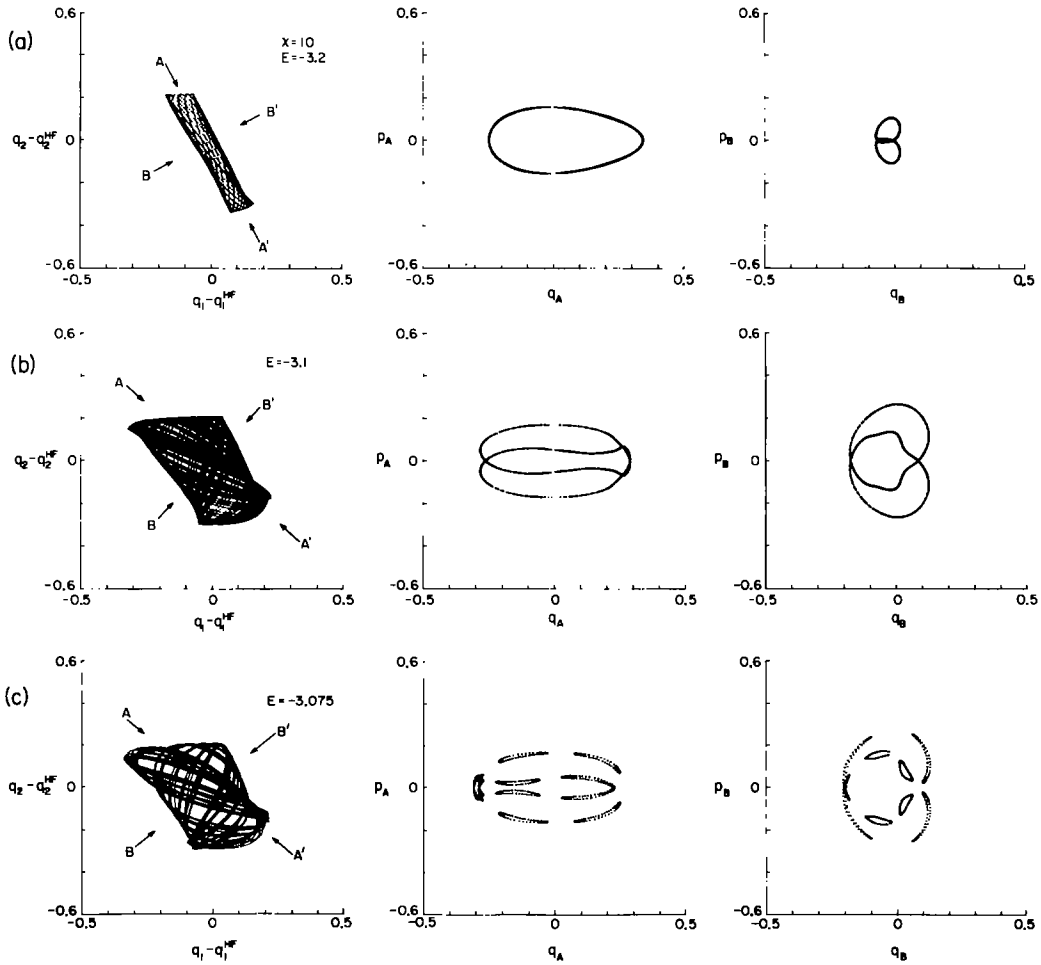


Fig. 2. Contour plots of the static hamiltonian, $H(q, p = 0)$, for the SU(3) model. (a) $\chi = 0.75$, one minimum; (b) $\chi = 2$, two minima; (c) $\chi = 10$, four minima.

The quantum hamiltonian only connects states with even differences in occupation numbers, which is reflected in the classical hamiltonian by symmetry about the q_1 and q_2 axes. Thus the states of the classical system are labelled by a positive or negative "parity" for each of the q_1, q_2 directions. When the classically allowed region is in four separate pieces, one expects the quantum energy levels to be approximately fourfold degenerate, similar to the parity doublet of a one-dimensional double well. However, since the classical approximation cannot reproduce this purely quantum mechanical effect, the splittings of the exact quantum levels are an indication of the validity of the classical approximation. For the levels we calculated in this regime ($\chi = 10$ and 100) these splittings were in the third significant figure. It may be possible to calculate these splittings semiclassically by instanton techniques, letting the action and momentum be imaginary [3]) or complex [32]), and calculating trajectories on the "inverted" energy surface.

We quantized the SU(3) model for three values of χ(0.75, 10 and 100) using both the surfaces of section and the BG method. For the former, Hamilton's equations require four initial conditions. We chose $p_1 = p_2 = 0$, and two "RPA actions" such that in the RPA limit these numbers are the exact actions. These initial conditions make the true actions a smooth single-valued function of the RPA actions. Hamilton's equations were

integrated by a fifth-order Runge-Kutta procedure in double precision and the trajectory was plotted in (q_1, q_2) space until it was clear whether or not it was quasiperiodic. A line was then chosen such that the line and its normal defined independent surfaces of section, as in subsect. 3.1. Quadratic inverse interpolation was used to calculate the points where the trajectory cut the section plane. Our procedure is self-checking for rounding error since points on a section may be very close in the plane but widely separated in time. Thus if a section is a smooth curve, even when highly magnified, the rounding error must be small. The area of the section was measured by reducing the figure to a single circuit, reflecting half of the points, ordering them, and using Simpson's rule for unequally spaced points. Fig. 3 illustrates a progression of the surfaces of section with increasing energy for $\chi = 10$. At low excitation, the system behaves like a pair of oscillators; as the energy increases, the torus becomes highly convoluted; at still higher energy, the system is stochastic.



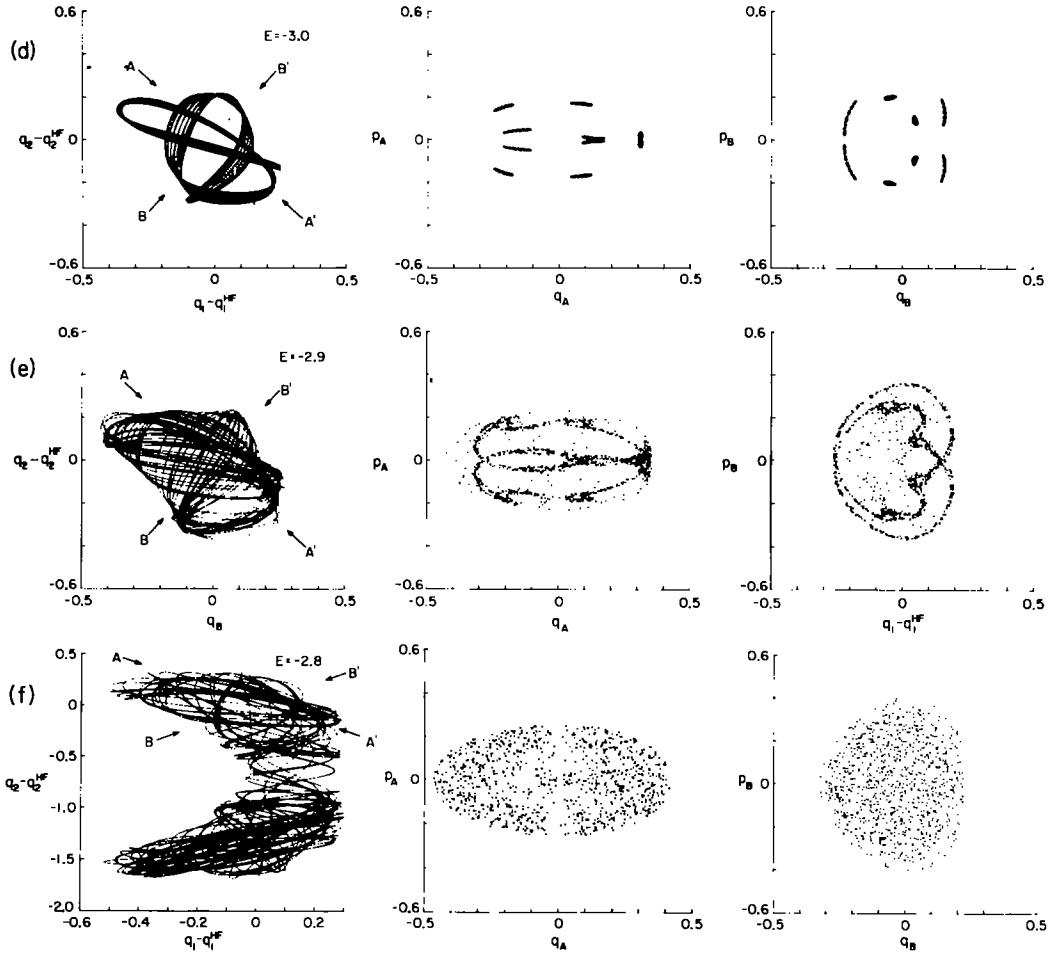


Fig. 3. Trajectory in q-space (left) and surfaces of section (center and right) for a progression of excitation energy. (a) Harmonic; (b) quasiperiodic, measurable by plane surface of section; (c), (d) quasiperiodic, unmeasurable by plane surface of section; (e), (f), stochastic.

From the above procedure we calculated the two actions, and applied the quantization condition

$$I_i = \frac{1}{2\pi}\int \boldsymbol{p}\cdot \mathrm{d}\boldsymbol{q} = \frac{1}{N}(n_i+\tfrac{1}{2}). \tag{4.10}$$

For both the $\chi = 10$ and $\chi = 100$ cases we could find few energy levels, with difficulty, due to the convolution of the surfaces of section and the rapid transition to stochasticity. The trajectories can be stochastic even when confined to a single minimum and were always stochastic when the energy was above the lowest saddle energy. For

$\chi = 0.75$, however, the surfaces of section were almost circles even for relatively high energies, enabling us to find many energy levels. For all three values of χ, the upper limit of energy at which we could quantize was often fixed by the insufficiency of planar surfaces of section; polyhedral surfaces could have been used to extend the procedure to higher energy, although at the cost of a greater computational complexity.

The BG procedure to quantize the system for all three values of χ was used to generate a Taylor series for the energy to fourth order in the actions. For $\chi = 10$ and $\chi = 100$, the same problems as before are evident, which the power series exhibited by being quickly and strongly divergent. For $\chi = 0.75$, however, the BG procedure provided almost as many levels as did the surface of section approach, though with less accuracy.

The calculated energy levels are illustrated in figs. 4 and 5. For ease of comparison, all exact quantal energies have been shifted by their "zero-point energy" (approximately

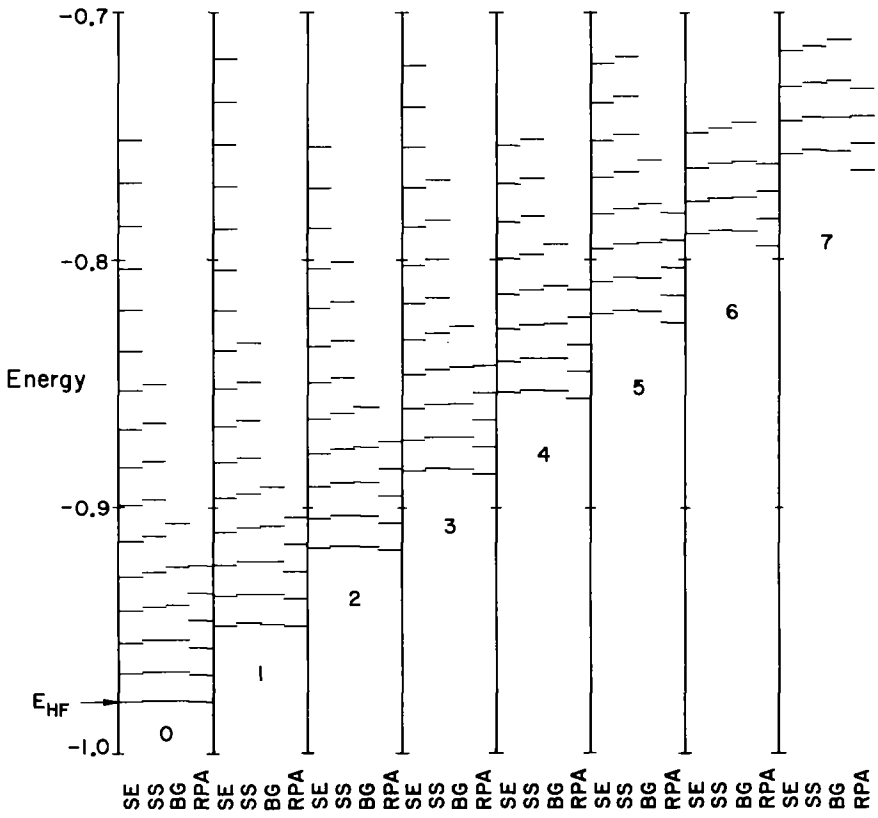


Fig. 4. Energy levels for the SU(3) model $N = 60$, $\chi = 0.75$. There are eight sets of four columns; each set corresponds to a particular number n_1 of oscillator quanta (0–7) while n_2 increases vertically. The four columns are: SE, shifted exact levels (to remove zero-point energy); SS, surface of section method; BG, Birkhoff-Gustavson method; RPA. The Hartree-Fock energy and the saddle energy are marked.

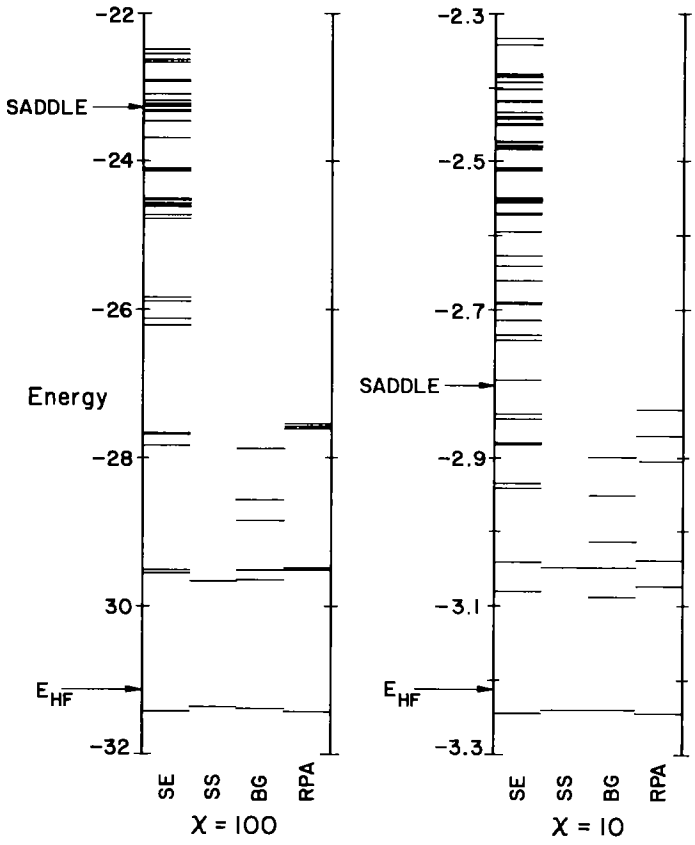


Fig. 5. Energy levels for SU(3) model, $N = 60$, $\chi = 10$ and $\chi = 100$. Each set of four columns is as in fig. 4. The (shifted) Hartree-Fock and (shifted) saddle energies are marked.

one-half the sum of the RPA frequencies) such that the energy of the shifted exact ground state is exactly equal to the RPA ground state. For $\chi = 0.75$, the exact levels can be easily classified by the two oscillator quantum numbers shown. For $\chi = 10$, and $\chi = 100$, though, the system is harmonic only for low excitation energy. We thus display the "raw" levels in these cases. Table 2 shows the comparison in numerical form for a few levels.

5. Summary and conclusions

This work has been an attempt to apply semiclassical methods to a nuclear shell-model hamiltonian. We showed that there are several equivalent ways to derive the classical hamiltonian system representing a given shell model: the TDHF variational

TABLE 2

Lowest energy levels for the SU(3) model

χ	State	Shifted exact	Surface of section	Birkhoff-Gustavson	RPA (harmonic)
0.75	(0, 0)	−0.97904	−0.97879	−0.97881	−0.97904
	(0, 1)	−0.96747	−0.96672	−0.96672	−0.96802
	(0, 2)	−0.95504	−0.95388	−0.95375	−0.95699
	(1, 0)	−0.94794	−0.94681	−0.94751	−0.94814
	(1, 1)	−0.93611	−0.93519	−0.93518	−0.93712
	(1, 2)	−0.92347	−0.92216	−0.92197	−0.92609
10	(0, 0)	−3.2446	−3.2407	−3.2407	−3.2446
	(0, 1)	−3.0807		−3.0883	−3.0731
	(1, 0)	−3.0410	−3.0484	−3.0488	−3.0386
100	(0, 0)	−31.419	−31.364	−31.376	−31.419
	(0, 1)	−29.549	−29.659	−29.652	−29.512
	(1, 0)	−29.511		−29.514	−29.478

States are labelled by the number of oscillator quanta, (n_1, n_2). Missing entries for $\chi = 10, 100$ are states where a corresponding classical trajectory could not be found.

principle using a Thouless state trial wave function, the WKB approximation to the Schrödinger equation for the coherent state wave function, and a path-integral representation for the propagator in terms of coherent states. All of these methods result in a generally multidimensional classical problem which must then be requantized to find the quantum eigenenergies of the system. This latter is a non-trivial and largely unsettled problem of high current interest, particularly in regard to intramolecular energy transfer. For a schematic three-level shell model, we found that the classical trajectories evolved from harmonic through quasiperiodic to stochastic as the excitation energy increased above the Hartree-Fock minimum. Among the methods we investigated to quantize these trajectories were EBK quantization using surfaces of section, the Birkhoff-Gustavson transformation to action-angle variables, and the ordinary harmonic (RPA) approximation. When the exact quantum level structure was harmonic (or nearly so) we found that all of these semiclassical methods predicted the excitation energies reasonably accurately. However, in more complicated situations all of these methods gave poor results and could, in fact, only find the few lowest energy levels.

As a practical tool, semiclassical quantization leaves much to be desired. It is far more laborious than the RPA yet produces results only when this approximation is already fairly accurate. Realistic situations involving many single-particle orbitals will certainly correspond to more complicated classical systems than the two-dimensional one we have used as our example, and here the situation can only be worse: the surface of section method is a very arduous proposition even in three dimensions and the computer implementation of the algebra for the Birkhoff-Gustavson procedure uses pro-

digious amounts of time for more than three or four dimensions. Moreover, it is difficult to find periodic solutions to an arbitrary hamiltonian in even two dimensions.

Of more basic interest, we have shown that these semiclassical methods, while derived from quantum mechanics, appear to have structure not present therein, such as stochasticity and entropy. Their connection with the properties of the exact quantum system and the insight that it might offer into nuclear problems seems a particularly intriguing area for future study.

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