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RSVP APPROACH TO THE QUANTIZATION AND TUNNELING IN MULTIDIMENSIONAL HALMITONIAN SYSTEMS

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Résumé - Nous montrons qu'en imposant aux solutions invariants de jauge de systèmes hamiltoniens quantiques d'être régulières et univoques, il est possible de décrire la fission spontanée et les états liés. Quelques exemples sont ensuite donnés.

Abstract - We show that the regularity and single-valuedness (RSVP) condition imposed on the gauge invariant solutions of quantal hamiltonian system allows to describe the spontaneous fission and quantized bound states. Few illustrative examples are summarized.

INTRODUCTION

A fundamental problem in quantum many-body theory is the formulation of a microscopic description of collective motion in any subspace of the Hilbert space. Some progress in this field has been achieved recently by applying the mean-field methods for bound states, fission and fusion cross section /1/. TDHF equation describing the evolution of a mean-field can be derived using the same time-dependent variational principle which leads, in the full Hilbert space, to the linear time-dependent Schrödinger equation. However, the TDHF equation is nonlinear and, consequently, the principle of superposition does not hold anymore. Moreover, TDHF method is formulated as an initial value problem. All that leads to the suspicion that the TDHF evolution exhibits classical features and, therefore, it cannot be applied for bound states and fission in the same fashion as the Schrödinger theory. Some of these difficulties could be removed by applying the regularity and single-valuedness principle (RSVP) to the gauge-invariant wave function /2/ or the functional integral representation (FIR) to the many-body propagator evaluated in the stationary phase approximation (SPA) /3/. In both approaches when applied for bound states the TDHF initial value problem is replaced by the TDHF time-periodic boundary problem. However, in contrast to FIR + SPA the RSVP quantization can be generalized for time-quasi-periodic boundaries in any subspace of the Hilbert space /2,4/. Below we apply the RSVP condition to describe spontaneous fission and quantized vibrational modes in quantal Hamiltonian system. The details of the method are presented in ref. 2 and only essential ideas and illustrative examples will be summarized here.

OUTLINE OF THE METHOD

Let us consider the subspace $\{\psi(\vec{\rho}, \vec{\pi})\}$ which is specified by the canonical conjugate variables $\vec{\rho} \equiv [\rho_1, \dots, \rho_k]$, $\vec{\pi} \equiv [\pi_1, \dots, \pi_k]$. Each element in this subspace can be written as $\psi(\vec{r}; t) \equiv \psi(\vec{r}; \vec{\rho}(t), \vec{\pi}(t))$. The Hamilton's equations of motion for $\vec{\rho}(t)$, $\vec{\pi}(t)$ can be obtained from the variational principle :

$$\delta \int_{t_1}^{t_2} \langle \psi(\vec{r}; t) | \hat{H} - i\hbar \partial_t | \psi(\vec{r}; t) \rangle dt = 0 \quad ; \quad \vec{r} = (\vec{r}_1, \dots, \vec{r}_A) \quad (1)$$

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assuming the norm conserving variations of $\psi(\vec{r};\vec{\rho},\vec{\pi})$ /5/. Obviously, the trajectory $\vec{\rho}(t), \vec{\pi}(t)$ for separable systems is conditionally periodic. Moreover, the KAM Theorem /6/ assures that even in the presence of a nonseparable conservative perturbation, the motion is conditionally periodic in the majority of the phase space. The phase factor of the wave function can be obtained considering the norm changing variations in $\{\psi(\vec{\rho},\vec{\pi})\}$. The full solution of (1) is :

$$\psi_c(\vec{r};t) = \psi_G(\vec{r};t) \exp\left\{-\frac{i}{\hbar} \mathcal{H}[\vec{\rho},\vec{\pi}]t\right\} \quad (2)$$

where $\psi_G(\vec{r};t) = \psi(\vec{r};\vec{\rho}(t),\vec{\pi}(t)) \exp\left\{\frac{i}{\hbar} \int_{\vec{\rho}_0}^{\vec{\rho}} \vec{\pi}' d\vec{\rho}'\right\}$; $\vec{\rho}_0 \equiv \vec{\rho}'(t_0), \vec{\rho} \equiv \vec{\rho}'(t)$ is the phase-

determined wave function which is invariant under the gauge transformation $\hat{H} \rightarrow \hat{H} + \beta(t)$. In the limit of infinitely long time-evolution in the regular region of the parametric space the trajectory of the Hamilton's system covers an invariant torus densely and uniformly. Thus, at each point \vec{r} one can define relation between the dynamical states $\psi(\vec{r};\vec{\rho},\vec{\pi})$ of the system for points $(\vec{\rho},\vec{\pi})$ on the invariant torus and the phase-determined gauge-invariant functions ψ_G . For each \vec{r} this relation should be a regular and single-valued function on the invariant torus, i.e. for any closed trajectory C_σ on the torus :

$$\oint_{C_\sigma} \vec{\pi} d\vec{\rho} = 2\pi n_\sigma \hbar \quad n_\sigma = 0, 1, \dots \quad (3)$$

This is an essential idea of the RSVP /2/. The RSV condition has much in common with conditions enforced upon the stationary solutions of the Schrödinger equation. Indeed the RSV condition can be expressed in the form of the canonically invariant quantization prescription which for the Schrödinger dynamics in the full Hilbert space yields only exact eigenstates and, moreover, all of them /2,4,7/. The invariant tori in RSVP are analogues of symmetries in the Schrödinger problem.

TUNNELING

A straightforward application of the RSVP in the many-body problem is the estimate of the tunneling probability. Let us consider a one dimensional potential barrier as shown in fig. 1. We assume that the gauge-invariant wave function in the classically allowed region I fulfils the RSV condition i.e. the system is in one of the states prescribed by the RSV quantization condition /2/. Consider now the wave packet passing from region I

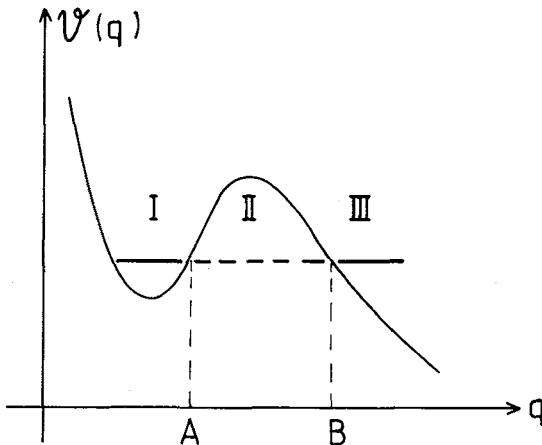


Fig. 1

Sketch of a potential well for a fissioning system with two classically allowed regions (I, III) separated by one classically forbidden region (II).

through the potential barrier to the region III. (Transformation to the classically forbidden region can be achieved by the so-called Wick rotation $t \rightarrow i\tau$ where τ is real. In this case the action integral becomes imaginary). The phase-determined wave function in regions I, II, III is :

$$\begin{aligned} \psi_G^{(I)}(\vec{r}; \rho, \pi) &= \psi(\vec{r}; \rho, \pi) \exp \left\{ \frac{i}{\hbar} \left[W_1(\rho, \pi) + \varphi_0^{(1)} \right] - \frac{1}{\hbar} \eta_0^{(1)} \right\} \\ \psi_G^{(II)}(\vec{r}; \rho_B, \pi_B) &= \psi(\vec{r}; \rho_B, \pi_B) \exp \left\{ - \frac{1}{\hbar} \left[W_2(\rho_B, \pi_B) + \eta_0^{(2)} \right] + \frac{i}{\hbar} \varphi_0^{(2)} \right\} \\ \psi_G^{(III)}(\vec{r}; \rho, \pi) &= \psi(\vec{r}; \rho, \pi) \exp \left\{ \frac{i}{\hbar} \left[W_3(\rho, \pi) + \varphi_0^{(3)} \right] - \frac{1}{\hbar} \eta_0^{(3)} \right\} \end{aligned} \quad (4)$$

where $\varphi_0^{(k)}, \eta_0^{(k)}$ ($k=1,2,3$) are the real and imaginary phases in the corresponding regions. The wave function (4) satisfies the RSVP in the whole space if and only : $\varphi_0^{(3)} = \varphi_0^{(2)} = W_1(\rho_A, \pi_A) + \varphi_0^{(1)}, \eta_0^{(2)} = \eta_0^{(1)}, \eta_0^{(3)} = W_2(\rho_B, \pi_B) + \eta_0^{(1)}$. In this case the solutions in regions I, II, III can be joined smoothly at the barrier and the transmission probability per unit time is

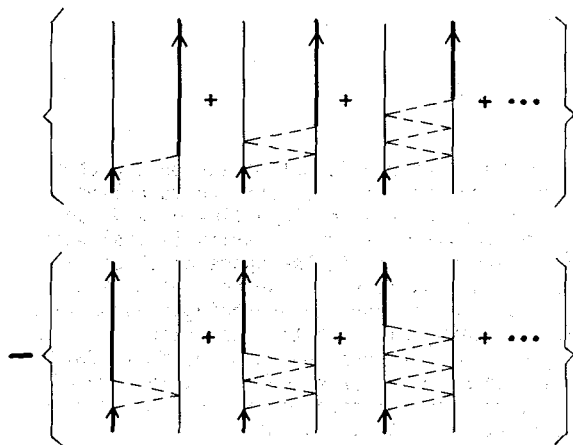
$$P = (\partial \bar{W}_1 / \partial E)^{-1} \exp \left\{ - \frac{1}{\hbar} W_2(\rho_B, \pi_B) \right\} \quad (5)$$

where $\bar{W}_1(E) = (2\pi)^{-1} \oint \pi' d\rho'$ and $(\partial \bar{W}_1 / \partial E) = T_1$ is the oscillation period in region I. Thus, in the restricted subspace of the Hilbert space the spontaneous fission width:

$$\Gamma_f = \hbar \left(\frac{\partial \bar{W}_1}{\partial E} \right)^{-1} e^{-W_2/\hbar} \quad (6)$$

resembles the WKB result. It should be stressed that in contrast to the FIR+ SPA the RSVP yields a correct premultiplying factor.

In deriving P we have neglected the multiple reflection of the wave packet inside a barrier as well as the feedback current. The true tunneling probability through the potential barrier is given by an infinite series of elementary transmission processes as shown schematically in fig. 2. Thick lines with arrows in fig. 2 denote the incoming and outgoing packets respectively whereas the dashed lines denote the reflected packets inside the barrier. For all independent processes depicted in fig. 2 the incoming current is the same. Graphs in the upper bracket contribute to the transmission probability whereas those included in the lower bracket increase the total reflectance of the barrier. Consequently, the total tunneling probability is given by a difference between the sum of probabilities for



" transmission graphs " and the sum of probabilities for

Fig. 2

A schematic presentation of graphs involved in the quantum mechanical transmission through the barrier. Direction of time is denoted by the arrows.

" feedback graphs ". This summation is equivalent to the averaging over the initial evolution time in I. All dynamical states on the invariant torus in region I can be reached in the course of infinitely long time-evolution of the systems. Physically, one cannot specify the dynamical state $\psi(\vec{r}, \rho(t_0), \pi(t_0))$ which at $t_0 < t_{in}$ leads to the penetration of a barrier. Thus, one should average over an ensemble of all initial dynamical states. This defines a quantized stationary state ψ_G in region I /2,8/. Different independent transmission processes from ψ_G are distinguished by the change of the phase $\exp\{-kW_2/2\hbar\}$ of the gauge-invariant wave function in region II, where k is the number of passages in II. Thus, one can easily calculate the total fission probability by summing contributions from different elementary fission processes :

$$\begin{aligned}
 P &= (\partial \bar{W}_1 / \partial E)^{-1} \left\{ e^{-W_2/\hbar} (1 + e^{-2W_2/\hbar} + \dots) - e^{-2W_2/\hbar} (1 + e^{-2W_2/\hbar} + \dots) \right. \\
 &= (\partial \bar{W}_1 / \partial E)^{-1} \left[1 + e^{-W_2/\hbar} \right]^{-1}
 \end{aligned}
 \tag{7}$$

This result agrees with a generalized JWKB formula for a spontaneous fission probability /8/.

The total penetrability of the barrier can also be calculated by summing the contributions from different processes in the course of infinitely long time evolution as presented schematically in fig. 3. The graphs in the upper part of fig. 3 describes the " history " of the wave packet which entered region II after " the first " hitting of a potential wall. The reflected wave packet comes back after one oscillation period T_1 initializing the next but one out of an infinite series of the independent " histories " of the system.

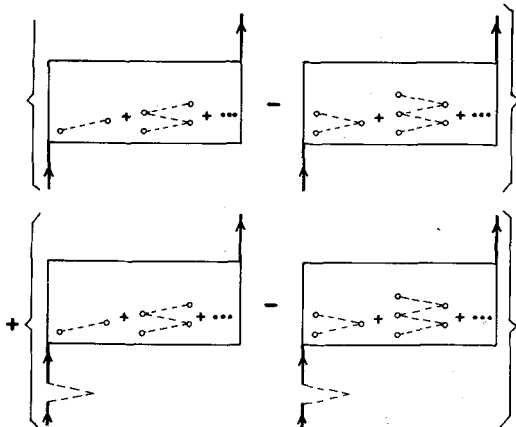


Fig. 3

The scetch of first two " histories " of the wave packet evolving in the infinite time from the classically allowed region I to the region III through the classically forbidden region II inside the barrier.

Obviously, the total penetrability of the barrier does not depend on the choice of a particular " history " of the system. The above results for the tunneling probability coincide with the WKB results suggesting a close link of RSVP and quasi-classical methods based on the \hbar -expansion. This similarity is misleading because in the RSVP approach one considers the path in the space of phase-determined wave functions and not in the classical configuration space. The choice of the variational subspace is here crucial because for the Schrödinger dynamics in the full Hilbert space, the RSVP gives nothing else but the conditions inforced upon solutions of the time-dependent Schrödinger equation. Consequently, RSVP yields a well known spectrum of quantized Schrödinger eigenstates, the tunneling probability, etc. /2,4/. To our knowledge, the coincidence of results for tunneling in JWKB and in RSVP approach suggests an ultimate relation between the low

order \hbar -expansion for Schrödinger dynamics and the violation of the superposition principle in the nonlinear quantum theories.

THE GAUGE INVARIANT QUANTIZATION

Conditions (3) express the RSVP for the gauge-invariant wave function (2) on the invariant torus. Topology of the torus specifies the set $\{C_i\}$ of independent basic closed curves such that each C_σ can be continuously deformed into a linear combination of C_i . Thus, eq. (3) can be rewritten in the form :

$$\oint_{C_\sigma} \vec{\pi} d\vec{\rho} = \sum_{i=1}^N M_i \oint_{C_i} \vec{\pi} d\vec{\rho} \quad (8)$$

which must hold for any choice of integers $[M_1, \dots, M_N]$. This implies :

$$I_i = (2\pi)^{-1} \oint_{C_i} \vec{\pi} d\vec{\rho} = n_i \hbar \quad i=1, \dots, N \quad (9)$$

Thus, the RSVP for $\psi_G(\vec{r}; \vec{\rho}, \vec{\pi})$ can be formulated in a form of the quantization prescription /2/. A particularly useful choice of C_i is such that :

$$I_i = (2\pi)^{-1} \oint_{C_i} \pi d\rho_i = (2\pi)^{-1} \iint d\pi_i d\rho_i \quad (10)$$

$2\pi I_i$ denotes the Poincaré surface of section in the direction i . For TDHF the above quantization procedure which is based on investigating phases of the A-particle wave function is impractical. However, one can still formulate the gauge-invariant quantization rules in terms of densities and currents allowing in this way for an easy inspection of the TDHF dynamics /10/. Let us consider the gauge-invariant wave function in the form of a Slater determinant :

$$\begin{aligned} \psi_G(\vec{r}_1, \dots, \vec{r}_A; t) &= \text{Det}\{\phi_j^G(\vec{r}_j, t)\} = \text{Det}\{\phi_j(\vec{r}_j)\} \exp\left\{\frac{i}{\hbar} \int_{t_0}^t \sum_j \langle \phi_j | i\hbar \partial_t | \phi_j \rangle dt'\right\} = \\ &= \psi(\vec{r}_1, \dots, \vec{r}_A; t) \exp\left\{\frac{i}{\hbar} \int_{t_0}^t \langle \psi | i\hbar \partial_t | \psi \rangle dt'\right\} \end{aligned} \quad (12)$$

where

$$\psi(\vec{r}_1, \dots, \vec{r}_A; t) = \varphi(\vec{r}_1, \dots, \vec{r}_A; t) \exp\left\{\frac{i}{\hbar} f(\vec{r}_1, \dots, \vec{r}_A; t)\right\} \quad (13)$$

We are looking for the equations of motion for ψ in such a representation that both φ and f are real functions, i.e. for each single particle (s.p.) wave function one has :

$$\phi_j(\vec{r}_j, t) = \varphi_j(\vec{r}_j, t) \exp\left\{\frac{i}{\hbar} f_j(\vec{r}_j, t)\right\} \quad (14)$$

where φ_j is a square root of the s.p. density ρ_j . Expressing the Lagrangian functional in terms of $\rho \equiv \varphi^2$ and f one obtains :

$$\mathcal{L}[\psi^*, \psi] = \int d\vec{r}_1 \dots d\vec{r}_A \left[\frac{d}{dt} \left(\frac{i\hbar}{2} \rho - f \rho \right) + f \rho \right] - \mathcal{H}(\rho, f) \quad (15)$$

where

$$\mathcal{H}(\rho, f) \equiv \langle \psi | \hat{H} | \psi \rangle = \frac{1}{2} \int \rho(\vec{r}_1, \dots, \vec{r}_A; t) (\vec{\nabla}_i f(\vec{r}_1, \dots, \vec{r}_A; t))^2 d\vec{r}_1, \dots, d\vec{r}_A + E(\rho)$$

This Lagrange functional is equivalent to :

$$\mathcal{L}'[\psi^*, \psi] \equiv \mathcal{L}'(\rho, f) = \int f \dot{\rho} d\vec{r}_1, \dots, d\vec{r}_A - \mathcal{H}(\rho, f) \quad (16)$$

because the solutions of equations of motion for both \mathcal{L} and \mathcal{L}' differ only by the \vec{r} -independent phase. Thus, the gauge-invariant function can be written as follows :

$$\psi_G(\vec{r}_1, \dots, \vec{r}_A; t) = \psi(\vec{r}_1, \dots, \vec{r}_A; t) \exp\left\{ \frac{i}{\hbar} \int_{t_0}^{t_0+t} [f \dot{\rho} d\vec{r}_1, \dots, d\vec{r}_A] dt' \right\} \quad (17)$$

and $\rho(\vec{r}_1, \dots, \vec{r}_A; t)$, $f(\vec{r}_1, \dots, \vec{r}_A; t)$ can now be considered as the canonical conjugate variables which fulfil the Hamilton's equations of motion :

$$\begin{aligned} \dot{f}(\vec{r}_1, \dots, \vec{r}_A; t) &= \frac{\delta \mathcal{H}(\rho, f)}{\delta \rho(\vec{r}_1, \dots, \vec{r}_A; t)} \\ \dot{\rho}(\vec{r}_1, \dots, \vec{r}_A; t) &= - \frac{\delta \mathcal{H}(\rho, f)}{\delta f(\vec{r}_1, \dots, \vec{r}_A; t)} \end{aligned} \quad (18)$$

The second equation in (18) is the continuity equation which depends only on the " collective part " $E_{coll} = \frac{1}{2} \sum_i \int \rho (\nabla_i f)^2 d\vec{r}_1, \dots, d\vec{r}_A$ of the Hamiltonian. RSV for ψ_G (eq. (17)) is satisfied if :

$$I = -(2\pi)^{-1} \int_{t_0}^{t_0+t} dt \int d\vec{r}_1, \dots, d\vec{r}_A f(\vec{r}_1, \dots, \vec{r}_A; t) \dot{\rho}(\vec{r}_1, \dots, \vec{r}_A; t) = n\hbar \quad (19)$$

(n = 0, 1, ...)

and the density functional is periodic (conditionally-periodic) in time. Obviously this expression is gauge-invariant. In the exemplaric case of a harmonic motion with the collective energy $E_{coll} = E^* \cos\left(\frac{2\pi}{T} t\right)$ the quantization condition (19) is :

$$\int_0^T 2E_{coll}(t') dt' = E^* T = 2\pi n\hbar \quad (20)$$

and $E_n^* = n\hbar(2\pi/T) = n\hbar\omega$. Thus, one obtains the correct separation distance between the levels of the harmonic oscillator.

THE COUPLED VIBRATIONS OF THE NON-SEPARABLE HAMILTON'S SYSTEM

RSV quantization method as formulated above is strictly valid for separable multi-dimensional Hamilton systems. For these systems at each excitation energy and for each i-mode one can always find an initial condition such that the ratio of action integrals $I_k/I_i = 0$ ($k \neq i$). Obviously, this requirement is not fulfilled for non-separable systems ($\epsilon \mathcal{H}_{ns} \neq 0$). However, the RSV quantization method may be still used as a valid approximation for non-degenerate Hamilton systems close to the separable ones. In this case invariant tori exist and the action integral \bar{I} exhibits only small oscillations around ($\bar{J} = \text{const}$) the action of the averaged system :

$$i\hbar \partial_t \bar{J} = (2\pi)^{-n} \int_0^{2\pi} \dots \int_0^{2\pi} \left[\partial_{\vec{\theta}} \epsilon \mathcal{H}_{ns}[\psi^*, \psi] \right] d\vec{\theta} \quad (21)$$

Below we discuss the RSV in connection with quantized isoscalar vibrations in the time-dependent deformed oscillator model (TDDOM). This model is applied for the description of giant resonances in light self-conjugate nuclei. The evolution is studied in the space of " boosted Slater determinants " which are build by filling the deformed harmonic oscillator field /2/. All states have the quantum numbers $J=L$, $S=T=0$ and the orbital symmetry [4, ..., 4]. Static s.p. states are the (n_x, n_y, n_z) eigenfunctions of the deformed harmonic oscillator potential with oscillator

lengths $b_x^{(0)}$, $b_y^{(0)}$, $b_z^{(0)}$. For all physically significant states in light nuclei if an individual s.p. state (n_x, n_y, n_z) is occupied then the s.p. states (n_x-1, n_y, n_z) , (n_x, n_y-1, n_z) , (n_x, n_y, n_z-1) are occupied as well. This property simplifies significantly the TDDO calculations and, moreover, it allows to eliminate the cm wave function. Thus the boosted s.p. wave function can be written as :

$$\overline{\langle x | n_x \rangle} = x^{n_x} \exp \left[-\frac{1}{2} (\rho_x(t) + i\pi_x(t)) \left(\frac{x}{b_x^{(0)}} \right)^2 \right] \quad (22)$$

where ρ_x , π_x depend on time. (The static solution corresponds to $\rho_x=1$, $\pi_x=0$). Equations of motion for $\psi(\vec{\rho}, \vec{\pi})$ are derived from (1) assuming the norm-conserving variations of $\psi(\vec{r}; \vec{\rho}(t), \vec{\pi}(t)) / 2$:

$$i\hbar \hat{S}_{\alpha\beta} \partial_t v_{\beta} = \partial_{v_{\alpha}} \mathcal{H} [\psi(\vec{v}), \psi^*(\vec{v}^*)] \quad (23)$$

$$\vec{v} \equiv [\rho_1 + i\pi_1, \dots, \rho_m + i\pi_m] ; \quad \vec{v}^* = [\rho_1 - i\pi_1, \dots, \rho_m - i\pi_m]$$

where $2m$ is the number of collective parameters. $\hat{S}_{\alpha\beta}$ is related to the Poisson bracket :

$$\hat{S}_{\alpha\beta} = \langle \psi | \psi \rangle^{-1} \langle \partial_{v_{\alpha}} \psi | \partial_{v_{\beta}} \psi \rangle - \langle \psi | \psi \rangle^{-2} \langle \partial_{v_{\alpha}} \psi | \psi \rangle \langle \psi | \partial_{v_{\beta}} \psi \rangle \quad (24)$$

Transformation to the canonical variables in (24) is straightforward because \hat{S} for s.p. wave functions in eq. (22) is real and diagonal. The relation between different possible sets of canonical variables is then provided by canonical transformations. Solving the TDDO equations we use the Hamiltonian which consists of the kinetic energy and the two-body Brink-Boeker B1 force which gives a good description of isoscalar giant resonances in light nuclei.

Evolution of the system can be initiated through the velocity field of the wave function (22). In TDDOM the initial excitation is then :

$$E^* \equiv E(\vec{Q}; \vec{P}) - E(\vec{Q}=0, \vec{P}=0) = \sum_{\text{all } i,j}^n A_{ij} P_i P_j \quad (25)$$

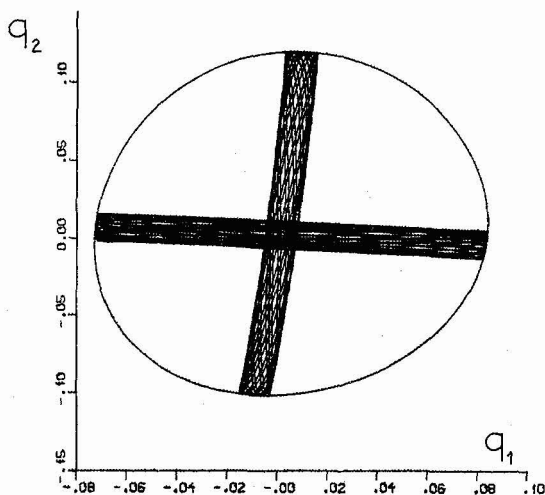


Fig. 4

The region swept out by trajectories for the $\tilde{\tau}^{(1)}$ and $\tilde{\tau}^{(2)}$ -excitations at $E^* = 1$ MeV in ^{20}Ne . The evolution is shown in the (q_1, q_2) -plane where $q_1 \equiv q_1 - 1$ and $q_2 \equiv q_2 - 1$. The circle encloses all

possible initial conditions for the time-evolution ($p_1 = p_2 = 0$).

For more details see the discussion in text.

For canonical variables involved in our description of coupled monopole and quadrupole vibrations ($q_b \equiv (\rho_{x_1} \rho_{x_2} \rho_{x_3})^{1/3}$, $q_B \equiv \rho_{x_3} (\rho_{x_1} \rho_{x_2})^{1/2}$ or $q \equiv (\rho_{x_1} \rho_{x_2})^{1/2}$, $q_z = \rho_{x_3}$), $A_{ij} = 0$ for $i \neq j$. Therefore, an initial energy sharing between modes can be uniquely specified by the parameters $f_i = A_{ii} p_i^2 / E^*$ ($\sum_{j=1}^m f_j = 1$). Thus, the separability of the Hamilton's system means that for each $\vec{f}^{(i)} \equiv [f_1 = 0, \dots, f_i = 1, \dots, f_n = 0]$ one has $I_k / I_i = 0$ for all $k \neq i$. In light nuclei, for the majority of coupled isoscalar vibrations if expressed in physically plausible set of canonical parameters, these conditions are approximately fulfilled. A typical example is ^{20}Ne nucleus (see fig. 4) in q, q_z -variables. In this nucleus we discuss the coupled symmetry conserving shape vibrations perpendicular and parallel to the symmetry axis. Fig. 5 shows the ratio of integrals I_k / I_i ($k \neq i$) for $\vec{f}^{(1)}$ -excitations ($i=1,2$) corresponding to the trajectory regions presented in fig. 4 (solid lines). In the range of excitation energies $E^* < 25$ MeV, $I_k / I_i < 0.05$ and, therefore, the RSV quantization method should

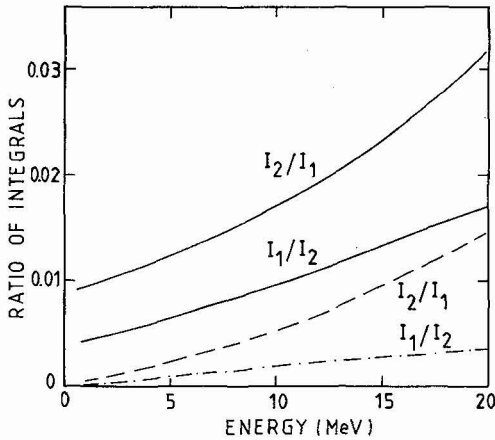


Fig. 5

The ratio of action integrals I_2 / I_1 for $\vec{f}^{(1)}$ - and I_1 / I_2 for $\vec{f}^{(2)}$ -excitations in ^{20}Ne . The solid lines denote actions which are calculated in the "rotated" canonical variables $\vec{q}' = \hat{R}(\theta_1, \theta_2) \vec{q}$. The rotation angles ($\theta_1 = -5^\circ$, $\theta_2 = -4^\circ$) are chosen in such a way that Poincaré surfaces of sections $q'_1 = 0$ and $q'_2 = 0$ determine actions I_j for exactly the same initial conditions as for trajectories in fig. 4. The dashed and dashed-dotted curves are obtained for "normal modes" in the least coupled system constructed by rotation ($\theta_1 = -5^\circ$, $\theta_2 = -4^\circ$) of initial variables and higher order non-linear transformations which do not change the initial condition.

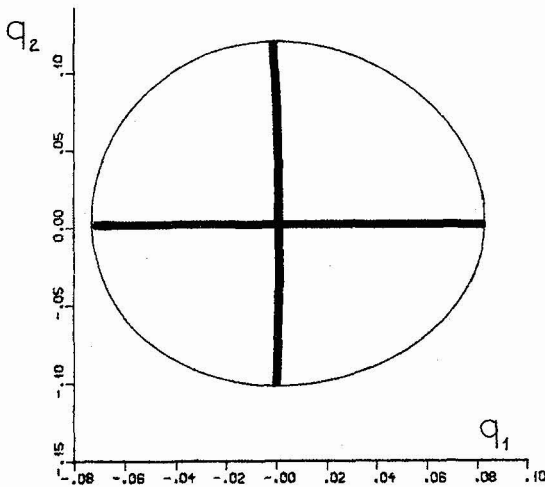


Fig. 6

The region swept out by trajectories in the "rotated" canonical variables ($\theta_1 = -5^\circ, \theta_2 = -4^\circ$) for $\vec{f}^{(1)}$ - and $\vec{f}^{(2)}$ excitations at $E^* = 1$ MeV in ^{20}Ne . For more details see the text and a caption of fig. 4.

yield an accurate approximation of the quantized states. One can notice immediately that the principal axes of the trajectory region in fig. 4 are not parallel to the coordinate axes. This observation provides a suggestion about the possible method of the systematic improvement of hamiltonian variables. One would like to transform the original coordinates to the new ones in which the trajectory region is more symmetric and to initiate in those new canonical variables the " normal modes " $\tilde{F}^{(i)}$. Such a procedure is equivalent to the consistent modification of the initial conditions so that the Hamilton's motion in the new canonical variables is less coupled. The group of unitary and linear canonical transformations covers all possible initial conditions while changing the two free parameters of the transformation (angles of the rotation θ_1, θ_2). This group is also simple enough for practical applications. The final improvement of the caustics can be achieved by certain non-linear transformations which do not modify the initial conditions but allow to calculate both I_1 and I_2 actions at the Poincaré surfaces of section. Fig. 6 presents the regions swept out by trajectories for $\tilde{F}^{(1)}, \tilde{F}^{(2)}$ -excitations in the " rotated " canonical variables $q_1 = Q_1 - 1, q_2 = Q_2 - 1$ where :

$$\begin{pmatrix} Q_1 \\ Q_2 \end{pmatrix} = \begin{pmatrix} \cos\theta_1 & \sin\theta_1 \\ -\sin\theta_2 & \cos\theta_2 \end{pmatrix} \begin{pmatrix} q \\ q_z \end{pmatrix} \tag{25}$$

and $P_i(p_1, p_2)$ ($i=1,2$) are given by the canonical transformation. Notice in fig. 6 a strong reduction of the trajectory regions. This leads to a decrease, by a factor 3-10, of the action integrals (dashed and dashed-dotted lines in fig. 5 as compared to the actions calculated for the original variables (the solid curves in fig. 5). One should stress that the above procedure of constructing the most decoupled system is not restricted to the weakly coupled, nondegenerate Hamilton's system. If one represents the vibrations of ^{20}Ne in terms of radius parameter q_b generating the breathing mode and the deformation q_β generating the volume

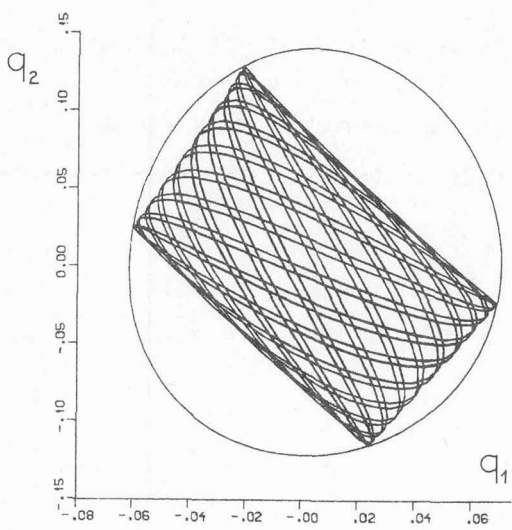


Fig. 7a

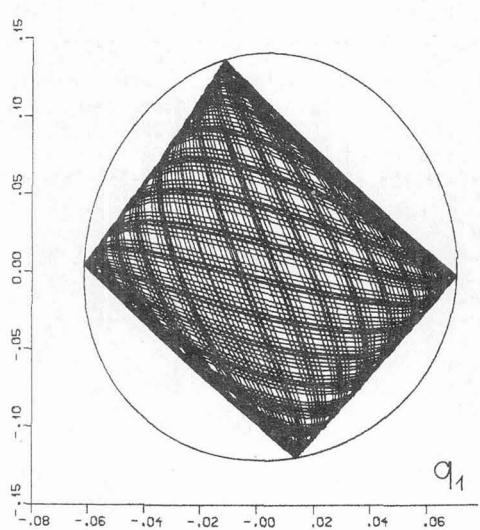


Fig. 7b

The region swept out by trajectories in the canonical variables $q_1 = q_b - 1, q_2 = q_\beta - 1$ for the $\tilde{F}^{(1)}$ - (fig. 7a) and $\tilde{F}^{(2)}$ (fig. 7b)-excitations of ^{20}Ne at $E^* = 1$ MeV.

conserving quadrupole vibrations then both modes are strongly coupled (see fig. 7). Nevertheless, applying both the linear transformation with $\theta_1 = 31^\circ$, $\theta_2 = 67.1^\circ$ and the initial condition preserving higher order nonlinear transformations one obtains the same trajectory region as shown in fig. 6. Having determined at each excitation energy the most decoupled system in the "rotated" canonical variables (25) one can calculate the energies of quantized states as prescribed in eq. (10). Thus, energies of the resonances $|I_1 = 1, I_2 \approx 0\rangle$, $|I_1 \approx 0, I_2 = 1\rangle$ are obtained by interpolating action integrals until the desired values of I_i are not found. These resonances are found at $E_1 = 25.0$ MeV for the q_1 -mode and at $E_2 = 16.46$ MeV for the q_2 -mode. The generator coordinate method (GCM) for equivalent generating functions $\phi(\vec{r}; \vec{p})$ and with the identical many-body Hamiltonian gives $E_1 = 25.06$ MeV and $E_2 = 16.54$ MeV /2/. Thus, both methods are in excellent agreement.

In summary, the RSVP presented here offers promise in a variety of applications in the many-body theory. However, several questions arise concerning the relation between the different descriptions of a quantum system in terms of either stationary or non-stationary states in the Hilbert space. The principal unresolved challenges are the understanding accuracy of RSVP and developing more powerful approximation techniques to deal with complicated dynamics in multidimensional hamiltonian system.

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