GEOMETRICAL QUANTIZATION IN DYNAMICAL VARIATIONAL APPROACH

E. CAURIER

Centre de Recherches Nucléaires,
F-67037 Strasbourg Cedex, France

S. DROŻDŻ*, J. OKOŁOWICZ AND M. PŁOSZAJCZAK**

Institute of Nuclear Physics,
31-342 Kraków, Poland

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The dynamical variational approach based on geometrical quantization is demonstrated to be capable in describing the most important quantum mechanical quantities. In particular, the consistent prescription for calculating the transition probabilities is presented. For several reasons, the method is expected to be better under control than the semiclassical methods in treating the systems whose classical counterparts are chaotic. The formal considerations are illustrated using an exactly solvable SU(3)--spin system.

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The quantum mechanical problems are rarely exactly solvable and one is forced to deal with approximate solutions. The semiclassical methods are of central importance in this connection but their applicability encounters serious technical difficulties when the phase-space displays stochastic structure [1]. The other kind of approach which we wish to advocate in this paper, is based on the time-dependent variational principle (TDVP):

$$\delta \int_0^t \langle \psi(x; t') | i\hbar\partial_{t'} - \widehat{H} | \psi(x; t') \rangle dt' = 0 , \tag{1}$$

* Present address: Institut für Kernphysik, 5170 Jülich, FRG.

** Present address: Gesellschaft für Schwerionenforschung GSI 6100 Darmstadt, FRG.

where $\hat{H}$ is the Hamiltonian operator. The idea is to reduce the infinite dimensional Hamiltonian problem by restricting the number of degrees of freedom to a most relevant few, parametrized by a vector $z(t)$. The resulting equations of motion for $\psi(x; t)$ are in general nonlinear and the stationary solutions cannot be found. The wave packet-type solutions of (1) for bound states $\psi(x; t) \equiv \psi(x; z(t))$ have to be localized in space. Then the time-evolution generates an additional phase and the full solution becomes:

$$\psi^C(x; t) \equiv \psi^C(x; z) = \psi(x; z) \exp\left(\frac{i}{\hbar} \int_0^t dt' \langle \psi | i\hbar \partial_{t'} | \psi \rangle\right) \times \exp\left(-i\langle \psi | \hat{H} | \psi \rangle t/\hbar\right), \tag{2}$$

where $z(t) = \left(z_1(t), \ldots, z_{2m}(t)\right)$. The first exponent in (2) depends solely on the geometry of a trajectory in the parametric space and can be identified with the geometrical phase. Phases of this type were appreciated first by the College Park group [2] in connection with the quantization of time-dependent Hartree-Fock (TDHF) solutions. The resulting method is known as the Gauge Invariant Periodic Quantization (GIPQ). Later on, the method was generalized to variational approaches based on any parametric space [3]. The most general formulation of the geometrical phase is due to Aharonov and Anandan [4] and in the adiabatic approximation it is known as the Berry phase [5]. Because of the gauge-invariance of the geometrical phase it is natural to extract from $\psi^C(x, t) = \psi^G(x; z) \exp(-i\langle \psi | \hat{H} | \psi \rangle t/\hbar)$, the gauge-invariant component ψ^G which is given by the product of $\psi(x; z)$ and the geometrical phase. ψ^G is a natural analog of a stationary-state wave function. The principle of regularity and single-valuedness (RSV) [6] is then imposed on ψ^G and provides a consistent prescription for selecting energies of quantized states. For periodic solutions $\psi^\alpha(x; z)$, associated with independent closed orbits $C_\alpha(z)$ in the parameter space, the RSV quantization condition reads

$$I_\alpha(C_\alpha) = (2\pi)^{-1} \int_0^{T_\alpha} \langle \psi^\alpha\left(x; z^{(\alpha)}(t')\right) | i\hbar \partial_{t'} | \psi^\alpha\left(x; z^{(\alpha)}(t')\right) \rangle dt' = n_\alpha \hbar \qquad (\alpha = 1, \ldots, m), \tag{3}$$

where m refers to the number of independent directions "α" and T_α is the oscillation period. By now there exist several methods to find those time-periodic solutions [7, 8].

The Eqs of motion in z can always be transformed into the Hamilton Eqs. in pairwise canonical variables $\{(p_i, q_i), (i = 1, \ldots, m)\}$ [9]. The RSV

conditions (3) become then particularly simple:

$$I_\alpha = (2\pi)^{-1} \oint_{C_\alpha} p_{(\alpha)}\, dq_{(\alpha)} = n_\alpha \hbar\,. \tag{4}$$

In that sense the geometrical quantization may become *technically* equivalent to the semiclassical quantization, even though, p, q are labels of the time-evolving phase-determined wave packet and not merely the classical momenta and coordinates. Such a wave packet is supposed to approximate the exact Schrödinger wave packet. These, however, evolve regularly in time even for classically chaotic systems. Therefore, the possible onset of chaos does not mean that the above quantization prescription is inapplicable but instead that the approximation fails and the parametric space has to be enlarged to include further quantum corrections in such a way that the regular time evolution in $z(t)$ is recovered.

This geometrical type of quantization has been extensively used to calculate the energies of nuclear vibrational states. Recently, based on the relationship between TDVP and the generator coordinate method [6], it has been successfully adopted to the calculation of transition probabilities between different quantized states [10].

The purpose of this paper is to address various aspects of the geometrical quantization and to demonstrate its efficiency on the example of SU(3) – quantum spin system [11] whose classical large-N limit [12] given by TDHF is non-integrable. The advantage of this quantum system lies both in its ability to mimic essential ingredients of the shell model and in the fact that it is exactly solvable. The SU(3) model consist of N distinguishable fermions, labeled by index n, each of which can be in three, N-time degenerate single-particle levels having energies $\epsilon_0 = -\varepsilon$, $\epsilon_1 = 0$, $\epsilon_2 = \varepsilon$. The Hamilton operator is:

$$\hat{H} = \sum_{k=0}^{K=2} \epsilon_k \hat{N}_{kk} + \tfrac{1}{2} \sum_{k,l=0}^{K=2} V_{kl} \hat{N}_{kl}^2\,, \tag{5}$$

where $V_{kl} = V(1 - \delta_{kl})$, $V < 0$, and $\hat{N}_{kl} = \sum_n a_{nk}^\dagger a_{nl}$ ($\sum_{k=0}^{K=2} \hat{N}_{kk} = \text{const}$) are SU(3) – generators which form basis for the Lie algebra of the coherent group G acting irreducibly on the Hilbert space of the SU(3) system. Finding the large-N limit of SU(3) quantum theory is associated with the construction of the corresponding coherent states. This can be achieved by applying each of the elements of the coherence group G to the noninteracting ground state of the system with all particles in the lowest level. The resulting states:

$$|\psi(z_1(t), z_2(t))\rangle = \exp\left(z_1(t)\hat{N}_{10} + z_2(t)\hat{N}_{20}\right)|z_1 = 0,\, z_2 = 0\rangle \tag{6}$$

are Slater determinants labelled by two complex particle-hole (p-h) amplitudes z_1 and z_2. The classical Hamiltonian $\overline{H}$ can now be identified with $\langle\psi(z)|\hat{H}|\psi(z)\rangle/\langle\psi(z^*)|\psi(z)\rangle$. Working with the normalized states, it is convenient to change to the parameters $\beta_i = z_i/\left(1+z_1z_1^*+z_2z_2^*\right)^{\frac{1}{2}}$ and separate out their real ($\boldsymbol{q}=[q_1, q_2]$) and imaginary ($\boldsymbol{p}=[p_1, p_2]$) parts which are the canonical conjugate variables [11]. The time-evolution of the classical SU(3) system is governed by the scaled Hamiltonian $\overline{H}[\boldsymbol{q}, \boldsymbol{p}] \equiv \overline{H}^{\infty}/N\varepsilon$ which, for a fixed, normalized strength of the two-body interaction $\chi \equiv NV/\varepsilon$, does not depend on the particle number. N appears only in the quantization condition.

Putting $\boldsymbol{p}=0$ in $\overline{H}$, one defines a static part $\overline{V}$ of this Hamiltonian. $\overline{V}(q_1, q_2)$ at $\chi > 3$ has four degenerate minima separated by the saddle points. For large N, the quantum motion is restricted to the narrow region in the phase space around each of the minima of $\overline{V}$. The high barriers between them prohibit strong mixing and the description of a quantum system using a single, time-evolving Slater determinant around each minimum of $\overline{V}$ separately can be justified. However, for small number of particles even the lowest excited state appears close to the saddle point and, therefore, mixing of the Slater determinants in the quantum wave function cannot be excluded. These quantum correlations are absent in the TDHF-field. One could approximate them by introducing projected manifolds $\{\psi_{\sigma_1,\sigma_2}(\beta_1, \beta_2)\} \equiv \{\hat{P}(\sigma_1, \sigma_2)\psi(\beta_1, \beta_2)\}$, where the projection operator is defined as $\hat{P}(\sigma_1, \sigma_2) \equiv (1+\sigma_1\hat{\Pi}_{\beta_1})(1+\sigma_2\hat{\Pi}_{\beta_2})$ with $\hat{\Pi}_{\beta_i}\psi(\beta_i, \beta_j) = \psi(-\beta_i, \beta_j)$ and σ_i $(i=1, 2)$ can take values $+1$ or -1 for the positive and negative parity states respectively. Hence, in each of the variational manifolds $\{\psi_{++}\}$, $\{\psi_{+-}\}$, $\{\psi_{-+}\}$, $\{\psi_{--}\}$ separately, the time-evolving wave-packet is a superposition of Slater determinants around each of the four minima of $\overline{V}$. Obviously, $\boldsymbol{q}$ and $\boldsymbol{p}$ are no longer canonical conjugate variables. With this form of variational manifolds, Eqs of motion take the form:

$$\sum_j S_{ij}\partial_t\beta_j = \frac{\partial}{\partial\beta_i^*}\langle\psi_{\sigma_1\sigma_2}|\hat{H}|\psi_{\sigma_1\sigma_2}\rangle \quad (i, j=1, 2), \tag{7}$$

where S_{ij} are the Poisson brackets:

$$S_{ij} = n^{-1}_{\sigma_1\sigma_2}\left(\langle\frac{\partial\psi_{\sigma_1\sigma_2}}{\partial\beta_i^*}|\frac{\partial\psi_{\sigma_1\sigma_2}}{\partial\beta_j}\rangle - n^{-1}_{\sigma_1\sigma_2}\langle\frac{\partial\psi_{\sigma_1\sigma_2}}{\partial\beta_i^*}|\psi_{\sigma_1\sigma_2}\rangle\langle\psi_{\sigma_1\sigma_2}|\frac{\partial\psi_{\sigma_1\sigma_2}}{\partial\beta_j}\rangle\right) \tag{8}$$

and $n_{\sigma_1\sigma_2} \equiv \langle\psi_{\sigma_1\sigma_2}|\psi_{\sigma_1\sigma_2}\rangle$.

Time-periodic solutions for $\beta(t)$ are selected to construct $\psi^G_{\sigma_1\sigma_2}$ and, then, the RSV quantization condition (3) is employed to select physical

states and their excitation energy. A stationary state wave function can be projected out by constructing [13] [6] the time-averaged wave function for a given quantized state $|\alpha\rangle$:

$$\psi^{G;\alpha}_{\sigma_1\sigma_2}(x) = \frac{1}{T_\alpha}\int_0^{T_\alpha} dt' \psi^{\alpha}_{\sigma_1\sigma_2}\left(x;\beta_{(\alpha)}(t')\right) \times \exp\left(\frac{i}{\hbar}\int_{\beta_{(\alpha)}(0)}^{\beta_{(\alpha)}(t')} \langle\psi^{*\alpha}_{\sigma_1\sigma_2}|i\hbar\partial_{t''}|\psi^{\alpha}_{\sigma_1\sigma_2}\rangle dt''\right). \quad (9)$$

The index "α" distinguishes among different periodic trajectories corresponding to different states. Each state is presented by the single stable trajectory so long as they can be defined uniquely. In the fully chaotic case, the individual families of periodic tarjectories proliferate exponentially and obviously the TDVP + RSV method cannot and ought not to be applied because at that moment the chosen approximation for the wave-packet does not make sense anymore. Using (9) one can calculate the transition probabilities between any two states $|\alpha\rangle$ and $|\alpha'\rangle$ and for any operator $\widehat{F}$.

Fig. 1 shows the results for diagonal and off-diagonal matrix elements of $\hat{s} \equiv \widehat{N}_{11} - \widehat{N}_{00}$ and $\hat{t} \equiv \widehat{N}_{22} + \widehat{N}_{11} - 2\,\widehat{N}_{00}$ between the first two excited states $|1\rangle$, $|2\rangle$ and the ground state $|0\rangle$. The calculations are performed for various particle numbers in the manifolds $\{\psi_{++}\}$, $\{\psi_{--}\}$ at $\chi = 10$. Solid lines exhibit results of RSV calculations in the projected manifolds, whereas dots show exact quantum results for each given N. The upper most plots in Fig. 1 exhibit the excitation energies $\langle 1|\widehat{H}|1\rangle$ and $\langle 2|\widehat{H}|2\rangle$ (in units of ε) for states with $(++)$ and $(--)$ parities. The dashed line in the upper figure for ψ_{++} denotes results of random phase approximation (RPA) for energies of the one-phonon states. Notice, that until $N \simeq 50$, the agreement between RPA and exact results is very good. Dashed–dotted line in the upper right figure for ψ_{--} presents results of the quantized TDHF. This is an improvement over RPA in the region $40 < N < 50$. For smaller number of particles ($N < 40$) one finds deviations mainly for the negative parity states. The positive parity states in turn, are still well described by TDHF for all N. In general, the agreement between exact SU(3) results and the large-N limit of SU(3) is excellent until $N \simeq 40$ for all diagonal matrix elements including those of $\hat{s}$ and $\hat{t}$. Below $N \simeq 40$ this good agreement deteriorates but can be recovered after the quantum correlations due to the parity projection are added. The agreement for the off-diagonal matrix elements of $\hat{s}$ and $\hat{t}$ operators is less spectacular. This is mainly due to the absence of quantum correlations in the ground state and reflects the strong sensitivity of the off-diagonal matrix elements to details of the wave function. For large-N,

these correlations are the familiar 2p – 2h, RPA correlations which do not influence the excitation spectrum or diagonal matrix elements but may have a strong effect upon the off-diagonal matrix elements for operators which connect to the ground state.

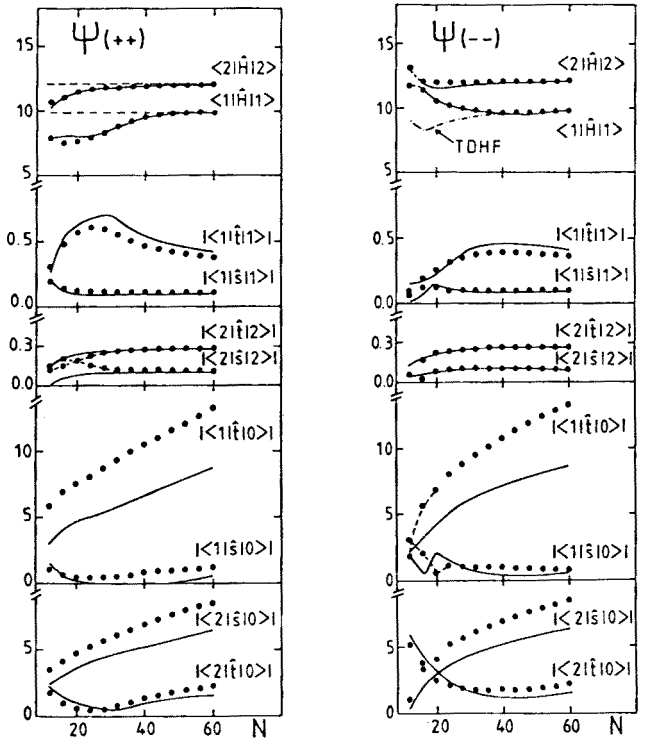

Fig. 1. The matrix elements for operators $\hat{H}$, $\hat{s} \equiv \hat{N}_{11} - \hat{N}_{00}$ and $\hat{t} \equiv \hat{N}_{22} + \hat{N}_{11} - 2\hat{N}_{00}$ as calculated exactly in SU(3) (dots) and in the projected manifolds $\{\psi_{++}\}$, $\{\psi_{--}\}$ for the first two excited states $|1\rangle$, $|2\rangle$ and the ground state $|0\rangle$ at $\chi = 10$. For more details see the description in text.

Fig. 2 shows the (q_1, p_1) surfaces of section at $q_2 = 0$, at the energy corresponding to the first excited state in the manifold $\{\psi_{++}\}$ at $\chi = 10$ and for various number of particles. In our case, a surface of section is given by set of points which are obtained by intersecting a trajectory with a plane $q_2 = 0$ in the three dimensional phase space (p_2 is fixed by the energy conservation). In the integrable system only closed curves are seen in the surface of section. For chaotic systems, on the contrary, the surface of section is evenly covered with the points in the whole energetically available phase space. It might seem paradoxical that the particle motion in

the phase space is more organized for large N. This, however, illustrates our introductory remark concerning the meaning of chaos in the variational dynamical approach. Here, decreasing the particle number, *i.e.* deviating more and more from the validity of the mean field approach, one sees an increase in the chaotic volume of the phase-space. Similar observations has been made recently in Ref. [14]. Finally, the chaotic trajectories fill the whole available phase-space ($N \simeq 12$). The stable periodic trajectories for quantized states of each parity could be found only until $N = 12$. For $N < 12$ the stable orbits disappear which signals the importance of further quantum corrections. Therefore, we did not continue calculations for $N < 12$ using unstable orbits. Notice however, that as long as we are able to localize the stable orbits in the parametric space, the agreement between results of SU(3)-quantum spin model and its classical, Large-N limit extended to include quantum correlations due to the parity projection, is very good.

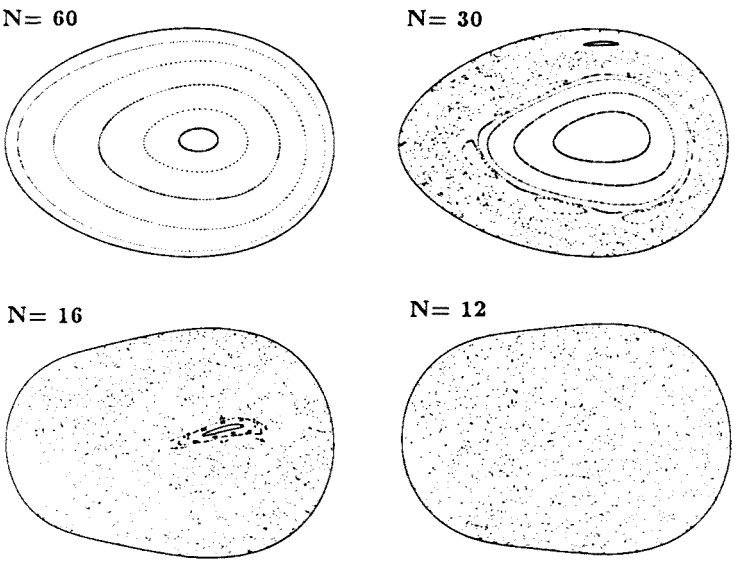

Fig. 2. (q_1, p_1)-surface of section at $q_2 = 0$ for different particle numbers as calculated for the state $|1_{++}\rangle$. For more details see the description in the text.

In conclusion, TDVP supplemented with the geometrical quantization condition, appears suitable for reproducing various quantum mechanical quantities. This method seems to be more efficient than the semiclassical method, particularly for the chaotic systems, in which the latter method requires many classical trajectories to built the wave function [1]. This is due to the fact that in variational approach the majority of quantum mechani-

cal effects is incorporated already from the beginning while the semiclassical methods aim at reconstructing the wave function from purely classical trajectories. In the above analysis, which relates properties of the wave function with the behaviour of periodic orbits in the subspace of phase--determined wave functions, the onset of chaos has no dramatic consequences and seems rather to indicate a gradually increasing importance of quantum corrections and, hence, a demand for revision of the variational manifold. Such a conclusion sounds consistent with the linearity of the Schrödinger equation which leads to the regular propagation of an exact wave packet in its multidimensional phase-space. Thus one would expect that its right approximant should behave similarly. Of course, the contrary is not necessarily true. A drastic reduction of the variational problem to one degree of freedom will always result in a regular motion although such an approach may be inadequate. Since on the level of stationary variational approach there exists no correctness criterion, the above aspect of the dynamical variational approach is particularly interesting and calls further clarification.

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