ANNALES
UNIVERSITATIS MARIAE CURIE-SKŁODOWSKA
LUBLIN—POLONIA
VOL. XL/XLI, 14 SECTIO AAA 1985/1986

Instytut Fizyki UMCS

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Collective Bohr Hamiltonian in the Generator Coordinate Method

Kolektywny hamiltonian Bohra w metodzie współrzędnej generującej

Коллективный гамильтониан Бора в методе генерирующей координаты

Dedicated to Professor
Stanisław Szpikowski on occasion
of his 60th birthday

1. INTRODUCTION

The collective Hamiltonian for quadrupole motion originally proposed by A. Bohr in 1952 [1] was successfully used for description of low lying collective nuclear states [2]. The parameters of the Hamiltonian at first were determined phenomenologically and afterwards on the basis of microscopic theories [2,3]. In the estimation of the inertial functions as well as the collective potential function different models have been used. The partially phenomenological pairing-plus-quadrupole model [4-6], TDHF approach [7], ATDHF theory of collective motion [8] and a direct application of the Inglis formula [9-11] provide only a few examples of a great variety of methods used to calculate the mass tensor and the potential energy surface. However, to obtain a quantal collective Hamiltonian all the methods require not unique procedure of quantization of a classical collective Hamiltonian [12]. In addition, e.g. in the popular cranking approach, the potential energy surface [13, 14] is chosen with accuracy to any arbitrary scalar function i.e. the quantal zero-point energy is not taken into account [15, 16].

The criticism of these quasi-quantal methods was a motivation to look for a more satisfactory approach. The generator coordinate method (GCM) offers a fully quantal theory [17-19] which together with the Gaussian overlap approximation [20] or its extension [21] allows for microscopical derivation of the collective Hamiltonian. This method allows to derive the collective Hamiltonian starting from stationary Schrödinger equation in a fermionic space. Contrary to the previous approaches no redundant variables are introduced and no quantization procedure of a classical Hamiltonian for collective motion is needed. The first attempts in this direction were already made nearly ten years ago. Using an approximate narrowing kernel approach [22] the rotational kinetic energy of the Bohr Hamiltonian has been obtained in [23]. However, the moments of inertia are derived only for the many-body Hamiltonians and not for the mean fields Hamiltonians. In addition the paper does not offer explicitly any expression for the zero-point correction to the potential energy. The full Bohr Hamiltonian is also not explicitly derived there because the analytical diagonalization of the five-dimensional metric tensor is needed.

It is the aim of the present paper to describe a quantal derivation of the full quadrupole collective Hamiltonian within the GCM and the extended Gaussian overlap approximation [21]. The recent GCM estimates of the mass parameters and potential energy [24-27] are different from those obtained by quantization of the classical collective Hamiltonian. However, to decide which approximation gives results more closer to the experimental data one needs to solve the full, including the most important degrees of freedom collective Hamiltonian. It will be a topic of our future publications. The present paper is only a preliminary step towards this goal; here we give only the outline of the theoretical formalism.

2. THE GENERATING FUNCTION AND THE METRIC TENSOR

The classical Bohr Hamiltonian is dependent on five quadrupole complex collective variables $\alpha_{\mu}^{(2)}$ ($\mu = -2,1,\ldots,2$) which one assumes as generating coordinates. One also assumes that the appropriate normalized generating function $|\alpha_{\mu}^{(2)}\rangle$ describing a quadrupole nuclear motion of many body system satisfies the conditions for the extended Gaussian overlap approximation [21] i.e. the overlap function $\langle\alpha_{-2}^{(2)},\ldots,\alpha_{2}^{(2)}|\alpha_{-2}^{\prime(2)},\ldots,\alpha_{2}^{\prime(2)}\rangle$ is a deformed in the variables $\alpha_{\mu}^{(2)}$ and $\alpha_{\mu}^{\prime(2)}$ Gaussian profile (for details see [21, 26 and 27]). After transformation [1] to the shape variables β and γ and three Euler angles $\Omega = (\Omega_1, \Omega_2, \Omega_3)$ the generating function can be factorized as

$$|\alpha_{-2}^{(2)},\ldots,\alpha_{2}^{(2)}\rangle = |\Omega\beta\gamma\rangle = \hat{R}(\Omega)|\beta\gamma\rangle \quad , \tag{1}$$

where $\hat{R}(\Omega) = e^{-i\Omega_1\hat{J}_3} e^{-i\Omega_2\hat{J}_2} e^{-i\Omega_3\hat{J}_3}$ is the rotation operator defined in the space fixed frame. The normalized "intrinsic" function $|\beta\gamma\rangle$ corresponds to the generating function $|\alpha_{\mu}^{(2)}\rangle$ at the moment when the "intrinsic" (rotating) and the laboratory (fixed space) frames coincide. In applications the intrinsic function $|\beta\gamma\rangle$ is usually chosen as a BCS-type function. Following the paper [23] one assumes that the intrinsic function $|\beta\gamma\rangle$ has the reflection (d_2-group) symmetry [2, 3]:

$$e^{-i\pi\hat{J}_k}|\beta\gamma\rangle = |\beta\gamma\rangle \, , \quad k = 1,2,3. \tag{2}$$

The symmetry allows to obtain the rotational inertia in respect to the principal axes. To apply directly the formulae of Refs. [21, 26, 27] one requires that the matrix elements $\langle\Omega\beta\gamma|\frac{\partial}{\partial q^k}|\Omega\beta\gamma\rangle$ ($q^k = \Omega_k$, k=1,2,3, $q^4 = \beta$, $q^5 = \gamma$) have to be equal zero. It is alyways fulfilled by the operators $\frac{\partial}{\partial\Omega_k}$ due to d_2-symmetry (2).

On the other hand, from the normalization property $\langle \beta\gamma | \beta\gamma \rangle = 1$, one can easily obtained that $\mathrm{Re} \langle \Omega\beta\gamma | \frac{\partial}{\partial q^k} | \Omega\beta\gamma \rangle = 0$ and the ap- priate choice of (β, γ)-dependent phase factor in the generating function (1) allows always to satisfy the required condition (see e.g. [27]).

Following [21, 27] the metric tensor in the collective space can be calculated from the formula

$$g_{\mu\nu} = \mathrm{Re} \langle q | \frac{\overleftarrow{\partial}}{\partial q^\mu} \frac{\overrightarrow{\partial}}{\partial q^\nu} | q \rangle \ , \qquad (3)$$

where $q = (q^\mu) = (\Omega_1, \Omega_2, \Omega_3, \beta, \gamma)$ and $\frac{\overleftarrow{\partial}}{\partial q}$ $\frac{\overrightarrow{\partial}}{\partial q}$ act on bra and ket, respectively. Owing to d_2-symmetry the metric tensor has a reduced form:

$$(g_{\mu\nu}) = \begin{bmatrix} (g_{\Omega_k \Omega_{k'}}) & & 0 \\ & & g_{\beta\beta} & g_{\beta\gamma} \\ 0 & & g_{\gamma\beta} & g_{\gamma\gamma} \end{bmatrix} \qquad (4)$$

Using the relation (it can be obtained by direct differentiation of the rotation operator)

$$\hat{R}^+(\Omega) \frac{\partial \hat{R}(\Omega)}{\partial \Omega_k} = -i \sum_{k'=1}^{3} b_{kk'}(\Omega) \hat{J}_{k'} \qquad (5)$$

where the matrix

$$(b_{kk'}(\Omega)) = \begin{bmatrix} -\sin\Omega_2 \cos\Omega_3 & \sin\Omega_2 \sin\Omega_3 & \cos\Omega_3 \\ \sin\Omega_3 & \cos\Omega_3 & 0 \\ 0 & 0 & 1 \end{bmatrix} \qquad (6)$$

one can obtain the expression for the "rotational" part of the metric tensor

$$g_{\Omega_k \Omega_{k'}} = \sum_{l=1}^{3} b_{kl}(\Omega)\, b_{k'l}(\Omega) \langle \hat{J}_l^2 \rangle \tag{7}$$

In (7) and further the notation $\langle \hat{A} \rangle = \langle \beta\gamma | \hat{A} | \beta\gamma \rangle$ is used. One can easily check that the corresponding contravariant components can be expressed in a similar way:

$$g^{\Omega_k \Omega_{k'}} = \sum_{l=1}^{3} \left(b^{-1}(\Omega) \right)_{lk} \left(b^{-1}(\Omega) \right)_{lk'} \langle \hat{J}_l^2 \rangle^{-1} \tag{8}$$

The "vibrational" part of the metric tensor is dependent on explicite definition of the generating function and in general can be written as (3) ($\mu, \nu = 4,5$):

$$g_{\mu\nu} = \langle \beta\gamma | \frac{\overleftarrow{\partial}}{\partial q^{\mu}} \frac{\overrightarrow{\partial}}{\partial q^{\nu}} | \beta\gamma \rangle \; ; \; q^4 = \beta \text{ and } q^5 = \gamma \tag{9}$$

Note that the vibrational components (9) do not depend on Euler angles. To derive expressions for the mass tensor and the potential energy one needs to calculate a part of Christoffel coefficients connected with the full metric tensor (g_{kl}). One can easily prove that

$$\Gamma^{\beta}_{\Omega_k \gamma} = \Gamma^{\gamma}_{\Omega_k \beta} = \Gamma^{\beta}_{\Omega_k \beta} = \Gamma^{\gamma}_{\Omega_k \gamma} = 0 \tag{10}$$

and in practice only the coefficients related to the vibrational tensor (9) have to be evaluated i.e.

$$\Gamma^{\varrho}_{\mu\nu} = \frac{1}{2} \sum_{h=4}^{5} g^{\varrho h} \left(\frac{\partial g_{\mu h}}{\partial q^{\nu}} + \frac{\partial g_{\nu h}}{\partial q^{\mu}} - \frac{\partial g_{\mu\nu}}{\partial q^{h}} \right) ; \; \mu,\nu,\varrho = 4,5 \tag{11}$$

3. THE MASS PARAMETERS AND THE ZERO-POINT ENERGY

Denote by $\hat{H}$ the many-body (or β, γ dependent mean field) Hamiltonian of the nucleus at the moment when the laboratory and intrinsic frames coincide i.e. for $\Omega = 0$. After rotation the Hamiltonian is equal

$$\hat{H}' = \hat{R}(\Omega)\,\hat{H}\hat{R}^{+}(\Omega). \tag{12}$$

Obviously, if $\hat{H}$ is a true many-body Hamiltonian then it is invariant under space rotation and $\hat{H}' = \hat{H}$. For the mean field Hamiltonians we assume only that $\hat{H}$ is invariant under d_2-group, i.e.

$$e^{-i\pi\hat{J}_k}\,\hat{H}\,e^{i\pi\hat{J}_k} = \hat{H}\;;\; k = 1,2,3. \tag{13}$$

It allows to avoid the asymmetry terms linear terms) [27] in the collective Hamiltonian which are not observed in experiment. The covariant components of the inverse mass tensor can be calculated from the formula [21, 26, 27]:

$$\begin{aligned}(m^{-1}(q))_{\mu\nu} = \mathrm{Re}\Big\{&\langle q|\frac{\overleftarrow{\partial}}{\partial q^{\mu}}\,\hat{H}'\,\frac{\overrightarrow{\partial}}{\partial q^{\nu}}|q\rangle_L +\\ &+\frac{1}{2}\langle q|\frac{\overleftarrow{\partial}}{\partial q^{\nu}}\,\frac{\partial\hat{H}'}{\partial q^{\mu}}|q\rangle - \frac{1}{2}\,\frac{\Delta h_{\nu}}{\Delta q^{\mu}}\Big\},\end{aligned} \tag{14}$$

where the linked matrix element is, as usually defined [18]

$$\langle q|\frac{\overleftarrow{\partial}}{\partial q^{\mu}}\hat{H}'\frac{\overrightarrow{\partial}}{\partial q^{\nu}}|q\rangle_L = \langle q|\frac{\overleftarrow{\partial}}{\partial q^{\mu}}\hat{H}'\frac{\overrightarrow{\partial}}{\partial q^{\nu}}|q\rangle - \langle q|\frac{\overleftarrow{\partial}}{\partial q^{\mu}}\,\frac{\overrightarrow{\partial}}{\partial q^{\nu}}|q\rangle\langle q|\hat{H}'|q\rangle \tag{15}$$

$$h_{\nu} \equiv \left(\frac{\partial}{\partial a^{\nu}}\,\frac{\langle a|\hat{H}'|a'\rangle}{\langle a|a'\rangle}\right)_{a=a'=q} \quad (\nu = 1,2,\ldots,5) \tag{16}$$

and $\frac{\Delta}{\Delta q^{\nu}}$ denotes a covariant derivative e.g.

$$\frac{\Delta h_{\nu}}{\Delta q^{\mu}} = \frac{\partial h_{\nu}}{\partial q^{\mu}} - \sum_{\varrho=1}^{5}\Gamma^{\varrho}_{\nu\mu}\,h_{\varrho}. \tag{17}$$

Using (10), d_2-symmetry property (2) and (13) one can show that the mass tensor has also a reduced form (4)

$$m^{-1} = \begin{bmatrix} ((m^{-1})_{\Omega_k \Omega_{k'}} & & 0 \\ & & (m^{-1})_{\beta\beta} & (m^{-1})_{\beta\gamma} \\ 0 & & & \\ & & (m^{-1})_{\gamma\beta} & (m^{-1})_{\gamma\gamma} \end{bmatrix} \tag{18}$$

After straightforward but lengthy calculation one can obtain the contravariant inverse mass tensor

$$(m^{-1})^{\Omega_k \Omega_{k'}} = \sum_{l=1}^{3} (b^{-1}(\Omega))_{lk} (b^{-1}(\Omega))_{lk'} \langle \hat{J}_l^2 \rangle^{-2} \cdot \tag{19}$$
$$\left\{ \langle \hat{J}_l \hat{H} \hat{J}_l \rangle_L + \frac{1}{4} \langle [\hat{J}_l, [J_l, H]] \rangle - \frac{1}{4} \sum_{\nu,\mu=4}^{5} h_\nu q^{\nu\mu} \frac{\partial}{\partial q^\mu} \langle J_l^2 \rangle \right\}$$

and for $u, \nu = 4,5$

$$(m^{-1})^{\mu\nu} = \sum_{\varrho=4}^{5} \sum_{\sigma=4}^{5} q^{\mu\varrho} q^{\nu\sigma} \,\mathrm{Re} \left\{ \langle \beta\gamma | \frac{\overleftarrow{\partial}}{\partial q^\varrho} \hat{H} \frac{\overrightarrow{\partial}}{\partial q^\sigma} | \beta\gamma \rangle_L \right.$$
$$\left. + \frac{1}{2} \langle \beta\gamma | \frac{\overleftarrow{\partial}}{\partial q^\sigma} \frac{\partial \hat{H}}{\partial q^\varrho} | \beta\gamma \rangle - \frac{1}{2} \frac{\Delta h_\sigma}{\Delta q^\varrho} \right\} . \tag{20}$$

Similarly to the vibrational part (9) of the metric tensor, the vibration part (20) of the inverse mass tensor does not depend on Euler angles.

The zero-point energy can be obtained from [21, 26, 27]

$$\mathcal{E}_0 = \frac{1}{2} \sum_{\mu,\nu=1}^{5} q^{\mu\nu} \,\mathrm{Re} \left\{ \langle q | \frac{\overleftarrow{\partial}}{\partial q^\mu} \hat{H}' \frac{\overrightarrow{\partial}}{\partial q^\nu} | q \rangle_L + \langle q | \frac{\overleftarrow{\partial}}{\partial q^\mu} \frac{\partial \hat{H}'}{\partial q^\nu} | q \rangle \right\} \tag{21}$$

and due to d_2-symmetry property reduces to a sum of the rotational $\mathcal{E}_0^{(rot)}$ and vibrational $\mathcal{E}_0^{(vib)}$ corrections to the standard collective potential energy $\langle \Omega\beta\gamma | \hat{H}' | \Omega\beta\gamma \rangle = \langle \beta\gamma | \hat{H} | \beta\gamma \rangle$:

$$\mathcal{E}_0 = \mathcal{E}_0^{(rot)} + \mathcal{E}_0^{(vib)} \tag{22}$$

In a similar way as for (19), making use of the formulae

$$\langle \Omega\beta\gamma| \frac{\overleftarrow{\partial}}{\partial\Omega_k} \hat{H}' \frac{\overrightarrow{\partial}}{\partial\Omega_{k'}} |\Omega\beta\gamma\rangle_L = \sum_{l=1}^{3} b_{kl}(\Omega)\, b_{k'l}(\Omega) \langle \hat{J}_l \hat{H} \hat{J}_l \rangle_L \tag{23}$$

and

$$\langle \Omega\beta\gamma| \frac{\overleftarrow{\partial}}{\partial\Omega_k} \frac{\partial\hat{H}'}{\partial\Omega_{k'}} |\Omega\beta\gamma\rangle = \sum_{l=1}^{3} b_{k'l}(\Omega)\, b_{kl}(\Omega) \langle \hat{J}_l [\hat{J}_l, \hat{H}] \rangle \tag{24}$$

one can obtain the rotational zero-point correction:

$$\varepsilon_0^{(rot)} = \frac{1}{2} \sum_{k=1}^{3} \langle \hat{J}_k^2 \rangle \left\{ \langle \hat{J}_k \hat{H} \hat{J}_k \rangle_L + \frac{1}{2} \langle [\hat{J}_l, [\hat{J}_l, \hat{H}]] \rangle \right\} \tag{25}$$

where, as it will be shown in next paragraph, $\mathcal{J}$ represents the rotational inertia:

$$\mathcal{J}_k^{-1}(\beta\gamma) = \langle \hat{J}_k^2 \rangle^{-2} \left\{ \langle \hat{J}_k \hat{H} \hat{J}_k \rangle_L + \frac{1}{4} \langle [\hat{J}_k, [J_k, H]] \rangle \right.$$
$$\left. - \frac{1}{4} \sum_{\nu,\mu=4}^{5} h_\nu q^{\nu\mu} \frac{\partial}{\partial q^\mu} \langle J_k^2 \rangle \right\} \tag{26}$$

Note that, the moments of inertia $\mathcal{J}(\beta\gamma)$ resembles the Peiers-Yoccoz and Une et al. [23] moments of inertia. The vibrational zero-point energy can be written as

$$\varepsilon_0^{(vib)} = \frac{1}{2} \sum_{l,l'=4}^{5} q^{ll'} \operatorname{Re} \left\{ \langle \beta\gamma| \frac{\overleftarrow{\partial}}{\partial q^l} \hat{H} \frac{\overrightarrow{\partial}}{\partial q^{l'}} |\beta\gamma\rangle_L + \right.$$
$$\left. + \langle \beta\gamma| \frac{\overleftarrow{\partial}}{\partial q^{l'}} \frac{\partial\hat{H}}{\partial q^l} |\beta\gamma\rangle \right\} \quad ; \; q^4 = \beta \;, q^5 = \gamma \tag{27}$$

4. THE COLLECTIVE HAMILTONIAN

The collective Hamiltonian derived in the GCM with extended gaussian overlap approximation [21] is very similar in form to the collective Hamiltonian obtained after the Pauli-Podolsky quantization procedure [3, 12]

$$\hat{\mathcal{H}}_{coll} = -\frac{1}{2\sqrt{|g|}} \sum_{l,l'=1}^{5} \frac{\partial}{\partial q^{l}} \sqrt{|g|}\, (m^{-1})^{ll'} \frac{\partial}{\partial q^{l'}} + \hat{V}(q) \tag{28}$$

where

$$g = \det (g_{\mu\nu}) \quad ; \quad \mu,\nu = 1, 2, \ldots, 5$$

and the potential energy is

$$\hat{V}(q) = \langle q|\hat{H}'|q\rangle - \mathcal{E}_0(q) \tag{29}$$

The main difference between (28) and the traditional collective Hamiltonian is that the metric tensor is different from the mass tensor and the potential is corrected by the zero-point energy.

In the case of the Bohr Hamiltonian (28) the rotational energy can be easily written in the standard form [23]:

$$\hat{T}_{rot} = \frac{1}{2} \sum_{k=1}^{3} \mathcal{J}_k^{-1}(\beta\gamma)(\hat{I}'_k)^2, \tag{30}$$

where the inertia parameters are explicitly given by (26) and

$$\hat{I}'_k = -i \sum_{l=1}^{3} (b^{-1}(\Omega))_{kl} \frac{\partial}{\partial \Omega_l} \tag{31}$$

are the angular momentum operators in the rotating (intrinsic) frame expressed in terms of Euler angles (see Chpt. 5 of [3]). In derivation of (30) the following relation was used

$$\sum_{k=1}^{3} \left[\frac{\partial}{\partial \Omega_k} , \sqrt{|g|}\, (b^{-1}(\Omega))_{lk} \right] = 0 . \tag{32}$$

The vibration kinetic energy does not depend on Euler angles and is given by the operator

$$\hat{T}_{vib} = -\frac{1}{2D} \Big\{ \frac{\partial}{\partial\beta} D(m^{-1})^{\beta\beta} \frac{\partial}{\partial\beta} + \frac{\partial}{\partial\beta} D(m^{-1})^{\beta\gamma} \frac{\partial}{\partial\gamma}$$
$$+ \frac{\partial}{\partial\gamma} D(m^{-1})^{\gamma\beta} \frac{\partial}{\partial\beta} + \frac{\partial}{\partial\gamma} D(m^{-1})^{\gamma\gamma} \frac{\partial}{\partial\gamma} \Big\} \tag{33}$$

where $D = \sqrt{|g_{\beta\beta} g_{\gamma\gamma} - (g_{\beta\gamma})^2| \langle J_1^2 \rangle \langle J_2^2 \rangle \langle J_3^2 \rangle}$

The potential energy (29), as it is expected, is a function of only shape parameters:

$$\hat{V}(\beta\gamma) = \langle \beta\gamma | \hat{H} | \beta\gamma \rangle - \mathcal{E}_0^{(rot)}(\beta\gamma) - \mathcal{E}_0^{(vib)}(\beta\gamma), \qquad (34)$$

where $\mathcal{E}_0^{(rot)}$ and $\mathcal{E}_0^{(vib)}$ can be calculated from (25) and (27). To complete formulae, one can quote the volume element

$$d\tau = \sqrt{|\det(g_{\mu\nu})|}\, d\beta\, d\gamma\, d\Omega_1 d\Omega_2 d\Omega_3 = \sqrt{|g_{\beta\beta} g_{\gamma\gamma} - (g_{\beta\gamma})^2|}\,\cdot$$

$$\cdot \langle J_1^2 \rangle \langle J_2^2 \rangle \langle J_3^2 \rangle \cdot d\beta\, d\gamma\, \sin\Omega_2\, d\Omega_1 d\Omega_2 d\Omega_3 \qquad (35)$$

which ensures the Bohr Hamiltonian

$$\hat{\mathcal{H}}_{coll} = \hat{T}_{rot} + \hat{T}_{vib} + \hat{V}(\beta\gamma) \qquad (36)$$

to be hermitian. It is also important to note that the Hamiltonian (36) is invariant under space rotations even when the Hamiltonian $\hat{H}'$, (12), is not invariant.

This way we derived the full quantal Bohr Hamiltonian with unique expressions for the mass tensor and potential energy for both a many-body and effective nuclear Hamiltonians. The derivation is independent on somewhat artificial quantization of a classical collective Hamiltonian as it was in the cranking or similar approaches. The collective Hamiltonian (36) has required symmetry properties and, on the other hand, allows for a very flexible choice of the collective subspace in the full fermion space. This fully quantal derivation of the Bohr Hamiltonian is limited only by rather general conditions under which the extended Gaussian overlap approximation can be used.

The author is greatly indebted to Professor K. Pomorski for suggesting this problem and for stimulating discussion. The author also would like to thank Professor M. Brack and E. Werner for warm hospitality at the University of Regensburg.

This work has been partially supported by contract CPBP 01.06.

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STRESZCZENIE

W pracy zastosowano metodę współrzędnej generującej (+ ogólnione przybliżenie gaussowskie) do otrzymania kwantowego hamiltonianu opisującego kwadrupolowe ruchy kolektywne jądra atomowego. Jako zmiennych kolektywnych użyto trzech kątów Eulera oraz dwóch standardowych parametrów deformacji β i γ. Uzyskano w pełni mikroskopowe wyrażenia na tensor masowy i potencjał kolektywny.

Р Е З Ю М Е

В работе применяется генерирующей координаты (+ обобщенное гауссово приблежение) для получения квантового гамильтониана, описывающего квадрупольные коллективные движения атомного ядра. Как коллективные переменные применялись три углы Эйлера и два стандартные параметры деформации β и γ. Получены полностью микроскопические выражения на массовый тензор и коллективный потенциал.