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Quasi-relativistic center-of-mass variables in applications

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Collective center-of-mass variables are introduced in the Lagrangian formalism of the relativistic classical mechanics of directly interacting particles. It is shown that the transition to the Hamiltonian formalism leads to the Bakamjian-Thomas model. The quantum-mechanical system consisting of two spinless particles is investigated. Quasi-relativistic corrections to the discrete energy spectrum are calculated for some Coulomb-like interactions having field theoretical analogues.

Key words: *quasi-relativistic mechanics, center-of-mass variables, Schrödinger equation*

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1. Introduction

There are two types of classical relativistic direct interaction theories (RDIT), namely, manifestly Poincaré-invariant four-dimensional formulations and three-dimensional approaches [1]. Applying each of them to the description of real physical N-particle systems we come across the problem of space-time interpretation of some formal constructions. In four-dimensional approaches difficulties are caused by the presence of redundant variables specific to many-time formalisms and in three-dimensional ones they are caused by the so-called no-interaction theorem. In the relativistic Hamiltonian mechanics, this theorem forbids identification (in the interaction zone) of canonical variables ${q_a}^i$ with physical (covariant) position coordinates ${x_a}^i$ ($a = \overline{1,N}$; $i = 1, 2, 3$) which transform as a space part of the events in the Minkowski space-time [2]. In the Lagrangian formulation [1,3–5] the no-interaction theorem asserts that the interaction Lagrangian depends inevitably on all higher time derivatives ${\overset{s}{x}_a}{}^i = \mathrm{d}^s {x_a}^i/\mathrm{d}t^s$, $s = 1, 2\ldots$, of the physical particle coordinates. This theorem is essentially related to the use of individual particle variables (PV) in both the Hamiltonian and Lagrangian approaches.

In papers [1,3–6] the following approach to the construction of RDIT was proposed. The starting point is the 3-dimensional Poincaré-invariant Lagrangian formalism [1,3] with using the physical coordinates ${x_a}^i$ and with allowing the connection to field theories via the Fokker-type formalism [6]. These aspects of the Lagrangian description along with the possibility to use the Nöther theorem for obtaining the conservation laws [4] are the main advantages of this approach from the point of view of the physical interpretation of the theory. The next step is a transition to the canonical Hamiltonian formalism admitting the quantization of the theory [5,7].

Another aspect of RDIT is the problem of how to separate the motion of the system as a whole from the internal motion of its constituents. This problem can be solved in a manner similar to that of the non-relativistic mechanics case by introducing center-of-mass variables (CMV). Relativistic generalization of the non-relativistic notion of the center-of-mass is ambiguous. The most frequently used are, firstly, the center-of-inertia (covariant center-of-mass) whose coordinates R^i are transformed by the Poincaré group as 3-coordinates of the Minkowski-space points, and, secondly, the center-of-spin (or canonical center-of-mass) with the canonical coordinates Q^i [8,9]. External variables Q^i and P_i describing the motion of a system as a whole, along with the corresponding set $({q_b}^i, p_{bi})$, $b = \overline{1, N-1}$ of $6(N-1)$ internal variables are often used in the relativistic Hamiltonian mechanics [10]-[13].

In the relativistic Lagrangian formalism it is natural to choose the coordinates of the center-of-inertia $\mathbf{R}$ as external position variables and to formulate the problem of constructing the relativistic Lagrangian mechanics of an N-particle system in terms of CMV. This set also contains $3(N-1)$ internal variables ${\rho_b}^i$ [14]-[17]. The internal variables ${\rho_b}^i$ may be introduced by postulating their transformation properties with respect to the Poincaré group. The corresponding relations which are written down in section 2 constitute the prerequisites which enable us to find a connection between CMV and PV and, accordingly, between the relativistic Lagrangians in terms of these two classes of variables. An important feature of CMV is the existence of the Poincaré-invariant interaction Lagrangians which depend only on a finite number of time derivatives (section 3). The transition to the Hamiltonian formalism (section 4) leads to the well-known Bakamjian-Thomas model supplemented by the relations between the canonical variables and the physical particle positions. In sections 5 and 6 the first-order quasi-relativistic approximation (up to c^{-2} terms) is considered from both the classical and the quantum mechanical viewpoints. Relativistic corrections to the energy spectrum of a two-particle system with Coulomb-like interactions are calculated as an illustration.

2. Realization of the Poincaré group $\mathcal{P}(1,3)$ in terms of the Lagrangian CMV

Since the external variables R^i describe the motion of an N-particle system as a whole, we require their transformation properties with respect to the Poincaré group to be the same as those of the physical coordinates ${x_a}^i$ of a single point particle. In the instant form of dynamics [3,1] they are [14,17]:

$$\mathcal{H}R_i = \dot{R}_i\,, \qquad \mathcal{P}_iR_j = \delta_{ij}\,, \quad \mathcal{J}_iR_j = -\varepsilon_{ijk}R_k\,, \tag{2.1}$$
$$\mathcal{K}_iR_j \;=\; -t\delta_{ij} + c^{-2}R_i\dot{R}_j\,. \tag{2.2}$$

Here $\mathcal{H} := D - \partial/\partial t$, $\mathcal{P}_i$, $\mathcal{J}_i$, and $\mathcal{K}_i$ are generators of time and space translations, space rotations, and boosts, respectively, and D is the total time derivation operator. As usual, the dot denotes the time derivation (e.g., $\dot{R}_i = DR_i$ are the components of the external velocity $\dot{\mathbf{R}}$). We postulate further that similar to the case of non-relativistic mechanics the internal CMV ${\rho_b}^i$ are the components of the translationally invariant 3-vectors $\boldsymbol{\rho}_b$ ($b = \overline{1, N-1}$) which do not depend explicitly on time:

$$\mathcal{H}\rho_{bi} = \dot{\rho}_{bi}\,, \quad \mathcal{P}_i\rho_{bj} = 0\,, \quad \mathcal{J}_i\rho_{bj} = -\varepsilon_{ijk}\rho_{bk}\,. \tag{2.3}$$

The transformation of these variables with respect to boosts is determined by the Poincaré group structure. It can be shown that the commutation relations of the Poincaré algebra $\mathcal{AP}(1,3)$, along with equations (2.1)–(2.3), lead to the following conditions [14,17]:

$$\mathcal{K}_i\rho_{bj} = c^{-2}\left(R_i\dot{\rho}_bj + \dot{R}_i\rho_{bj} - \delta_{ij}(\dot{\mathbf{R}}\boldsymbol{\rho}_{\mathbf{b}})\right)\,. \tag{2.4}$$

The expressions for generators $\mathcal{X}_\alpha = \{\mathcal{H}, \mathcal{P}_i, \mathcal{J}_i, \mathcal{K}_i\}$ of the Poincaré group in terms of CMV may be obtained from equations (2.1)–(2.4) immediately [14].

3. Poincaré-invariance of the Lagrangian description

The evolution of a particle system is described by the solutions of the Euler-Lagrange-Ostrogradsky equations

$$\sum_{s=0}^{\infty}(-D)^s\frac{\partial L}{\partial \overset{s}{z}_\nu} = 0\,, \quad \{z_\nu\} = \{R_i, \rho_{bj}\}, \tag{3.1}$$

following from the variational principle $\delta\int L\mathrm{d}t = 0$. The conditions of Poincaré invariance of equations (3.1) may be expressed by the system of first-order differential equations for the Lagrange function:

$$\mathcal{X}_\alpha L = D\Omega_\alpha\,, \tag{3.2}$$

where the auxiliary functions Ω_α have to satisfy the compatibility conditions:

$$\mathcal{X}_\alpha\Omega_\beta - \mathcal{X}_\beta\Omega_\alpha = {c_{\alpha\beta}}^\gamma\Omega_\gamma\,, \tag{3.3}$$

with ${c_{\alpha\beta}}^\gamma$ being the structure constant tensor of the Poincaré group $\mathcal{P}(1,3)$. For this group the relations (3.3) admit the following set of functions Ω_α:

$$\Omega_{\mathcal{H}} = L\,, \quad \Omega_{\mathcal{P}_i} = 0\,, \quad \Omega_{\mathcal{J}_i} = 0\,, \quad \Omega_{\mathcal{K}_i} = c^{-2}R_iL\,. \tag{3.4}$$

In which case the conditions (3.2) of Poincaré invariance take on the form:

$$\mathcal{P}_i L = 0\,, \qquad \mathcal{J}_i L = 0\,, \quad (\mathcal{H} - D)L \equiv -\frac{\partial L}{\partial t} = 0\,,$$
$$(\mathcal{K}_i - c^{-2} R_i D)L - c^{-2}\dot{R}_i L = 0\,. \tag{3.5}$$

The structure of equations (3.5) is quite different from the structure of the Poincaré invariance conditions in terms of PV ${x_a}^i$ [3,4]. Whereas the interaction Lagrangian as a function of the particle variables is defined on $J^\infty\pi$, equations (3.5) admit Lagrangians that depend on CMV and their time derivatives of finite orders. The simplest structure of L is given by

$$L(\dot{\mathbf{R}}, \ddot{\mathbf{R}}, \boldsymbol{\rho}_b, \dot{\boldsymbol{\rho}}_b) = \Gamma^{-1} F(\boldsymbol{\alpha}_b, \boldsymbol{\beta}_b, \boldsymbol{\gamma})\,, b = \overline{1, N-1}; \tag{3.6}$$

here $\Gamma^{-1} = \sqrt{1 - c^{-2}\dot{\mathbf{R}}^2}$ and F is an arbitrary function of scalar products of the vectors

$$\boldsymbol{\alpha}_b \;=\; \boldsymbol{\rho}_b + c^{-1}\Gamma[\dot{\mathbf{R}}\boldsymbol{\rho}_b]\,, \qquad \boldsymbol{\beta}_b = \Gamma\dot{\boldsymbol{\alpha}}_b - c^{-1}\Gamma^2[\ddot{\mathbf{R}}\boldsymbol{\alpha}_b]\,, \tag{3.7}$$
$$\boldsymbol{\gamma} \;=\; \Gamma\ddot{\mathbf{R}} + c^{-1}\Gamma^2[\dot{\mathbf{R}}\ddot{\mathbf{R}}] + c^{-2}\Gamma(\dot{\mathbf{R}}\ddot{\mathbf{R}})\dot{\mathbf{R}}\,. \tag{3.8}$$

Contrary to $\boldsymbol{\alpha}_b$ and $\boldsymbol{\beta}_b$, the $\boldsymbol{\gamma}$ dependence of L is not necessary. The Lagrangian (3.6) depending on a finite number of CMV can be made equivalent to the Lagrangian defined on an infinite-dimensional set of PV $\overset{s}{x}_a{}^i$, only if the CMV are functions of all these PV. The set of equations (2.1)–(2.4) with generators $\mathcal{H}$, $\mathcal{P}_i$, $\mathcal{J}_i$, and $\mathcal{K}_i$, determined in terms of PV [3,4], may be regarded as the basis for determining these functions [17].

Using the Nöther theorem for Lagrangians with higher derivatives [1]-[4] we found ten integrals of motion $(E, \mathbf{P}, \mathbf{J}, \mathbf{K})$ corresponding to the Poincaré-invariance of the theory, based on Lagrangian (3.6). From their analysis we obtain [14,17] the following equation of external motion

$$M\mathbf{R} + c^{-2}[\dot{\mathbf{R}}, \mathbf{s}] = \mathbf{K}_0 \tag{3.9}$$

in the rest frame of reference ($E = E_0 = Mc^2$, $\mathbf{P} = 0$, $\mathbf{J} = \mathbf{s}$, $\mathbf{K} = \mathbf{K}_0$)). It should be noted that the equation

$$M\ddot{\mathbf{R}} + c^{-2}[\dddot{\mathbf{R}}, \mathbf{s}] = 0\,, \tag{3.10}$$

being the consequence of (3.9), was obtained in [18] for classical particles with a spin; it is a three-dimensional form of the well-known Mathisson equation. Spin $\mathbf{s}$ is equal to the internal angular momentum of the system.

Solving (3.9) in a coordinate system with the origin at point $\mathbf{R}_0 = \mathbf{K}_0/M$, where $\mathbf{K}_0$ is the value of integral $\mathbf{K}$ in the rest frame and the Oz axis is directed along spin $\mathbf{s}$, we see that point $\mathbf{R}(t)$ describes a circular motion in a plane orthogonal to the spin:

$$R_x(t) = A\sin(\omega_0 t - \alpha)\,, \quad R_y(t) = A\cos(\omega_0 t - \alpha)\,, \quad R_z = 0\,. \tag{3.11}$$

Here, frequency $\omega_0 = Mc^2/s$; A and α are constants of the integration. Taking into account the usual non-relativistic limit procedure, in accordance with which the center of mass is at rest as measured in the rest frame, we must set $A = 0$. Indeed, as $c^{-2} \to 0$ ($\omega_0 \to \infty$), the limits of the trigonometric functions in equation (3.11) do not exist. This means that in the set of solutions of equations (3.1) for the Lagrangian (3.6) we keep only those which satisfy the standard free-particle equation $\ddot{\mathbf{R}} = 0$.

4. The Hamiltonian description

There are several ways to obtain the Hamiltonian formulation corresponding to the Lagrangians with higher derivatives and with supplementary conditions, like $\ddot{\mathbf{R}} = 0$ [7,19,20]. Here we use an approach close to that of [19]. Let us perform a change of the variables $(\mathbf{R}, \boldsymbol{\rho}_b) \mapsto (\mathbf{Q}, \mathbf{q}_b)$, where

$$\mathbf{Q} = \mathbf{R} + \frac{[\mathbf{P}, \mathbf{s}]}{M(E + Mc^2)}, \tag{4.1}$$

$$\mathbf{q}_b = \Gamma \boldsymbol{\rho}_b - \frac{c^{-2}\Gamma^2}{\Gamma + 1} \dot{\mathbf{R}}(\dot{\mathbf{R}}\boldsymbol{\rho}_b). \tag{4.2}$$

Relation (4.1) is a definition of the canonical center-of-mass [8]. In terms of new variables, the Lagrangian (3.6) has the form:

$$L(\dot{\mathbf{R}}, \ddot{\mathbf{R}}, \boldsymbol{\rho}_b, \dot{\boldsymbol{\rho}}_b) = L(\dot{\mathbf{Q}}, 0, \mathbf{q}_b, \dot{\mathbf{q}}_b) + L' \equiv \tilde{L}(\dot{\mathbf{Q}}, \mathbf{q}_b, \dot{\mathbf{q}}_b) + L', \tag{4.3}$$

where L' contains only the terms which do not contribute to the equations of motion if the external equation of motion $\ddot{\mathbf{R}} = 0$ is satisfied. Therefore, the term L' may be omitted in equation (4.3) and, thus, the transformation to the Hamiltonian description may be performed in the usual manner on the basis of Lagrangian $\tilde{L}$. Using the Legendre transformation we construct Hamiltonian H corresponding to Lagrangian $\tilde{L}$:

$$H = \sqrt{c^2\mathbf{P}^2 + M^2(\mathbf{q}_b, \boldsymbol{\pi}_b)c^4}, \tag{4.4}$$

where

$$\mathbf{P} = \frac{\partial \tilde{L}}{\partial \dot{\mathbf{Q}}}, \quad \boldsymbol{\pi}_b = \frac{\partial \tilde{L}}{\partial \dot{\mathbf{q}}_b}, \quad Mc^2 = \sum_{b=1}^{N-1} \boldsymbol{\beta}_b \frac{\partial F}{\partial \boldsymbol{\beta}_b} - F \bigg|_{\ddot{\mathbf{R}}=0}. \tag{4.5}$$

We note that the external momentum variable $\mathbf{R}$ is a motion integral (the total momentum of the system).

Expression (4.4) for H reproduces the particle-system Hamiltonian of the Bakamjian-Thomas model [10]. The advantage of our way of constructing this model is the possibility to express the internal Hamiltonian $M(\mathbf{q}_b, \boldsymbol{\pi}_b)$ in terms of the interaction Lagrangian which, in turn, may be related to some field models [6]. On the other hand, in our approach the canonical variables $\mathbf{Q}, \mathbf{P}, \mathbf{q}_b$, and $\boldsymbol{\pi}_b$ have a definite relation to the Lagrangian CMV $\mathbf{R}$, $\boldsymbol{\rho}_b$ and their time derivatives $\dot{\mathbf{R}}$, $\dot{\boldsymbol{\rho}}_b$ and, therefore, to the individual particle variables $\mathbf{x}_a$, at least in the approximations in the parameter c^{-2}.

5. Quasi-relativistic approximation

Let us consider the main steps of our approach in the first-order approximation in c^{-2} (i.e. quasi-relativistic or post-Newtonian approximation). We use the following sufficiently general form of a quasi-relativistic two-particle Lagrangian with static non-relativistic potential $U(r)$ [21,1,4]:

$$\begin{aligned} L &= \sum_{a=1}^{2}\left(\frac{m_a v_a^2}{2}+\frac{m_a v_a^4}{8c^2}\right)-U(r)-\frac{1}{2c^2}\Big((-\mathbf{v}_1\mathbf{v}_2+2Av^2)U(r)+ \\ &+ \left((\mathbf{r}\mathbf{v}_1)(\mathbf{r}\mathbf{v}_2)+2B(\mathbf{r}\mathbf{v})^2\right)\frac{1}{r}\frac{\mathrm{d}U}{\mathrm{d}r}+2u_1(r)\Big)\,, \end{aligned} \tag{5.1}$$

where $\mathbf{r}=\mathbf{x}_1-\mathbf{x}_2, \mathbf{v}=\mathbf{v}_1-\mathbf{v}_2$, A and B are arbitrary constants and $u_1(r)$ is an arbitrary function. For interactions which correspond to the linear field theories, we have $u_1(r)=0$ and constants A and B depend on the tensor structure of interaction [1,21]. For example, we have $A=B=0$ for a vector interaction, and $A=-1, B=0$ for a scalar interaction.

Further we consider a specific case of interactions which correspond to the non-relativistic long-range potential

$$U(r)=\frac{\alpha}{r}\,, \tag{5.2}$$

where α is a constant of the interaction. We suppose that the Galileo-invariant function $u_1(r)$ has the form:

$$u_1(r)=\frac{\alpha_1}{r^2}\,, \tag{5.3}$$

where α_1 is the constant. Let us note five significant cases covered by the interaction described in a quasi-relativistic approximation by the Lagrangian of type (5.1) where functions (5.2) and (5.3) enter:

- $\alpha=e_1e_2, A=B=0$, and $\alpha_1=0$: the Darwin Lagrangian which describes an electromagnetic interaction of two point charges;

- $\alpha=-Gm_1m_2, 2A=3, B=0$, and $2\alpha_1=G^2m_1m_2m(m=m_1+m_2)$: the Einstein-Infeld-Hoffmann Lagrangian which describes a gravitational interaction of two point masses;

- $\alpha=e_1e_2-Gm_1m_2, 2A=-3Gm_1m_2/\alpha, B=0$, and $2\alpha_1=G(Gm_1m_2m+e_1^2m_2+e_2^2m_1-2e_1e_2m)$: a gravitational interaction of charged bodies (the Bażański Lagrangian [22]);

- $\alpha=-Gm_1m_2, 2A=1+2\gamma, B=0$, and $2\alpha_1=(2\beta-1)G^2m_1m_2m$: a gravitational interaction in the PPN-formalism [23] which classifies suitable theories of gravitation (i.e. those which do not contradict the four classical experiments, satisfy the conditions of the Lorentz-invariance, and admit N-particle Lagrangian functions) in the first-order approximation in c^{-2};

- $\alpha = -Gm_1m_2, A = -2B = 1$, and $\alpha_1 = 0$: the Lagrangian of the quasi-relativistic approximation of the Whitehead-Shield theory of gravitation [24] where the massless tensor field of the second rank as an intermediate field is assumed.

The correspondence between CMV and PV for a two-particle system in the first-order quasi-relativistic approximation has the following form [17] :

$$\begin{aligned}\mathbf{x}_a &= \mathbf{R} + (-1)^b\frac{m_b}{m}\boldsymbol{\rho} + \frac{1}{c^2}\left\{(-1)^b\frac{m_b}{m}\left(\frac{1}{2}\dot{\mathbf{R}}^2\boldsymbol{\rho} - (\dot{\mathbf{R}}\boldsymbol{\rho})\dot{\mathbf{R}}\right) - \right.\\ &- \left.\frac{m_b^2}{m^2}(\dot{\mathbf{R}}\boldsymbol{\rho})\dot{\boldsymbol{\rho}} + \frac{m_1 - m_2}{2m^2}\left(\mu\dot{\boldsymbol{\rho}}^2 + U(\rho)\right)\boldsymbol{\rho}\right\}, \qquad (5.4)\end{aligned}$$

where $a, b = 1, 2, b \neq a, m = m_1 + m_2, \mu = m_1m_2/m$. Using these relations in the Lagrangian (5.1) leads to the following two-particle quasi-relativistic Lagrangian in terms of CMV:

$$\begin{aligned}L &= \frac{m\dot{\mathbf{R}}^2}{2} + \frac{\mu\dot{\boldsymbol{\rho}}^2}{2} - U(\rho) + \frac{m\dot{\mathbf{R}}^4}{8c^2} + \frac{\mu\dot{\boldsymbol{\rho}}^4}{8c^2}\left(1 - \frac{3\mu}{m}\right) + \frac{3\mu}{4c^2}\dot{\mathbf{R}}^2\dot{\boldsymbol{\rho}}^2 - \\ &- \frac{\mu}{2c^2}(\dot{\mathbf{R}}\dot{\boldsymbol{\rho}})^2 + \frac{\mu}{c^2}\left(\dot{\mathbf{R}}[\boldsymbol{\rho}[\ddot{\mathbf{R}}\dot{\boldsymbol{\rho}}]]\right) + \frac{1}{2c^2}\left\{\left(\dot{\mathbf{R}}^2 - \left(\frac{\mu}{m} + 2A\right)\dot{\boldsymbol{\rho}}^2\right)U(\rho) + \right.\\ &+ \left.\left(\left(\frac{\mu}{m} - 2B\right)(\boldsymbol{\rho}\dot{\boldsymbol{\rho}})^2 - [\dot{\mathbf{R}}\boldsymbol{\rho}]^2\right)\frac{1}{\rho}\frac{\mathrm{d}U}{\mathrm{d}\rho}\right\} - \frac{1}{c^2}u_1(\rho)\,. \qquad (5.5)\end{aligned}$$

This expression agrees with the corresponding approximation of the Lagrangian (3.6).

In the quasi-relativistic approximation the canonical external variable (4.1) becomes

$$\begin{aligned}\mathbf{Q} &= \mathbf{R} + \left.\frac{[\mathbf{P}, \mathbf{s}]}{M(E + Mc^2)}\right|_{\ddot{\mathbf{R}}=0} \equiv \\ &\equiv \mathbf{R} + \frac{\mu}{2mc^2}\left[\dot{\mathbf{R}}[\boldsymbol{\rho}\dot{\boldsymbol{\rho}}]\right]. \qquad (5.6)\end{aligned}$$

The total momentum

$$\mathbf{P} = \mathbf{P}|_{\ddot{\mathbf{R}}=0} \equiv \frac{E}{c^2}\dot{\mathbf{R}} \qquad (5.7)$$

is canonically conjugated to $\mathbf{Q}$. Quasi-relativistic inner canonical variables are defined by the relations

$$\mathbf{q} = \boldsymbol{\rho} + \frac{\left[\dot{\mathbf{R}}[\boldsymbol{\rho}\dot{\boldsymbol{\rho}}]\right]}{2c^2} + \frac{1}{\mu c^2}\frac{\partial\lambda}{\partial\dot{\boldsymbol{\rho}}}, \qquad (5.8)$$

$$\boldsymbol{\pi} = \left(1 - \frac{\dot{\mathbf{R}}^2}{2c^2}\right)\frac{\partial L}{\partial\dot{\boldsymbol{\rho}}} - \frac{1}{c^2}\frac{\partial\lambda}{\partial\boldsymbol{\rho}}, \qquad (5.9)$$

where $\lambda(\boldsymbol{\rho}, \dot{\boldsymbol{\rho}})$ is an arbitrary Galileo-invariant function. Choosing this function in the form

$$\lambda(\boldsymbol{\rho}, \dot{\boldsymbol{\rho}}) = (\boldsymbol{\rho}\dot{\boldsymbol{\rho}}) \left(\frac{\mu \dot{\boldsymbol{\rho}}^2}{8} \left(1 - \frac{3\mu}{m}\right) + \frac{1}{4}\left(1 - \frac{\mu}{m} - 4B\right) U(\rho) \right), \tag{5.10}$$

we obtain the Hamiltonian function depending on the square of the inner momentum $\boldsymbol{\pi}$ and therefore being convenient for quantization:

$$H = \frac{\mathbf{P}^2}{2m} - \frac{\mathbf{P}^2}{2m^2c^2}\left(\frac{\boldsymbol{\pi}^2}{2\mu} + U(q)\right) - \frac{\mathbf{P}^4}{8m^3c^2} + \frac{\boldsymbol{\pi}^2}{2\mu(q)} + v(q)\,. \tag{5.11}$$

Here

$$\frac{1}{\mu(q)} = \frac{1}{\mu} + \frac{1}{4\mu^2c^2}\left\{2\left(1 + \frac{\mu}{m} + 4A - 4B\right)U(q) - \left(1 - \frac{3\mu}{m}\right) q\frac{dU}{dq}\right\} \tag{5.12}$$

and

$$v(q) = U(q) + \frac{1}{c^2}\left\{u_1(q) - \frac{1}{4\mu}\left(1 - \frac{\mu}{m} - 4B\right) U(q) q\frac{dU}{dq}\right\}. \tag{5.13}$$

6. Quasi-relativistic Schrödinger equation

Starting with the Hamiltonian function (5.11) we write down the stationary Schrödinger equation:

$$(\hat{H} - E)\langle \mathbf{Q}, \mathbf{q} \mid E, \mathbf{P}\rangle = 0\,. \tag{6.1}$$

The total wave function $\langle \mathbf{Q},\mathbf{q}|E,\mathbf{P}\rangle$ of the system is equal to the product $\Psi(\mathbf{Q})\psi(\mathbf{q})$ of the external wave function $\Psi(\mathbf{Q})$ and the inner one $\psi(\mathbf{q})$. We consider the states with sharply defined total momentum $\mathbf{P}$, so the external wave function is then a plane wave, $\Psi(\mathbf{Q}) = \exp(i\mathbf{kQ})$, where the wave vector $\mathbf{k} = \mathbf{P}/\hbar$. Due to the separation of the external and internal variables in equation (6.1), we obtain the following wave equation:

$$(\hat{h} - \mathcal{E})\psi(\mathbf{q}) = 0\,, \tag{6.2}$$

where

$$\mathcal{E} = E - \frac{P^2}{2m} + \frac{EP^2}{2m^2c^2} - \frac{P^4}{8m^3c^2}\,. \tag{6.3}$$

Here E and $\mathbf{P}$ are eigenvalues of the non-relativistic Hamiltonian and total momentum operators, respectively.

The internal Hamiltonian operator is defined by the formula

$$\hat{h} = \frac{1}{2}\hat{X} + v(q)\,, \tag{6.4}$$

where the first term is some Hermitian operator which corresponds to the classical function $\pi^2/\mu(q) \equiv a(q)\pi^2$. We use the following sufficiently general quantization rule:

$$\hat{X} = a(q)\hat{\pi}^2 + \delta^{ij}[\hat{\pi}_i, a(q)]\hat{\pi}_j + \lambda\hat{\pi}^2(a(q))\,, \tag{6.5}$$

where the inner momentum operator is chosen in the usual form:

$$\hat{\pi}_i = -i\hbar\frac{\partial}{\partial q^i}\,; \qquad \hat{\pi}^2 = -\hbar^2\Delta\,. \tag{6.6}$$

This rule preserves the rotational invariance of the inner Hamiltonian and depends on one parameter $\lambda \in \mathbb{R}$. The value $\lambda = 1/2$ corresponds to the symmetrization $(\hat{\pi}^2 a(q) + a(q)\hat{\pi}^2)/2$.

To illustrate our approach we consider the Coulomb-like potential (see equations (5.2) and (5.3)). In this case the functions $a(q) := \mu^{-1}(q)$ and $v(q)$ take the form:

$$a(q) = \frac{1}{\mu}\left(1 + \frac{1}{\mu c^2}C_1\frac{\alpha}{q}\right), \quad C_1 = \frac{3}{4} - \frac{\mu}{4m} + 2A - 2B\,, \tag{6.7}$$

$$v(q) = \frac{\alpha}{q}\left(1 + \frac{1}{\mu c^2}C_2\frac{\alpha}{q}\right), \quad C_2 = \frac{1}{4} - \frac{\mu}{4m} - B + \frac{\mu\alpha_1}{\alpha^2}\,. \tag{6.8}$$

Here $\mu = m_1 m_2/m$ and the parameters A, B, α_1, and α are defined by the type of interaction (see section 5).

After some calculations we arrive at the following Hamiltonian operator:

$$\hat{h} = \frac{\hbar^2}{2}\left(-\frac{1}{\mu(q)}\Delta + \frac{\alpha}{\mu^2 c^2}C_1\frac{\mathbf{q}}{q^3}\frac{\partial}{\partial\mathbf{q}} + \frac{4\pi\alpha\lambda}{\mu^2 c^2}C_1\delta(\mathbf{q})\right) + v(q)\,, \tag{6.9}$$

where π denotes a well-known transcendental number instead of the value of the inner momentum.

We shall study the discrete spectrum of H, when $\alpha < 0$. The use of methods of the perturbation theory (e.g., see [25]) allows us to obtain quasi-relativistic corrections to the non-relativistic Bohr expression

$$\mathcal{E}_n^{(0)} = -\frac{\mu\alpha^2}{2\hbar^2}\frac{1}{n^2}\,, \tag{6.10}$$

where n is the main quantum number. Let us rewrite the Hamiltonian operator (6.9) in the form

$$\hat{h} = \frac{\mu}{\mu(q)}\hat{h}^{(0)} + \frac{C_2 - C_1}{\mu c^2}\frac{\alpha^2}{q^2} + \frac{\hbar^2}{2}\frac{\alpha}{\mu^2 c^2}C_1\left(\frac{\mathbf{q}}{q^3}\frac{\partial}{\partial\mathbf{q}} + 4\pi\lambda\delta(\mathbf{q})\right)\,, \tag{6.11}$$

where

$$\hat{h}^{(0)} = -\frac{\hbar^2}{2\mu}\Delta + \frac{\alpha}{q} \tag{6.12}$$

is a non-relativistic energy operator possessing spectrum (6.10). According to the stationary perturbation theory [25], the quasi-relativistic term $\mathcal{E}_{nl}^{(1)}$ is equal to the matrix element

$$\mathcal{E}_{nl}^{(1)} = \int \mathrm{d}^3 q\, \psi_{nlm}^{*(0)}(\mathbf{q}) V \psi_{nlm}^{(0)}(\mathbf{q}) \equiv \langle V\rangle_0\,, \tag{6.13}$$

where $\psi^{(0)}_{nlm}(\mathbf{q})$ are the eigenfunctions of operator (6.12) and

$$V = \frac{1}{\mu c^2} C_1 \frac{\alpha}{q} \hat{h}^{(0)} + \frac{C_2 - C_1}{\mu c^2} \frac{\alpha^2}{q^2} + \frac{\hbar^2}{2} \frac{\alpha}{\mu^2 c^2} C_1 \left(\frac{\mathbf{q}}{q^3} \frac{\partial}{\partial \mathbf{q}} + 4\pi\lambda\delta(\mathbf{q}) \right) , \tag{6.14}$$

is a quasi-relativistic perturbation of the non-relativistic energy operator (6.12). While calculating (6.13) we take into consideration that $\psi^{(0)}_{nlm}(\mathbf{q})$ are the eigenfunctions of $\hat{h}^{(0)}$. We also use the average values of the following functions of $\mathbf{r} = \mathbf{q}$ [25]:

$$\langle r^{-1} \rangle_0 = -\frac{\mu\alpha}{\hbar^2} \frac{1}{n^2} , \qquad \langle r^{-2} \rangle_0 = \frac{\mu^2 \alpha^2}{\hbar^4} \frac{2}{n^3(2l+1)},$$
$$\langle \delta(\mathbf{r}) \rangle_0 = |\psi^{(0)}_{nlm}(0)|^2 = \frac{\mu^3 |\alpha|^3}{\pi \hbar^6 n^3} \delta_{0l} \, . \tag{6.15}$$

One can easily check that the average value is

$$\int \mathrm{d}^3 q \psi^{*(0)}_{nlm}(\mathbf{q}) \frac{\mathbf{q}}{q^3} \frac{\partial}{\partial \mathbf{q}} \psi^{(0)}_{nlm}(\mathbf{q}) = 2\pi |\psi^{(0)}_{nlm}(0)|^2. \tag{6.16}$$

Therefore, the quasi-relativistic correction to the energy spectrum is given by

$$\mathcal{E}^{(1)}_{nl} = \frac{\mu\alpha^4}{2\hbar^4 c^2} \frac{1}{n^3} \left(\frac{C_1}{n} - \frac{4(C_1 - C_2)}{2l+1} - (2\lambda - 1) \frac{2C_1}{n^3} \delta_{0l} \right) . \tag{6.17}$$

We note a dependence of the obtained spectrum on the quantization parameter λ.

For the case of an electromagnetic interaction, when the parameters $A = B = 0$, $\alpha_1 = 0$ (see section 5), spectrum (6.17) agrees with the results of the conventional quantum electrodynamics provided that $\lambda = 1/2$. Let us consider a hydrogen-like atom. Then the constant of interaction $\alpha = -Ze^2$, where Ze is the charge of the nucleus. Since the mass of the nucleus is much greater than the rest mass of electron m_e, we have $\mu \to m_e$ and, therefore, the ratio $\mu/m \to 0$. Here m is the total mass of the atom. Introducing these parameters into equations (6.7) and (6.8) we obtain $C_1 = 3/4$ and $C_2 = 1/4$. According to equation (6.17), the quasi-relativistic correction is equal to

$$\mathcal{E}^{(1)}_{nl} = \frac{m_e (Ze^2)^4}{\hbar^4 c^2} \frac{1}{n^4} \left(\frac{3}{8} - \frac{n}{2l+1} \right) . \tag{6.18}$$

It is in good agreement with the quasi-relativistic correction to the hydrogen-like spectrum which follows from the Dirac equation (see [25, p.216]).

Now let us consider parapositronium. The mass of an electron is equal to the mass of a positron and, therefore, $\mu = m_e/2$ and the ratio $\mu/m = 1/4$. Whence the constants $C_1 = 11/16$ and $C_2 = 3/16$. Putting these parameters into equations (6.17) we re-obtain an expression for the quasi-relativistic splitting of the parapositronium spectrum which is conventionally found by using the Breit equation [26]:

$$\mathcal{E}^{(1)}_{nl} = \frac{m_e (e^2)^4}{2\hbar^4 c^2} \frac{1}{n^3} \left(\frac{11}{32n} - \frac{1}{2l+1} \right) . \tag{6.19}$$

7. Conclusions

The transformation of particle variables into center-of-mass ones for a class of two-particle quasi-relativistic Lagrangians with interactions having field-theoretical analogues has been carried out. As a result, the motion of a system as a whole was separated from its inner motion. A set of canonical variables in terms of which the Hamiltonian has a quadratic dependence on the inner momentum variable is found. The problem is quantized. The quasi-relativistic splitting of the discrete energy spectrum is obtained. As expected, the degeneracy in the orbital quantum number is eliminated.

In the specific case of an electromagnetic interaction between particles, the quasi-relativistic corrections to the non-relativistic discrete spectrum are in agreement with the corresponding approximation of the spectrum of a hydrogen-like atom obtained by using the Dirac equation (modulus of the spin of the electron which was not taken into account). For parapositronium (where the summary spin is equal to zero) the spectrum obtained within the frame of the CMV-formalism coincides with the one derived by using the Breit equation.

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Квазірелятивістичні змінні центра мас у застосуваннях

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У лаґранжевому формалізмі релятивістичної класичної механіки прямо взаємодіючих частинок введені колективні змінні центра мас. Показано, що відповідний гамільтонів формалізм веде до моделі Бакамджіяна–Томаса. Вивчається квантово-механічна система із двох безспінових частинок. Для низки кулоноподібних взаємодій, що мають теоретико-польові аналоги, підраховано квазірелятивістичні поправки до дискретного енерґетичного спектру.

Ключові слова: *квазірелятивістична механіка, змінні центра мас, рівняння Шредінґера*

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