ON THE TWO-BODY PROBLEM IN QUANTUM MECHANICS

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Following the representation of a two-body system in classical mechanics, we build up a quantum picture which is free of spurious effects and retains the intrinsic features of the internal bodies. In the coordinate space the system is represented by the real particles, individually bound to a center of forces which in a certain limit coincides with the center of mass and the wave function writes as product of the individual wave functions with correlated arguments.

Key words: bound systems, center of mass states, constrained systems.

1. THE CENTER OF MASS PROBLEM

The usual approaches to the two body problem in classical and quantum mechanics (see, for instance, [1, 2] pp. 306–308) start with the replacement of the particle position vectors \( \mathbf{r}_1, \mathbf{r}_2 \) and momenta \( \mathbf{p}_1, \mathbf{p}_2 \) by the center of mass variables

\[
\mathbf{R} = \frac{m_1}{m_1 + m_2} \mathbf{r}_1 + \frac{m_2}{m_1 + m_2} \mathbf{r}_2
\]

\[
\mathbf{P} = \mathbf{p}_1 + \mathbf{p}_2
\]

(1)

and the relative ones

\[
\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2
\]

\[
\mathbf{p} = -\frac{m_2}{m_1 + m_2} \mathbf{p}_1 - \frac{m_1}{m_1 + m_2} \mathbf{p}_2
\]

(2)

where \( m_1 \) and \( m_2 \) are the particle masses. If the interaction potential depends only on the relative distance, the replacement results in the separation of the Hamiltonian \( \mathcal{H} \) in two independent parts:

\[
\mathcal{H} = H_{\text{int}} + H_{\text{CM}}
\]

(3)

where

\[
H_{\text{int}} = \frac{1}{2m_r} \mathbf{p}^2 + V(r)
\]

(4)

and

\[ H_{CM} = \frac{1}{2M} \tilde{P}^2 \]  

(5)

which may be seen as the Hamiltonians of two fictitious particles: a particle with the reduced mass \( m_r = m_1 m_2 / (m_1 + m_2) \) in the external potential \( V(r) \) and a free particle with the mass \( M = m_1 + m_2 \) having the momentum \( \tilde{P} \) and the position vector \( \tilde{R} \) of the center of mass.

Following the usual quantization procedure, the wave function of the two-body system in stationary state is the product of the eigenfunctions of \( H_{int} \) and \( H_{CM} \) and the energy is the sum of the corresponding eigenvalues. As it is well known, a problem arises in connection with the eigenfunctions of \( H_{CM} \), since the attempt to localize the center of mass by imposing adequate boundary conditions violates the invariance at translations and generates an infinite series of spurious states with arbitrary high energy levels. These states have no classical analog and are not the result of a dynamical mechanism. They are spurious and hence have to be separated out from the physical solutions.

The problem has been extensively studied in nuclear many body models [3], where the achievement of a translational invariant, independent particle picture requires a clear separation of the center of mass energy and states from the physical ones. The solution proposed by Lipkin, de Shalit and Talmi [4] is to introduce in the internal Hamiltonian the contribution of the redundant (or superfluous) coordinates which assure the independent treatment of nucleons. These ones generate new spurious states and a new term in the internal Hamiltonian which compensates the kinetic energy of the center of mass in the approximation of equal masses. Finally its contribution has to be subtracted from \( E_{int} \) and the spurious solutions have to be separated out. The separation requires special technics which, excepting the case of the harmonic oscillator, is rather hard to be done (see, e.g., Ref. [3] (par. 11.3), [4–6]).

The existence of spurious states seem to confirm the deeply rooted opinion that the center of mass problem reflects the uncertainty relations and is characteristic to quantum mechanics. Contrary to this belief, we show that the problem may be solved by properly defining the classical system which has to be quantized. We demonstrate that the spurious effects can be eliminated if the rest condition of the bound system is explicitly written as a constraint on the position of the center of mass.

Specifically, we consider the bound system in the rest frame where the center of mass position is fixed, i.e. \( \tilde{R}(t) = \tilde{R}_0 \) and follow Dirac’s Hamilton method of treating the constrained systems (see [7], [8]).

According to Dirac, whenever the “naive” Hamiltonian (in our case the “naive” Hamiltonian is \( H_{CM} \)) is incompatible with the constraints, it has to be
replaced by a right one. To find it, one has to build up the whole algebra generated with the aid of Poisson brackets from the “naive” Hamiltonian and the initial constraints and look for its center, i.e. for the elements whose Poisson brackets with every element of the algebra are zero. If the algebra is closed, there is at least an element with this property. This is either a Casimir invariant of the algebra or another element of its center and represents the right Hamiltonian which guarantees the preservation of constraints, inclusively of the “naive” Hamiltonian.

In the center of mass problem the algebra is generated by $H_{CM}$, the constraint $\bar{R} - \bar{R}_0 = 0$ and the results of the Poisson brackets

$$\{H_{CM}, \bar{R} \} = \frac{1}{M} \bar{P}$$

and

$$\{R_i, P_j \} = \delta_{ij}.$$  \hspace{1cm} (6)

From the above it results that this algebra is closed and, besides the variables $\bar{R}$ and $\bar{P}$, it contains also the identity. The latter and its multiples form the center of this algebra and are the only elements whose Poisson brackets with every element of the algebra are zero. According to our prescription, one of these multiples having the dimension of energy is the right center of mass Hamiltonian. It results that $H_{CM}$ has to be replaced by a constant supposed to be the sum of masses and hence the right Hamiltonian of a two body system at rest reads

$$H = m_1 + m_2 + \frac{1}{2m_r} \bar{P}^2 + V(r).$$ \hspace{1cm} (8)

Obviously, the Poisson brackets of the Hamiltonian $\mathcal{H}$ with all the elements of the above algebra are zero.

Closing the discussion on the center of mass problem, we remark that, unlike the previous approaches to the bound state problem, the center of mass variables are absent form the Hamiltonian $\mathcal{H}$. This is explicitly due to the rest condition $\bar{R} - \bar{R}_0 = 0$ and has important consequences in the quantization process.

2. THE PROBLEM OF THE INTERNAL MOTION

According to the results quoted in the preceding section, the dynamics of the bound system at rest is ruled by $\mathcal{H}$ and the solution of the equations of motion expresses in terms of the relative vector $\tilde{r}$ which has a fixed point: the center of mass.
Introducing the notations \( \mu_1 = m_1/(m_1 + m_2) \), \( \mu_2 = m_2/(m_1 + m_2) \) and denoting by \( \vec{r}_1 \) and \( \vec{r}_2 \) the position vectors of the internal particles with respect to the center of mass we find:

\[
\begin{align*}
\mu_1 \vec{r}_1 + \mu_2 \vec{r}_2 &= 0 \\
\vec{r} &= \vec{r}_1 - \vec{r}_2 \\
\vec{r}_1 &= \mu_2 \vec{p} = (1 - \mu_1) \vec{p} \\
\vec{r}_2 &= -\mu_1 \vec{p} = -(1 - \mu_2) \vec{p}
\end{align*}
\]  

and draw the following representation of the two-body system: the particles are at the ends of a segment of variable length, \( r(t) \), rotating around the center of mass which divides it in two parts, \( r_1(t) \) and \( r_2(t) \), whose length is inverse proportional to the masses \( m_1 \) and \( m_2 \).

On the other hand, we notice that considering the internal particles as distinct physical systems and using the pairs of individual canonical conjugate variables \( r_1, p_1 \) and \( r_2, p_2 \) where \( \vec{r}_1 \) and \( \vec{r}_2 \) satisfy (11) and (12), the Hamiltonian \( \mathcal{H} \) writes as sum of two individual Hamiltonians

\[
\mathcal{H} = H_1 I_2 + H_2 I_1
\]

where

\[
\begin{align*}
H_1 &= m_1 + (1 - \mu_1) H_{int} \bigg|_{r = (1 - \mu_1)^{-1} \vec{r}_1; \vec{p} = (1 - \mu_1) \vec{p}_1} = \\
&= m_1 + \frac{(1 - \mu_1)^2}{2m_1} \vec{p}_1^2 + V_1(\vec{r}_1) \\
H_2 &= m_2 + (1 - \mu_2) H_{int} \bigg|_{r = (1 - \mu_2)^{-1} \vec{r}_2; \vec{p} = (1 - \mu_2) \vec{p}_2} = \\
&= m_2 + \frac{(1 - \mu_2)^2}{2m_2} \vec{p}_2^2 + V_2(\vec{r}_2)
\end{align*}
\]  

and \( I_1 \) and \( I_2 \) are the identity operators on the phase space of the first and second particle respectively.

In the new form, \( \mathcal{H} \) appears as the Hamiltonian of a system made of two particles with the masses \( m_1 \) and \( m_2 \) individually bound to the same center of forces which coincides with the center of mass \( (\vec{r}_1 = \vec{r}_2 = \vec{r} = 0) \) through the external potentials \( V_1(\vec{r}_1) = (1 - \mu_1) V(r) \big|_{r = (1 - \mu_1)^{-1} \vec{r}_1} \) and \( V_2(\vec{r}_2) = (1 - \mu_2) V(r) \big|_{r = (1 - \mu_2)^{-1} \vec{r}_2} \).

For consistency, the position vectors \( \vec{r}_1 \) and \( \vec{r}_2 \) with respect to the center of forces have to satisfy (11) and (12). This guarantees that the real particles have collinear instantaneous position vectors with respect to the center of mass and move on similar trajectories.
Moreover, it can be easily checked that, thanks to the proportionality relations (11) and (12), the sum of the kinetic and potential energy of the first and second particle in the potentials $V_1(r_1)$ and $V_2(r_2)$ respectively is equal to the total energy of the particle with the reduced mass in the potential $V(r)$. Also, the angular momentum of the particle with the reduced mass $\vec{L} = \vec{r} \times \vec{p}$ is equal to $\vec{L}_1 = \vec{r}_1 \times \vec{p}_1$ and $\vec{L}_2 = \vec{r}_2 \times \vec{p}_2$ are the angular momenta of the internal particles with respect to the center of mass.

This is the classical representation of a two-body system which is subject to the quantization procedure.

First we remark that, due to the absence of center of mass variables from the Hamiltonian $\mathcal{H}$, there are no center of mass operators and hence no spurious center of mass states.

According to the quantization procedure, the individual variables $\vec{r}_1, \vec{p}_1$ and $\vec{r}_2, \vec{p}_2$ in $H_1$ and $H_2$ are replaced by the canonical conjugated operators $\vec{r}_1, -i\vec{V}_1$ and $\vec{r}_2, -i\vec{V}_2$ and the real particles are assigned the individual wave functions $\Psi_{v_1}(\vec{r}_1)$ and $\Psi_{v_2}(\vec{r}_2)$ which satisfy the time-independent Schrödinger equations:

$$m_1 - \frac{(1-\mu_1)^2}{2m_1} \vec{V}_1 \Psi_{v_1}(\vec{r}_1) = 0 \quad (16)$$
$$m_2 - \frac{(1-\mu_2)^2}{2m_2} \vec{V}_2 \Psi_{v_2}(\vec{r}_2) = 0 \quad (17)$$

Then, assuming that, just as in the classical representation, the coordinates of the real particles are related by (11) and (12) the wave function of the bound system writes as follows:

$$\Psi(\vec{r}) = \Psi_{v_1}(\vec{r}_1) \big|_{\vec{r}_1 = \vec{r}} \psi_{v_2}(\vec{r}_2) \big|_{\vec{r}_2 = -(1-\mu_2)\vec{r}}.$$

(18)

In the general case where $\vec{r}_1$ and $\vec{r}_2$ are the position vectors with respect to an arbitrary point in the rest frame, $\Psi(\vec{r})$ writes as

$$\Psi(\vec{r}) = \int d^3\rho \, \psi_{v_1}(\vec{r}_1 - \vec{\rho}) \psi_{v_2}(\vec{r}_2 - \vec{\rho}) \delta^3(\vec{\rho} - \vec{r}_{CM})$$

(19)

where $\vec{r}_{CM} = \mu_1 \vec{r}_1 + \mu_2 \vec{r}_2$.

Further, noticing that the coordinates of the internal particles as well as $H_1$ and $H_2$ are related by scale transformations, it results that $\Psi_{v_1}(\vec{r}_1)$ and $\Psi_{v_2}(\vec{r}_2)$ are also related by scale transformations, just as the particle trajectories in
classical mechanics. In quantum mechanics this means that the main, the orbital
and the magnetic quantum numbers of the individual and of the relative wave
functions satisfy the following relations \( n_1 = n_2; l_1 = l_2; m_1 = m_2 \).

Closing, we notice that (18) satisfies all the requirements imposed to the
bound state wave function in the independent particle picture: it depends only on
the relative vector \( \vec{r} \) and hence it is invariant at translations; in the same time, it
is in agreement with the classical picture of a bound system and, as product of
the individual wave functions, it retains the intrinsic properties of the internal
particles.

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