§6. Quantum Mechanical and Semiclassical Study of the Collinear Three-Body Coulomb Problem

Tolstikhin, O.I. (Kurchatov Inst., Moscow, Russia), Namba, C.

Accurate quantum mechanical (QM) solutions of the problems encountered in the theory of atomic collisions are rarely accessible. Even if they are, because of complexity of the calculations such solutions often have the character of a *virtual experiment* rather than a *theory*, and another theory is required for their qualitative interpretation. On the other hand, the semiclassical (SC) theory (by which we mean the asymptotic solution of the problem for small values of some parameter, h, characterizing the collision system, which is not necessarily Planck's constant) is simpler in implementation and usually permits one to consider a wider range of problems as well as to identify major mechanisms governing the collision processes. Thus, the SC theory could be very useful. However the results obtained in the leading order of this theory have limited accuracy, e.g. $\sim O(h)$, and usually cannot be improved because in the next order the theory becomes prohibitively difficult. But the asymptotic estimate of the error $\sim O(h)$ doesn't tell anything about its actual numerical value. To appreciate the meaning of $\sim O(h)$ for the given class of problems it is desirable to study those rare 'boundary' situations in which accurate QM solution can be obtained with confidence and simultaneously a SC solution is expected to be valid and to analyze in detail how these two solutions converge with each other as the asymptotic parameter h tends to zero. A study of this type, whose goal is to develop a SC understanding of the low-energy dynamics of the three-body Coulomb problem (TBCP), is initiated in the present work.

Our previous QM studies of the TBCP [1] have shown that the dynamics of heavy-light-heavy systems reveals features whose understanding is most naturally and easily provided by the SC theory. In the extreme limit when two mass ratios become vanishingly small, which is the case for systems consisting of two nuclei and an electron (ion-atom collisions), a SC theory of slow collisions has been developed by Solov'ev [2]. This theory, now known as the hidden crossing method, can be extended to the case of arbitrary masses of particles on the basis of the hyperspherical approach proposed by Macek [3]. A first step in this direction was done recently [4], where a classification of hyperspherical hidden crossings in the TBCP was developed; the next step would be to study the dynamics. Here we do this for a simplified model, namely, we consider the collinear TBCP. In this case, after approapriate rescaling of hyperspherical coordinates, the Schrödinger equation can be presented in such a form that an asymptotic parameter emerges which is given by

$$h = \frac{2}{\pi} \arctan \sqrt{\frac{m_3 m_{\mathrm{tot}}}{m_1 m_2}}, \tag{1}$$

where m_i are particle masses and m_{tot} is the total mass of the system. Note that for all possible combinations of masses $0 \leq h \leq 1$ and that $h \to 0$ for heavy-light-heavy systems. We plan to consider the whole spectrum of low-energy collision phenomena including bound states, resonances, elastic scattering, excitation, charge transfer and ionization and to analyze the convergence of QM and SC results in families of systems that differ only by the value of h. Some preliminary results are shown in Fig.1.

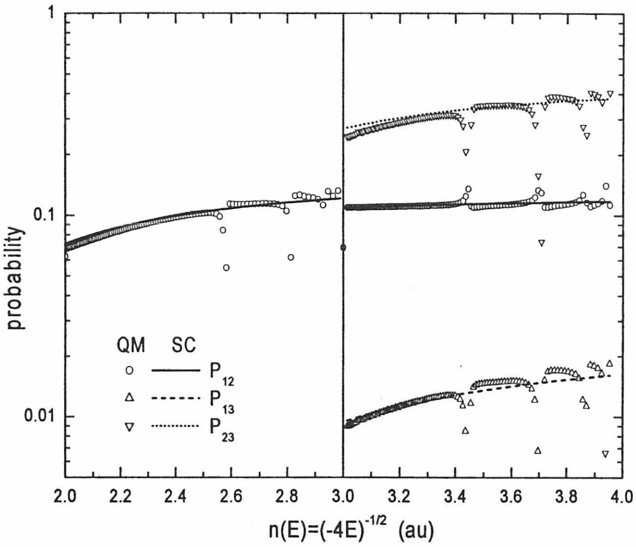

Fig.1 Comparison of QM and SC results for the probabilities P_{nm} of inelastic collisions $ee^{+}(n) + e \leftrightarrow ee^{+}(m) + e$ in the energy range below $n = 4$ threshold. For this system $h = 2/3$.

References

[1] O.I. Tolstikhin, I.Yu. Tolstikhina, and C. Namba, Phys. Rev. A **60**, 4673 (1999); O.I. Tolstikhin and C. Namba, Phys. Rev. A **60**, 5111 (1999); V.N. Ostrovsky, Phys. Rev. A **61**, 032505 (2000).

[2] E.A. Solov'ev, Sov. Phys. - Usp. **32**, 228 (1989).

[3] J. Macek, J. Phys. B **1** 831, (1968).

[4] E.A. Solov'ev and O.I. Tolstikhin, J. Phys. B **34**, L439 (2001).