Comment on "Degenerate Wannier Theory for Multiple Ionization"

The recent Letter of Pattard and Rost [1] suggests new threshold laws for the processes of the breakup of a particle into several charged fragments, which, regretfully, is incorrect. Previous studies, starting from the classical paper by Wannier [2] derived fragmentation cross section σ in a power-law form

$$\sigma(\epsilon \to 0) \sim \epsilon^{\mu}, \tag{1}$$

where ϵ is the energy excess above the breakup threshold. The primary task of the theory is to evaluate the threshold index μ for different multiparticle systems, a comprehensive bibliography can be found in Ref. [3]. Pattard and Rost [1,4] suggest the threshold law of novel functional form, namely, with an extra logarithmic ϵ dependence:

$$\sigma(\epsilon \to 0) \sim \epsilon^{\mu} |\ln\epsilon|^{-\nu}. \tag{2}$$

According to Wannier's [2] original idea, for the Coulomb interaction between the fragments the threshold law is defined by the motion along the *potential ridge* as the constituent particles fly apart. This motion is unstable; survival on the ridge corresponds to the system fragmentation, whereas sliding from it means that the breakup is not achieved. The instability of the motion is characterized by a set of Lyapunov exponents λ_i. The threshold index μ is expressed via the *sum of all Lyapunov exponents* [3,4]. In this Comment we discuss the key result obtained by Pattard and Rost in [1], and repeated in [4], namely, the novel threshold law (2).

The standard approach to the derivation of threshold laws relies on the analysis of classical trajectories in the vicinity of the potential ridge, where the equations of motion are *linearized* over coordinates transversal to the ridge. The system is described by a set of coupled linear equations that is differential over the time variable t. The time dependence of the coefficients is eliminated by introducing the effective time τ. The solutions of these equations $q(\tau)$ depend on the effective time as $\exp(\lambda_i \tau)$, where the set of λ_i eigenvalues is found by solving the characteristic equation. The threshold index μ is expressed via λ_i (see, for details, Refs. [2,3] and references therein).

Pattard and Rost [1,4] essentially retain the traditional framework, but argue that the situation is changed when the Lyapunov exponents happen to be *degenerate*. They refer to the standard mathematical textbook [5] saying that, "If n eigenvalues are degenerate, the general solution contains additional terms $\tau^k \exp(\lambda\tau)$, $(k < n)$." Further, they relate the logarithm in the alleged coordinate time dependence,

$$q(\tau) = \tau^k \exp(\lambda\tau) \equiv \exp(\lambda\tau + k \ln\tau) \qquad (k < n), \tag{3}$$

to the logarithmic factor in the energy dependence (2).

This reasoning is invalid. Consider harmonic vibrations of a system with many degrees of freedom (for example, a polyatomic molecule) around an equilibrium position. Some eigenfrequencies might be degenerate due to symmetry reasons, or accidentally. The argumentation by Pattard and Rost fully applies to this case; however, as is universally known, the *logarithmic solutions* (3) in fact do not emerge [see Eq. (23.6) in Ref. [6] and subsequent discussion]. The reason is clear: *in the harmonic approximation all of the normal modes are fully decoupled* and hence a character of the time dependence in each mode does not depend on whether or not some other degenerate mode exists.

This argument is directly related to the motion in the vicinity of the potential ridge. The problem is described by the Hamiltonian that is quadratic both in transversal coordinates and in momenta, similar to the harmonic approximation for a polyatomic molecule. The only difference is that the equilibrium is unstable and some eigenfrequencies are complex valued [3]. Obviously this fact does not influence the functional form of solutions of the same equations of motion which still reveal no *logarithmic terms*. The degenerate Lyapunov exponents are related to the *different modes* which are *fully decoupled*, therefore the logarithmic solutions (3), being mathematically feasible for general linear differential equations, do not emerge in the physical applications concerned.

In summary, the threshold law is given by Eq. (1) while the modification (2) is never valid.

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