Wannier threshold law and the classical-quantum correspondence in three-body Coulomb breakup

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We derive the classical threshold law for the breakup of three charged particles interacting via long-range Coulomb forces for the case of a charge ratio of 1/4 between the particles involved. The Wannier exponent in canonical Wannier theory is known to diverge in this case. We find that the classical threshold law, which is proportional to $\exp(-\lambda/\sqrt{E})$, shows exponential suppression of the ionization probability at threshold. We thus identify the possibility that exponential behavior in breakup processes, typically attributed to quantum-mechanical tunneling, can arise as a completely classical dynamical effect. We show that in the limit of zero energy, the behavior of the cross section is characterized by a classical to quantum transition. We discuss the regime of parameters in which this transition occurs and the possibility of an experimental observation of this transition.

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The first study of the complete fragmentation of three charged particles for small total fragmentation energy $E \to 0$ dates back to Wannier's seminal paper from 1953 [1]. In this paper, he derived a power law $P(E) \propto E^{\xi_+}$ for the fragmentation probability based on purely classical arguments. The threshold exponent ξ_+ depends on the charges and masses of the individual particles. In the case where one of the particles has mass m and charge q and the other two particles have equal masses M and charges $-Q$ (q and Q have the same sign), the exponent is given by [2,3]

$$\xi_+ = \frac{3}{4}\sqrt{1+\frac{16}{9}\,\frac{1+2M/m}{1-Q/4q}} - \frac{1}{4}. \qquad (1)$$

In the case $m \gg M$, $Q=1$, and $q=1$, the original Wannier result $\xi_+ = 1.127$ for electron-impact ionization of neutral atoms is recovered.

Quantum-mechanical formulations [4,5] for the breakup were subsequently proposed that led to the same threshold law as derived classically by Wannier. More recently, semiclassical S-matrix theory has been used to confirm and extend the range of Wannier's classical theory of fragmentation [6]. The success of Wannier's classical analysis of the threshold region for three-body Coulomb breakup raises the question as to the extent of its validity and as to how classical and quantum-mechanical threshold laws in atomic physics are related.

A situation that is especially interesting with respect to this question arises when the charge ratio between the particles taking part in the break-up process has the value $q/Q = 1/4$. A possible experimental realization is the ionization of Be^{3+} in a collision with a Be^{4+}. Wannier's original analysis seems to fail for this process since the Wannier exponent diverges for charge ratio 1/4. A recent analysis of this breakup process therefore started from a quantum-mechanical picture using hidden-crossing theory [7]. The results can be summarized as follows: (a) The quantum-mechanical fragmentation probability is not a power law in the energy but has the form

$$P_{\mathrm{qm}}(E) \propto \exp\left[\frac{-\kappa}{E^{1/6}}\right] \qquad (2)$$

with a numerical factor κ depending on the fragments, and (b) the semiclassical limit of the threshold law *differs* from the quantum-mechanical threshold law; it is given by $P_{\mathrm{sc}}(E) \propto \exp[-\lambda E^{-1/2}]$.

The question that naturally arises and that we answer in this paper is the following: Is it possible to derive the *semiclassical* threshold law resorting to a completely classical picture? Intuitively one might guess the answer to be negative since semiclassically the breakup probability is exponentially suppressed (albeit with a different energy exponent than the quantum-mechanical threshold law), pointing toward a possible interpretation in the form of a tunneling mechanism involved in the breakup process. However, as we will show, the exponential behavior can be interpreted purely in terms of the classical dynamics of the system. We thus put the breakup process with diverging Wannier exponent on an equal footing with Wannier's original analysis for $q/Q \neq 1/4$. The derivation of the classical threshold law is followed by a discussion that puts special emphasis on the relation between the classical threshold law $P_{\mathrm{cl}}(E)$ derived here and the previously derived quantum-mechanical threshold law $P_{\mathrm{qm}}(E)$.

As a required preliminary to the derivation of the threshold law for the divergent case, we will provide Wannier's derivation in brief. To look for electronic trajectories leading to double escape, Wannier [1] argued that one has to look for unstable ridges or points in the equipotential plot. For a system consisting of two electrons and a fixed nucleus (charge Z), the potential energy can be written in hyperspherical coordinates R, α, and θ, with $R=\sqrt{(r_1^2+r_2^2)}$, $\tan\alpha = r_2/r_1$,

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where r_1 and r_2 are the distances of the electrons from the nucleus and θ the interelectronic angle. The potential energy is $V=C(\alpha,\theta)/R$ and

$$C(\alpha,\theta)=-\frac{Z}{\cos\alpha}-\frac{Z}{\sin\alpha}+\frac{1}{(1-\sin 2\alpha\cos\theta)^{1/2}}. \quad (3)$$

This has a saddle point at $\alpha=\pi/4$; $\theta=\pi$.

The variables $\beta=\pi/4-\alpha$ and $\gamma=\pi-\theta$ are introduced with origin at the Wannier saddle point and the Hamiltonian of the system in terms of the hyperspherical coordinates and these variables are written as

$$H(\equiv E)=\frac{1}{2}p_R^2+\frac{1}{2R^2}p_\beta^2+\frac{2}{R^2\sin^2(2\alpha)}p_\gamma^2+\frac{C}{R}. \quad (4)$$

The momenta p_R, p_β, and p_γ are given by

$$p_R=\dot{R},\ p_\beta=R^2\dot{\beta},\ p_\gamma=\frac{R^2\sin^2(2\alpha)}{4}\dot{\gamma}, \quad (5)$$

and the equations of motion are

$$\ddot{R}=R\dot{\beta}^2+\frac{1}{4}R\sin^2(2\alpha)\dot{\gamma}^2+\frac{C}{R^2}, \quad (6)$$

$$\frac{d}{dt}[R^2\dot{\beta}]=\frac{1}{2}R^2\sin(2\alpha)\cos(2\alpha)\dot{\gamma}^2-\frac{1}{R}\frac{\partial C}{\partial\beta}, \quad (7)$$

$$\frac{d}{dt}\left[\frac{R^2\sin^2(2\alpha)}{4}\dot{\gamma}\right]=-\frac{1}{R}\frac{\partial C}{\partial\gamma}. \quad (8)$$

The motion in the coordinate γ proves incidental for the threshold behavior of the cross section since γ always tends asymptotically to zero (the interelectronic angle θ focuses at π).

To form an equation that describes the β coordinate dynamics near the ridge the function $C(\alpha,\theta)$ is expanded as a power series about the saddle point and Eq. (7) is linearized to get

$$2R\dot{R}\dot{\beta}+R^2\ddot{\beta}=-\frac{1}{R}\left(-\frac{12Z-1}{\sqrt{2}}\beta\right). \quad (9)$$

The finite energy (E) hyper-radial momentum along the saddle for the linearized system is

$$\dot{R}=\sqrt{2E+\frac{4\sqrt{2}\left(Z-\frac{1}{4}\right)}{R}} \quad (10)$$

and time is eliminated from Eq. (9) by using Eq. (10). This gives an equation of motion in R for the angle β:

$$\frac{d^2\beta}{dR^2}R^2[2ER+k]+\frac{d\beta}{dR}R\left[4ER+2k-\frac{k}{2}\right]-\beta\left[\frac{12Z-1}{\sqrt{2}}\right]=0, \quad (11)$$

where $k=4\sqrt{2}(Z-\frac{1}{4})$.

This equation is crucial in finding the ionization probability. Wannier chose to work with the $E=0$ solutions. Equation (11) then becomes Euler's equation with the general solution found by reducing it to a constant coefficient equation by means of the substitution $R=R_b\exp(q)$. The general solution is

$$\beta=\frac{\pi}{4}-\alpha=C_1e^{[-(1/2)\mu-1/4]q}+C_2e^{[(1/2)\mu-1/4]q} \quad (12)$$

with $\mu=\frac{1}{2}[(100Z-9)/(4Z-1)]^{1/2}$. The solution with exponent $-\frac{1}{2}\mu-\frac{1}{4}(\equiv\xi_-)$ is associated with trajectories that converge to the ridge and the solution $+\frac{1}{2}\mu-\frac{1}{4}(\equiv\xi_+)$ with diverging trajectories. The proportion of converging trajectories that correspond to ionization cannot be limited and the critical behavior when evaluating the energy dependence of the ionization cross section is due to the diverging trajectories.

The energy dependence of the ionization probability is given by finding the ratio of an angular trajectory spread (β_b) at a radius R_b (this radius is a constant in the limit $E\to 0$ [8]) to a fixed angular spread (β_c) that is not dependent on energy at large R ($=R_c$),

$$P(E)\propto\frac{\beta_b}{\beta_c}=\frac{C_2R_b^{\xi_+}}{\beta_c}. \quad (13)$$

Keeping β_c fixed results in an energy dependence of the integration constant C_2. In the generic Wannier theory, one constructs different solutions [the ones approximated by $E=0$ in the Coulomb zone ($ER\ll 1$) and the "free" ones for $ER\gg 1$] and matches them. So in the generic case the solutions in the Coulomb zone do not depend on the energy at all, classical scaling comes in through the matching condition at $ER_c\approx 1$ where R_c is

$$R_c=\frac{(4Z-1)}{\sqrt{2}E}\ \left(\equiv\frac{k}{2E}\right). \quad (14)$$

The result is Wannier's threshold power law

$$P(E)\propto(ER_b)^{\xi_+}. \quad (15)$$

Quantum-mechanical derivations [4,5] lead to an identical threshold law. In addition, hidden-crossing theory [5] has been used to extend Wannier's results near threshold by introducing corrections to the power law. Corrections can also be obtained within the framework of classical Wannier theory by extending the theory to finite E. The key is to use Eq. (11), keeping E as a parameter. We find that the results from hidden-crossing theory and the extended Wannier theory for the $Z=1$ system are indistinguishable up to and beyond 8 eV above threshold [9]. This demonstrates the equivalence between the quantum-mechanical and classical results in the generic Wannier case.

The divergence of the Wannier exponent when the ratio of nuclear charge to wing particle charge is $q/Q=1/4$, or equivalently when $Z=1/4$ in the above, *does not* mark a

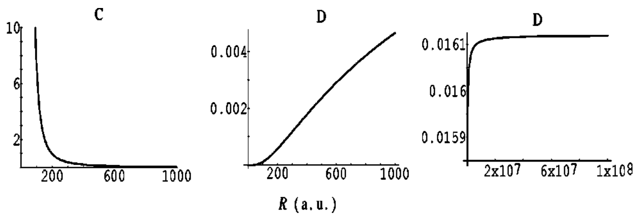

FIG. 1. Plots of solutions I_1 and K_1 as a function of the hyperradius R at total energy $E=0.02$ eV. The label C indicates the convergent solution $I_1[x]$, and the label D corresponds to the divergent solution, $K_1[x]$. For the divergent solution, we plot it separately for radii near the nucleus and at asymptotic distances.

failure of Wannier theory. To find a solution for this case demands that we use Eq. (11), keeping E as a parameter. For $Z=1/4$ $(k=0)$ this becomes

$$\frac{d^2\beta}{dR^2}R^3[2E]+\frac{d\beta}{dR}R^2[4E]-\beta\sqrt{2}=0. \tag{16}$$

We cast this equation into normal form by letting $\beta(E,R)=u(R)v(E,R)$ and choosing u so that the first derivative term in v' vanishes. This gives

$$u=\frac{A}{R} \tag{17}$$

and hence the equation for v

$$\frac{d^2v}{dR^2}=f(E,R)v, \tag{18}$$

where $f(E,R)=(E\sqrt{2}R^3)^{-1}$. This equation has solutions involving the modified Bessel functions ($I_n[x]$ and $K_n[x]$) [10], and when the product is taken with $u(R)$ we get

$$\beta(E,R)=A_1\sqrt{\frac{1}{R}}\,I_1\left[2^{3/4}\sqrt{\frac{1}{ER}}\right]+A_2\sqrt{\frac{1}{R}}\,K_1\left[2^{3/4}\sqrt{\frac{1}{ER}}\right]. \tag{19}$$

This solution shows the scaling property of the classical Hamiltonian since it depends on ER. So even with a vanishing Coulomb potential on the saddle (which is manifest through the solutions being Bessel functions) the Coulombic nature of the problem shows through the argument of the Bessel functions.

To be able to construct the ionization probability using Wannier's arguments, it is important that one of these solutions can be identified with trajectories that diverge from the ridge and the other with those that converge. In Fig. 1 we plot the two solutions in Eq. (19) at a fixed energy E. We see that the $K_1[x]$ solution gives the required diverging behavior and that the $I_1[x]$ solution gives the converging behavior that does not affect the energy dependence of the ionization cross section.

The ionization probability can therefore be constructed by calculating the ratio of the angular spread in β at a fixed radius R_b to the fixed angular spread at an asymptotically large distance. Since Eq. (19) is the solution for *all* values of ER we take $R_c\to\infty$. This means that we should write

$$P(E)\propto\beta(E,R_b)/\beta(\infty). \tag{20}$$

So to get the correct threshold law we must take the limit $R\to\infty$ at *fixed finite E* before taking $E\to 0$ for the threshold behavior.

The angle β for the diverging $K_1[x]$ solution at one particular energy E converges to $E^{1/2}2^{-3/4}$ as $R\to\infty$, so to have a constant asymptotic angle one has to choose

$$A_2=2^{3/4}E^{-1/2}. \tag{21}$$

To get $\beta(R_b)$ we need the behavior of the solution at *small* $ER_b\ll 1$. This is precisely the condition for the applicability of a WKB solution of Eq. (18). The general solution is a linear combination of the two WKB solutions

$$v(E,R)=f(R)^{-1/4}\exp\left[\pm\int^R f(t)^{1/2}dt\right]. \tag{22}$$

Evaluating the integral in Eq. (22) and taking the product with $u(R)$ gives

$$\beta(E,R)=B_1R^{-1/4}\exp\left[\frac{+2^{3/4}}{\sqrt{ER}}\right]+B_2R^{-1/4}\exp\left[\frac{-2^{3/4}}{\sqrt{ER}}\right]. \tag{23}$$

The second (B_2) solution corresponds to the diverging $K_1[x]$ solution and gives the $\beta(R_b)$ behavior. The additional energy dependence of B_2 [same as A_2 in Eq. (21)] is not important in the threshold behavior since the exponential part dominates, so the ionization cross section is $\sigma(E)\propto\exp[-2^{3/4}/\sqrt{ER_b}]$. With both electrons on the ridge the initial distance x_0 of each electron from the nucleus is $x_0=R_b/\sqrt{2}$ so that $R_b=\sqrt{2}x_0$ and hence,

$$\sigma(E)\propto\exp\left[\frac{-\lambda}{\sqrt{E\,x_0}}\right], \tag{24}$$

where $\lambda=\sqrt{2}$. This is the exact same formula as obtained in [7] by taking the semiclassical limit of the quantum expression obtained from hidden-crossing theory. It also agrees with the classical Monte Carlo calculation of Dimitrijević *et al.* [11] who found that an identical exponential function with $\lambda=1.364$ (a difference of only 5% from our analytical value) best fitted their numerical data.

The classical threshold law Eq. (24) is based on the quasifree motion of the particles along the Wannier ridge $\beta=0$. The coupling between the motion in the hyperangle β and the hyperradius R is described by Eq. (23). It determines the classical threshold law. The threshold regime is characterized by the condition $ER_b\ll 1$ under which the classical threshold law Eq. (24) was derived. Quantum mechanically, R_b can be interpreted as the binding radius of the initially bound particles. R_b is thus inversely proportional to the binding energy E_b of the initially bound complex. In terms of the binding energy the condition to be in the threshold regime is $E/E_b \ll 1$.

We now ask the following question: Suppose we are in the threshold regime $E/E_b \ll 1$. An experiment is performed in which the break-up cross section is measured at different values of energy E, and the target is always prepared in the same state with binding enegy E_b. Will one measure the classical threshold behavior all the way down to zero breakup energy? Surprisingly, the answer is negative. Instead, a transition from the classical threshold behavior Eq. (24) to the quantum-mechanical threshold law Eq. (2) will take place. The reason is the following: As shown in Ref. [7], where the quantum-mechanical threshold law Eq. (2) was derived, the quantum-mechanical motion in β is related to a quantum-mechanical zero point energy $E_0(R)$ that depends on the hyper-radius as $E_0(R) \sim 1/R^{3/2}$. The classical threshold law holds when the motion along the saddle is quasifree corresponding to the condition $E \gg E_0$ or $ER^{3/2} \gg 1$ for $R > R_b$. Expressed in terms of the initial binding energy, this gives the condition $E \gg E_b^{3/2}$ for the classical threshold law to hold. In the opposite limit, the zero point energy E_0 dominates over the breakup energy and the quantum-mechanical version of the threshold law holds.

Measuring the near-threshold breakup cross section of the three-body Coulomb system with charge ratio $q/Q = 1/4$ as a function of energy opens—at least in principle—a way to investigate the classical to quantum transition in a problem of atomic collision dynamics. The classical threshold law shows an exponential suppression of the breakup probability near zero energy. We have shown that exponential threshold behavior need not necessarily involve quantum-mechanical tunneling but can arise as a classical dynamical effect.

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