Three-particle breakup near threshold when the Wannier exponent diverges

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Wannier theory predicts an infinite threshold exponent for the breakup of three charged particles if two of the particles have equal charges and the ratio of the charge of one of these to the charge of the third particle has the value (-4). We show that the Wannier picture of ridge propagation remains valid and that the threshold law changes to the form $\sigma \propto E^{-1/6}\exp(-\kappa/E^{1/6})$. The classical and quantum results differ, which is in contrast to the generic Wannier case. We show that the classical limit of the threshold law explains the threshold behavior obtained numerically by classical trajectory calculations. [S1050-2947(97)08106-7]

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I. INTRODUCTION

Wannier theory of three-particle breakup has been successfully extended to the case of arbitrary masses and charges over recent years [1,2]. It predicts a power law

$$\sigma \propto E^{\zeta} \tag{1}$$

for the breakup cross section near the threshold $E \rightarrow +0$. E is the total energy of the system. The threshold exponent ζ 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 [1,2]

$$\zeta = \frac{3}{4}\left(1 + \frac{16}{9}\,\frac{1+2M/m}{1-Q/4q}\right)^{1/2} - \frac{1}{4}. \tag{2}$$

In the cases $m \gg M$, $Q=1$, and $q=1$ the original Wannier result $\zeta = 1.127$ for electron impact ionization of neutral atoms is recovered [3].

One question however has so far remained unanswered: What happens when the ratio of the charges of the wing particles to the charge of the third particle is $Q/q=4$ and the Wannier exponent becomes infinite? The classical equations of motion in the vicinity of the Wannier ridge do not allow an analytical solution in this case [4], in contrast to what we call the generic Wannier case $Q/q<4$ [3]. Wannier's picture of trajectories converging to and diverging from the potential ridge, however, is still valid even for this exceptional case. Quantum mechanically these trajectories are related to convex and concave wave fronts traveling along the potential ridge [5]. We show how this picture can be incorporated into this borderline case. We derive the quantum mechanical threshold law and the leading-order terms of the aymptotic series near threshold. We also derive the semiclassical limit for the threshold law, and show how the numerically determined classical threshold law [4] emerges analytically from our analysis.

A possible experimental realization of the situation analyzed in this paper would be the measurement of the integrated ionization cross section of the beryllium antiprotonic ion $[Be^{4+}+p^{-}]$ by another beryllium ion Be^{4+}. We predict a strongly suppressed, though finite cross section for finite positive energies. Due to the exponential suppression an experimental determination of the threshold law may be difficult; however, our main emphasis is to demonstrate that the theory presented here heals a shortcoming of the Wannier theory, which cannot make any predictions about the slope of the cross section for $Q/q=4$ at all. In this context we aim to clarify the relation between the Wannier picture of ridge propagation and classical mechanics. It has been shown that the breakup of three charged particles reduces to a purely classical process [6] in the generic Wannier case, even if the starting point is a quantum-mechanical or semiclassical one. However, we will demonstrate that this statement does not hold in general, but depends on the final state interaction.

In Sec. II we present the theory, which is employed in Sec. III to derive the quantum-mechanical threshold law. The relation to the classical threshold law is then discussed in Sec. IV.

II. THEORY

We use the same set of Jacobi coordinates as in Ref. [2]. $\mathbf{R}$ denotes the vector between the wing particles of mass M, and $\mathbf{r}$ is the vector from the third particle of mass m to the center of mass of the wing particles. The latter is written in components parallel and orthogonal to the axis defined by the wing particles: $\mathbf{r} = x\hat{\mathbf{R}} + y\hat{\mathbf{R}}_{\perp}$. The hat denotes unit vectors. We also introduce the reduced masses $\mu_R = M/2$ and $\mu_r = 2Mm/(2M+m)$. Threshold breakup is characterized by $R\rightarrow\infty$, and motion in the vicinity of the Wannier saddle by $x\sim 0$ and $y\sim 0$. Quantum mechanically the Schrödinger equation must be solved in a region around the Wannier ridge incorporating appropriate boundary conditions. We use atomic units throughout, but keep the dependence on $\hbar$ in the equations explicitly in order to take the classical limit later on.

In the Wannier theory the potential is expanded around the equilibrium configuration $x=0$ and $y=0$ up to second order:

$$V(\mathbf{R},\mathbf{r}) = -\frac{C_0}{R} - \frac{C_{x2}}{2}\,\frac{x^2}{R^3} + \frac{C_{y2}}{2}\,\frac{y^2}{R^3}, \tag{3}$$

with the coefficients

$$C_0 = Q(4q-Q), \quad C_{x2} = 32qQ, \quad C_{y2} = 16qQ. \tag{4}$$

The wave function is written as

$$\Psi(\mathbf{R},\mathbf{r}) = \frac{1}{R}\psi(R)\varphi(R;x,y). \tag{5}$$

The wave function for the relative motion of the wing particles is written as a WKB ansatz with outgoing wave boundary conditions

$$\psi(R) = \frac{1}{\sqrt{K(R)}}\exp\left[\frac{i}{\hbar}\int_{R_0}^{\infty} K(R)\,dR\right], \tag{6}$$

where the momentum is given by

$$K(R) = \sqrt{2\mu_R[E + C_0/R - \varepsilon(R)]}. \tag{7}$$

The effective potential $\varepsilon(R)$ takes the coupling between the relative motion of the wing particles and the bending and stretching motion around the Wannier configuration into account. It can be derived directly from a diabatic solution for $\varphi(R,x,y)$ [2,5]. Alternatively, substituting potential (3) into the Schrödinger equation and fixing R leads to the adiabatic Schrödinger equation

$$\left[-\frac{\hbar^2}{2\mu_r}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{1}{y}\frac{\partial}{\partial y}\right) - \frac{C_{x2}x^2}{2R^3} + \frac{C_{y2}y^2}{2R^3}\right]\varphi_{\text{asy}}(R;x,y) = \varepsilon(R)\varphi_{\text{asy}}(R;x,y) \tag{8}$$

for the motion in x and y. The transformation between adiabatic and diabatic ionization channels was carried out in Ref. [7]. It can be seen from Eq. (11) in [7] that the adiabatic and diabatic channels coincide to order $1/R^{3/2}$ for the case where $C_0 = 0$, i.e., when $Q/q = 4$. It is therefore sufficient to consider Eq. (8), which has the form of a one-dimensional inverted harmonic oscillator in x, and a two-dimensional harmonic oscillator in y. The energy for the lowest-lying state with ${}^1S$ symmetry is

$$\varepsilon(R) = -\frac{i}{2}\omega_x + \omega_y, \quad \omega_x = \frac{\hbar}{\mu_r^{1/2}R^{3/2}}\sqrt{C_{x2}},$$

$$\omega_y = \frac{\hbar}{\mu_r^{1/2}R^{3/2}}\sqrt{C_{y2}}, \tag{9}$$

which, taking Eq. (4) into account, become

$$\varepsilon(R) = \frac{\hbar|C_1|}{R^{3/2}}\exp\left[-i\tan^{-1}\frac{1}{\sqrt{2}}\right], \quad |C_1| = 2\sqrt{\frac{6Qq}{\mu_r}}. \tag{10}$$

The minus sign in the first term of Eq. (9) was chosen to meet outgoing wave boundary conditions for the asymptotic wave function in x. This corresponds to the picture of wing particles falling off the Wannier ridge as they move toward larger interparticle distance. Such events lead to single ionization only. Since $C_0 = 0$, the Coulomb term in Eq. (7) vanishes, and the leading-order contribution comes from the effective potential $\varepsilon(R)$, which is of leading order $1/R^{3/2}$. This is the essential difference with the generic Wannier case.

The effective potential $\varepsilon(R)$ has an imaginary part because the Schrödinger equation is solved in a finite region of configuration space. Since $\pi/2 < \arg[E - \varepsilon(R)] < \pi$, the real and imaginary parts of the momentum $K(R)$ are both positive, and the wave function in Eq. (6) is indeed an outgoing wave with decaying amplitude. The decaying amplitude is associated with particles contributing to single escape instead of three particle breakup. The wave function for the bending and stretching motion asymptotically has the form

$$\varphi_{\text{asy}}(R;x,y) = N_x\exp\left[i\frac{\omega_x}{2}x^2\right]N_y\exp\left[-\frac{\omega_y}{2}y^2\right]. \tag{11}$$

The wave function in y, which corresponds to angular correlations, has a Gaussian peak around the equilibrium configuration. The wave function in x is related to the energy distributions, which is uniform around the equilibrium configuration corresponding to an equal energy sharing of the energies of the wing particles. These two features of the standard Wannier theory remain unchanged in the case when the Wannier exponent becomes infinite. Since φ_{asy} determines the angular and energy distribution we call it the distribution function for matters of abbreviation.

The normalization constant N_y is chosen to normalize the integral of the square of the oscillator in y to unity. The choice of the normalization constant N_x has to be addressed carefully. In Ref. [7] the transformation from adiabatic to diabatic wave functions φ_{asy} was treated on an equal footing for the harmonic and antiharmonic oscillators, resulting in equal forms of the coupling matrix elements. This requires a normalization of the wave functions of the antiharmonic oscillator in the same way as for the harmonic oscillator. From the view point of the adiabatic or ''hidden crossing'' theory, the emergence of the normalization constant was clarified in Ref. [8]. It is proportional to $R^{1/8}$. This scaling of the normalization constant with R had to be taken into account in the diabatic theory of Ref. [7] as well to derive the correct Wannier exponent. There it was attributed to a phase-space factor.

The break-up cross section is proportional to the survival probability $P(E)$ on the saddle which is given by the square of the exponential part of the wave function [7,9,8,11]:

$$P(E) = \exp\left[-\frac{2}{\hbar}\text{Im}\int_{R_0}^{\infty} K(R)\,dR\right]. \tag{12}$$

To arrive at the cross section, the survival probability must be multiplied by the square of the distribution function taken at a value $R = R_C$, where the asymptotic distribution emerges. The relation between R_C and the energy E will be addressed in Sec. III. The square of the distribution function must be integrated over the coordinates x and y, and the integrated ionization cross section for a given angular momentum L then gives

$$\sigma(E) \propto \frac{\pi}{E+I}(2L+1)R_C^{1/4}P(E). \tag{13}$$

I denotes the ionization potential of the target.

III. QUANTUM-MECHANICAL THRESHOLD LAW

A. Limit as $E \to +0$

In the generic Wannier case $Q/q<4$ the dominating interaction in the final channel (6) is an attractive Coulomb potential. A valid approximation in this case is to expand the survival probability as

$$P(E)=\exp\left[-\frac{2}{\hbar}\int_{R_0}^{\infty}\frac{\mathrm{Im}[-\varepsilon(R)]}{K_0(R)}dR\right], \tag{14}$$

with the zero-order momentum

$$K_0(R)=\sqrt{2\mu_R(E+C_0/R)}. \tag{15}$$

This is, however, not possible for $Q/q=4$, because the Coulomb potential vanishes and the dominant interaction in the ionization channel is the potential (10). The full expression (12) must be calculated instead. The radius R_0 characterizes the boundary of the reaction zone where all three particles are close together. In the reaction zone the correlated motion of the three particles must in principle be treated fully quantum mechanically. As has been shown elsewhere [8], the reaction zone contributes with an additional factor to the double escape probability which goes to a nonzero constant at $E=0$, and which depends only very weakly on the total energy near threshold. It therefore plays no role for the behavior of the ionization probability as a function of the excess energy, and need not concern us further. The value of R_0 should be chosen on physical grounds. If one of the wing particles is initially bound to the particle with mass m, the binding energy is $E_b=-\mu(Qq)^2/(2\hbar^2n^2)$ depending on the quantum number n of the initial state. Here the reduced mass $\mu=mM/(M+m)$ has been introduced. In a classical picture the incoming particle polarizes the bound particle in its orbit, and a reasonable choice for R_0 is twice the distance x_0 of the expectation value of the radius of the bound particle in its orbit, which is

$$R_0\sim\frac{2\hbar^2n^2}{\mu(Qq)}. \tag{16}$$

Threshold breakup is characterized by the condition that the excess energy E is much less than the binding energy E_b. With the above choice (16), it can be easily verified that this is equivalent to the condition

$$E\ll\hbar|C_1|/R_0^{3/2}. \tag{17}$$

This in turn means that the motion on the Wannier ridge starts in a region where the effective potential dominates over the kinetic energy of the particles. Notice that the real part of the potential (10) is repulsive, and thus introduces a potential barrier through which the system has to tunnel on the Wannier ridge because of condition (17). This can be understood as a purely quantum-mechanical effect: The bending motion in y has a quantum-mechanical zero point energy which must be subtracted from the total energy E for the relative motion of the two wing particles. However, it must be emphasized that even with the real part of $\varepsilon(R)$ absent, the imaginary part arising from the stretching motion in x only leads to an imaginary part in $K(R)$. Neglect of the real part of the effective potential (10) does not change the form of the threshold law to be deduced, but only the numerical constants.

The survival probability (12) is calculated in the Appendix under condition (17). The leading term is independent of the starting radius R_0 and gives the threshold behavior

$$P_{\mathrm{thr}}(E)=\exp[-\kappa/E^{1/6}],\quad E\to+0 \tag{18}$$

where κ is given in the analytical form

$$\kappa=\frac{1}{\hbar^{1/3}}\left(\frac{2\mu_R}{\pi}\right)^{1/2}\Gamma(\tfrac{1}{3})\Gamma(\tfrac{1}{6})|C_1|^{2/3}\sin\left[\frac{2}{3}\left(\pi-\arctan\frac{1}{\sqrt{2}}\right)\right]. \tag{19}$$

To relate this result to the cross section, Eq. (13), the radius R_C must be specified. In the standard Wannier theory the radius at which the asymptotic energy distribution emerges is characterized by the transition from the Coulomb zone in which the potential energy dominates to the asymptotic free zone where the Coulomb energy can be neglected. The boundary between the two zones scales as $R_C\sim 1/E$, giving rise to an additional factor $E^{-1/4}$ in the near-threshold cross section [8]. Since the attractive Coulomb potential is missing in our case, standard Wannier theory has to be modified at this point. The Coulomb zone is replaced by the coupling zone which is dominated by the effective potential (10). The boundary between the coupling zone and the asymptotic free zone then scales as $R_C\sim E^{-2/3}$. This leads to the threshold behavior

$$\sigma_{\mathrm{thr}}(E)\propto E^{-1/6}\exp[-\kappa/E^{1/6}]. \tag{20}$$

B. Leading-order corrections to threshold law

We now discuss corrections to the threshold law (20) arising from higher-order terms in the evaluation of the survival probability, and estimate the range of validity of the threshold law. The first correction of the survival probability depends on the starting radius R_0 and gives (see the Appendix)

$$P(E)=P_{\mathrm{thr}}(E)\exp\left[\left(\frac{2\mu_R}{\hbar}\right)^{1/2}\cos\left(\frac{1}{2}\arctan\frac{1}{\sqrt{2}}\right)\times\left(8|C_1|^{1/2}R_0^{1/4}-\frac{4R_0^{7/4}}{7\hbar|C_1|^{1/2}}E\right)\right]. \tag{21}$$

The energy-dependent part of the correction determines the energy range over which the threshold law (18) is valid. As the criterion for the critical energy E_C above which the threshold behavior is modified, we choose

$$\exp\left[-\sqrt{2\mu_R}\cos\left(\frac{1}{2}\arctan\frac{1}{\sqrt{2}}\right)\frac{4R_0^{7/4}}{7\hbar^{3/2}|C_1|^{1/2}}E_C\right]\approx 0.9, \tag{22}$$

which translates into the condition

$$\frac{E_C}{|E_b|}\approx 0.17\left(\frac{n\mu^3}{\mu_R^2\mu_r}\right)^{1/4}. \tag{23}$$

For the fictitious case of electron impact ionization of a neutral atom with charge $q=\frac{1}{4}$, which has been treated in Ref. [4], one has the threshold coefficient $\kappa=12.056$ a.u., and the critical energy is $E_C/|E_b|\approx 0.2$. The Wannier law for electron-impact ionization on hydrogen ($q=1$) is known to be valid up to approximately 2.7 eV [10]. Thus, while the form of the threshold law itself changes the departure from the threshold behavior still relates to approximately the same ratio of the excess energy to the binding energy. For the real case of ionization of the beryllium antiprotonic ion $[\mathrm{Be}^{4+}+p^-]$ by another beryllium ion Be^{4+} the threshold coefficient is much larger, namely $\kappa=409.2$ a.u., and the ratio of the critical excess energy to the binding energy is $E_C/|E_b|\approx 0.075$ which corresponds to $E_C\approx 0.54 m_p=27$ keV. Another, less esoteric example is the single ionization of Be^{3+} in a collision with a Be^{4+} ion. Here the exponential suppression of the energy behavior of the cross section is even more dramatic due to the small mass ratio of the electron to the remaining Be^{3+} ions. The threshold coefficient is $\kappa=4922$ for this case. Effectively such a large threshold exponent leads to a threshold behavior of the cross section which can be interpreted as resulting from an infinite Wannier exponent. However, because of the small efficiency in creating the Beryllium antiprotonic ion, the latter example may be better suited for an experimental study, and *absolute* values of the cross section near threshold will be larger compared to the first.

C. Extension to other potentials

A simple argument for the threshold behavior of the survival probability (18) can be given on the basis of a scaling argument. Neglecting the total energy in the coupling zone the integrand in Eq. (12) scales as $R^{-3/4}$. Instead of taking the upper limit of the integral to be infinite the survival probability is integrated up to the boundary $R_C=(\hbar|C_1|/E)^{2/3}$ between the coupling zone and the asymptotic free zone where the kinetic energy of the particles dominates the potential energy. The probability therefore scales as $P(E)\propto\exp[-\kappa R_C^{1/4}]$, which corresponds to the previously derived result (18). Since the argument is rather general we conclude that any motion which is governed asymptotically by a potential of the form

$$\varepsilon(R)=\frac{C}{R^{\nu}}\quad(\ \mathrm{Im}C\leqslant 0\ \ \text{and}\ \ \mathrm{Re}C>0,\ \ 0<\nu<2\ )\tag{24}$$

in the final channel results in a threshold law of the form

$$P_{\mathrm{thr}}(E)\propto\exp[-\kappa E^{1/2-1/\nu}].\tag{25}$$

Especially for the case $Q/q>4$, which we have not dealt with so far, we recover the result for the tunneling probability through a repulsive Coulomb potential ($\nu=1$). In this case the threshold law does not arise from the effect of the potential $\varepsilon(R)$ but from the Coulombic nature of the final-state interaction. Note that this differs from the generic Wannier case $Q/q<4$, where the Coulomb interaction is attractive and the coupling potential is essential to derive the Wannier law (1). However, care has to be taken if the dependence of the interaction in the final channel has a dependence on R with a power $\nu\geqslant 2$. Since the radial kinetic energy itself behaves typically like $1/R^2$, it dominates over the effective potential, and the above result does not apply [12].

IV. CLASSICAL LIMIT

In this section we discuss the classical limit of the survival probability. Dimitrijević, Grujić, and Simonović performed classical trajectory calculations for the above-mentioned fictitious case $q=\frac{1}{4}$ and fitted the results to a threshold law of the form [4]

$$P_{\mathrm{cl}}(E)\sim\exp[-\lambda/\sqrt{x_0E}],\quad x_0=R_0/2\tag{26}$$

(cf. Sec. 3.1 of their paper). They obtained the numerical value $\lambda=1.364$. The breakup probability depends explicitly on the starting radius R_0 of the outgoing trajectories. This can be linked to the scaling properties

$$\mathbf{r}\to\tau\mathbf{r},\quad \mathbf{p}\to\mathbf{p}/\sqrt{\tau},\quad E\to E/\tau,\quad \tau>0\tag{27}$$

of classical Coulomb systems [3]. The findings of Ref. [4] are purely numerical, and no explanation could be given for the energy dependence of the classical cross section and the value of the coefficient λ.

The classical calculations of Ref. [4] as well as the quantum-mechanical approach presented here treat the breakup process as a half-collision reaction. However, apparently the results differ completely, which needs explanation. In the following we will show that the behavior (26) of the breakup cross section can be recovered as the classical limit of the theory presented here. The classical limit corresponds to $\hbar\to 0$, while keeping the excess energy E and the binding energy E_b constant. The later condition implies $\hbar n=\mathrm{const}$ and therefore the starting radius must be kept fixed at a certain value R_0. The effective potential (10) scales linearly with $\hbar$, so the classical limit corresponds to the condition

$$\frac{\hbar|C_1|}{R^{3/2}}\ll E,\quad R_0\leqslant R<\infty.\tag{28}$$

This is the opposite of condition (17) for the quantum-mechanical threshold law to hold. The proper interpretation of the above condition (28) is that in the classical limit the absolute value of the zero point energy of the effective potential (10) is small compared to the excess energy E. [Note that the values chosen in the classical calculations of Ref. [4] namely, $R_0=0.1$ a.u., $R_0=1$ a.u. and energies $E\leqslant 0.1$ a.u. actually fall within the threshold regime (17) if treated quantum mechanically.]

The survival probability (12) with the momentum given by Eq. (7) and $C_0=0$ is expanded under condition (28), which gives the classical threshold law

$$\begin{aligned}P_{\mathrm{cl}}(E)&=\exp\left[-\frac{2}{\hbar}\sqrt{2\mu_RE}\int_{R_0}^{\infty}\frac{\mathrm{Im}[-\hbar C_1]}{ER^{3/2}}dR\right]\\&=\exp\left[-\left(\frac{32(Qq)\mu_R}{\mu_r}\right)^{1/2}\frac{1}{\sqrt{x_0E}}\right].\end{aligned}\tag{29}$$

The bending and stretching motion decouple in the expression for the classical ionization probability, and the bending motion in y is irrelevant because it contributes with a real part only in the effective potential.

The analytical expression (29) has the same form as the fit to the numerical results of [4]. For the values $q=\frac{1}{4}$, $Q=1$, $\mu_R=\frac{1}{2}$, and $\mu_r=2$ of the fictitious system, the value of the coefficient is $\lambda=\sqrt{2}$, which departs from the numerical value by only 5%. Residual differences between the analytical value and the fit value may be related to the quadratic approximation (3) of the potential energy around the Wannier ridge, while the classical trajectory calculations were performed without this approximation. Quantum mechanically ($\hbar=1$), condition (28) corresponds to the high-energy limit. This also explains the observation of Ref. [4] that the classical limit of the ionization probability has the same behavior as the far-from-threshold probability for ionization by heavy ions [13].

The classical [3] and quantum-mechanical derivation [5,8] of the threshold law (1) for the generic Wannier case lead to identical results. This is in contrast to the exceptional case $Q/q=4$ discussed here. In the generic Wannier case, Eq. (14) is valid because of the dominance of the scale-independent attractive Coulomb potential in the final channel. Since the potential $\varepsilon(R)$ is proportional to $\hbar$, the dependence on $\hbar$ drops out, and the quantum-mechanical and classical results coincide to lowest order in $\hbar$.

V. SUMMARY

We have derived the threshold law for three-particle breakup near threshold in the case when the Wannier exponent is infinite. The threshold law changes from a power law to an exponential behavior as a function of the the excess energy. An experimental realization of this behavior should be feasible, although the strong suppression of the cross section near threshold will probably make it difficult to confirm the analytically derived threshold coefficient κ.

The Wannier picture of propagation on the ridge of the three-particle potential remains valid. The classical threshold law, however, differs from its quantum-mechanical counterpart. This fact requires a refinement of the statement that Wannier theory is essentially a classical theory. The derived analytic form of the classical threshold law explains the behavior of previous numerical classical trajectory calculations.

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APPENDIX

The survival probability (12) is calculated with the momentum (7), $C_0=0$, and the coupling potential given by Eq. (10). We change the integration variable to $x=R^{3/2}$. The survival probability takes the form

$$P(E)=\exp\left[-\frac{2}{\hbar}\mathcal{J}(2\mu_R E,-2\mu_R\hbar C_1)\right], \tag{A1}$$

with the integral

$$\mathcal{J}(a,b)=\tfrac{2}{3}\,\mathrm{Im}\int_{x_0}^{\infty}x^{-1/3}\sqrt{a+b/x}\,dx. \tag{A2}$$

Partial integration gives

$$\mathcal{J}(a,b)\equiv\mathcal{J}_1+\mathcal{J}_2=\mathrm{Im}[x^{2/3}\sqrt{a+b/x}]_{x_0}^{\infty}+\mathrm{Im}\frac{b}{2}\int_{x_0}^{\infty}\frac{dx}{x^{4/3}\sqrt{a+b/x}}. \tag{A3}$$

For a real and positive, which corresponds to $E>0$, the upper limit of the first term $\mathcal{J}_1$ vanishes. The contribution of the lower limit is calculated in the limit $a\ll|b|/x$, which corresponds to Eq. (17). It gives

$$\mathcal{J}_1(a,b)=-R_0^{1/4}\mathrm{Im}\sqrt{b}-\frac{a}{2}R_0^{7/4}\mathrm{Im}\frac{1}{\sqrt{b}}+o(R_0^{13/4}), \tag{A4}$$

with

$$\mathrm{Im}\sqrt{b}=\sqrt{2\mu_R\hbar}|C_1|^{1/2}\sin[\tfrac{1}{2}\arg(b)],$$
$$\arg(b)=\pi-\tan^{-1}\frac{1}{\sqrt{2}}. \tag{A5}$$

The term $\exp[-2/\hbar\mathcal{J}_1]$ contributes to the correction term in Eq. (21). So does $\exp[-2/\hbar\mathcal{J}_2]$. The later also determines the threshold behavior of the survival probability. The integral is available in closed form:

$$\mathcal{J}_2(a,b)=\mathrm{Im}\left(\frac{3b}{2x_0^{1/3}\sqrt{a}}\ {}_2F_1[\tfrac{1}{3},\tfrac{1}{2};\tfrac{4}{3};-b/(ax_0)]\right). \tag{A6}$$

Expansion for $ax_0/|b|\ll1$ gives

$$\mathcal{J}_2(a,b)=\frac{a^{-1/6}}{2\sqrt{\pi}}\Gamma(\tfrac{1}{3})\Gamma(\tfrac{1}{6})\mathrm{Im}[b^{2/3}]-3R_0^{1/4}\mathrm{Im}\sqrt{b}+\frac{3a}{14}R_0^{7/4}\mathrm{Im}\frac{1}{\sqrt{b}}+o(R_0^{13/4}). \tag{A7}$$

When the expansions (A4) and (A7) for $\mathcal{J}_1$ and $\mathcal{J}_2$ are inserted into (A1) expressions (18), (19), and (21) for the threshold behavior of the breakup cross section and the threshold coefficient κ result.

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