Hidden Crossing Theory of Threshold Ionization of Atoms by Electron Impact

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The hidden crossing theory, familiar in the context of ion-atom collisions, is adapted to the computation of ionization cross sections and spin asymmetries for electron impact on atomic hydrogen. Computed ionization cross sections and spin asymmetry agree within 10% with measurements. A rapid variation of the spin asymmetry near threshold is found, and its origin is traced to anharmonic corrections to the Wannier threshold law for triplet spin states.

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The collective motion of charged particles is fundamental to atomic physics [1,2]. One of the most dramatic, and well-studied manifestations of collective motion is the Wannier threshold law [3] for the fragmentation of a neutral species into two electrons and a positively charged ionic core. Despite the extensive development of quantal theories of electron correlations in atoms, the correlation effects described by Wannier are difficult to fit into standard theories of ionization [4–8]. Present theory, for example, has not been able to give a complete *ab initio* description, over an extended energy range, of the correlations first treated classically by Wannier. A calculation by Crothers [9] for of the ionization of helium atoms by electron impact did incorporate the electron correlations, but did not consider higher order terms in the asymptotic development underlying Wannier's theory and was therefore unable to represent the correlations over an extended energy range. The difficulties of incorporating Wannier's correlations in quantal theories has prompted many researchers to resort to purely classical calculations [10,11]. This is quite natural, since the Wannier correlations are readily computed for classical orbits, but are difficult to include in quantal wave functions. Such classical descriptions can only be provisional, however, and a fully quantal theory represents a constant goal [8].

We have shown how the Wannier threshold law for the ionization of hydrogen atoms by proton impact emerges from the hidden crossing theory [12,13] which employs adiabatic electron eigenfunctions computed at fixed internuclear distance, Solov'ev [14]. For electron impact, theory employs the hyperspherical representation [2,15–17]. In this work we report the first calculations of ionization of atomic hydrogen by electron impact using the hidden crossing theory. Our computations generally agree well with experiment over an extended energy range, thus the hidden crossing theory provides a means to incorporate the many fragmentary insights that have emerged over the years into a complete *ab initio* theory of electron correlations near the Wannier threshold.

The adiabatic energy eigenvalues $\varepsilon(R)$ at complex hyperadius R represent the fundamental quantities in the hidden crossing theory. As in the theory for proton impact, the existence of a region where the eigenfunctions have harmonic oscillator structure [18] is essential to realize the Wannier threshold law. Integration through the harmonic oscillator region gives an asymptotic expression, the first term being the Wannier power law E^{ζ_W}, where E is total energy of the ionized electrons and ζ_W is the Wannier index, equal to 1.127 for electron impact on neutral atoms. Higher order anharmonic corrections give additional nonanalytic $\sqrt{E}$ and $E \ln E$ terms. Integration through the near zone connects the initial state with the harmonic oscillator region and determines an analytic function of E which sets the absolute cross section at $E = 0$.

We use the hyperspherical Hamiltonian in the form given by Lin and co-workers [16] and basis-spline codes developed by Boettcher and co-workers [19,20] to compute $\varepsilon(R)$ for complex R. The real part of the effective quantum number $n(R) = 1/\sqrt{-2\varepsilon(R)}$ plotted vs R represents a Riemann surface on which $\varepsilon(R)$ is single valued for negative $\varepsilon(R)$. Figure 1 shows the surface for the ^1S state. Notice the broad, flat, sloping region extending to infinite R separated from the real axis by a series of branch points. In this region, the wave functions $\varphi(R;\theta,\alpha)$ of the angle θ between the electron position vectors $\mathbf{r}_1$, $\mathbf{r}_2$ and the hyperangle $\alpha = \arctan(r_2/r_1)$ are harmonic oscillator eigenfunctions with energy eigenvalues given by

$$\varepsilon_{\text{ays}}(R) = -C_0/R - C_1/R^{3/2} + C_2/R^2 + \cdots, \quad (1)$$

where C_i are known constants derived from expansions about the potential saddle whose values need not concern us here. Terms R^{-n} with $n \geq 2$ give nonanalytic $\sqrt{E}$ contributions to the Wannier threshold law.

The transition matrix element in the hidden crossing theory involves the action integral $J = \int_{R_0}^{\infty}[K(R) - K_0(R)]\,dR$ evaluated along a path that starts at a small value R_0 on the real axis, goes around the first top-of-barrier branch point,

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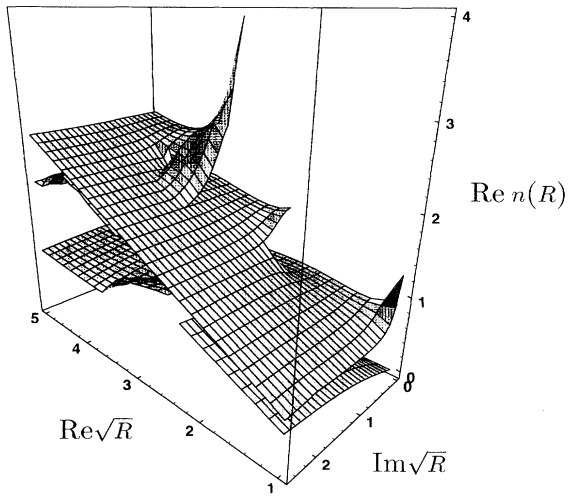

FIG. 1. Plot of the real part of $n(R) = 1/[-2\varepsilon(R)]^{1/2}$ vs $R^{1/2}$ for two electrons in the field of a proton.

and then to infinity along a path through the harmonic oscillator region as shown in Fig. 2. Here $K(R) = \sqrt{2E - \varepsilon(R)}$ and $K_0(R) = \sqrt{2(E + C_0/R)}$. At R_Q the exact $\varepsilon(R)$ is replaced by $\varepsilon_{\rm ays}(R)$. Because $\varepsilon_{\rm ays}(R)$ has no branch points, the integral from R_Q to infinity can be taken along a path that returns to R_0 and then to infinity along the real axis so that $J = \int_{R_0}^{\infty}[K_{\rm ays}(R) - K_0(R)]\,dR + \int_{R_0}^{R_Q}[K(R) - K_{\rm ays}(R)]\,dR$.

The ionization cross section for a given spin is given by

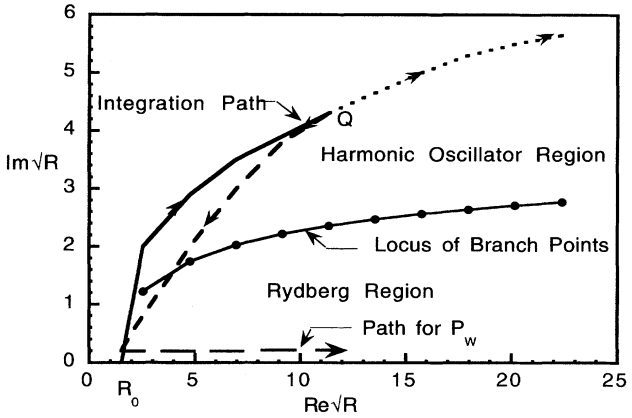

FIG. 2. Plot showing the integration path in the complex R plane to determine the ionization cross section. The locus of branch points separates the Rydberg region from the harmonic oscillator region. The integration path (solid path) for the ionization channel starts at R_0 on the real axis and goes around the first top-of-barrier branch point to infinite distances through the harmonic oscillator region. At R_Q the exact $\varepsilon(R)$ is replaced by the first few terms in its asymptotic expansion $\varepsilon_{\rm ays}(R)$ (dotted path). The integration path may be distorted to return to R_0 (dashed path) and then to infinity along the real axis. Integration of the asymptotic expression along this latter path determines the function $P_W(E)$.

$$\sigma^S = \frac{\pi}{2E+1}\sum_L (2L+1)P_L^S(E)P_W^{(L,S)}(E), \qquad (2)$$

where the asymptotic "Wannier" function $P_W^{(L,S)}(E)$ is given by

$$P_W^{(L,S)}(E) = \left|\exp\left[i\int_{R_0}^{\infty}[K_{\rm ays}(R) - K_0(R)]dR\right]\right|^2 \times \int_0^{\pi}\int_0^{\pi/2}|\varphi(R_E;\theta,\alpha)|^2 d\alpha\,\sin\theta\,d\theta\,. \qquad (3)$$

The functions $P_L^S(E)$ relate to the integration connecting the initial channel to harmonic oscillator region at R_Q. For S and P singlet and triplet channels, computations of the hyperspherical $\varepsilon(R)$ show that the initial state connects to the harmonic oscillator region at a top-of-barrier branch point as in Fig. 1. In this circumstance, there are always two paths around the branch point which contribute. In the semiclassical sense, one path c_1 represents ionization as the incident electron approaches the atom and another c_2 as it leaves. Then $P_L^S(E)$ is given by

$$P_L^S(E) = \left|\exp\left[i\int_{c_1}^{R_Q}[K(R) - K_{\rm ays}(R)]dR\right] + \exp\left[i\int_{c_2}^{R_Q}[K(R) - K_{\rm ays}(R)]dR\right]\right|^2. \qquad (4)$$

For L greater than 1, the initial channel and the harmonic oscillator regions are not connected by a top-of-barrier branch point. The ^1D and ^3F channels are indirectly connected, however. Letting ℓ_1, ℓ_2 denote the single-electron orbital angular momentum numbers we have, for example, that at $R = 0$ the initial $(\ell_1, \ell_2) = (0,2)^1D$ channel mixes with the $(1,1)$ channel, since the eigenvalues are degenerate [21]. The $(1,1)$ channel does have a top-of-barrier branch point so that the harmonic oscillator region is reached by a transition near $R = 0$ followed by a transition to the harmonic oscillator region. In this case only the path c_2 contributes.

The energy eigenvalues have been computed exactly (to within our numerical accuracy) using the basis-spline technique as discussed above. Equation (4) was then used to calculate $P_L^S(E)$. The asymptotic Wannier function $P_W^{(L,S)}(E)$ is known in closed form [13], thus the cross sections σ^S and spin asymmetry A are computed using Eq. (2) and the definition

$$A = \frac{\sigma^{(1)} - \sigma^{(3)}}{\sigma^{(1)} + 3\sigma^{(3)}}. \qquad (5)$$

Figure 3(a) compares the computed and measured [22] cross section for the ionization of atomic hydrogen by electron impact. Good agreement in shape for $E < 1$ eV is expected since $P_W^{(L,S)} \to E^{\zeta_W^{ad}}$, where ζ_W^{ad} differs from the exact Wannier index by less than 3%. The overall normalization is given by the "inner" function $P_L^S(E)$. The

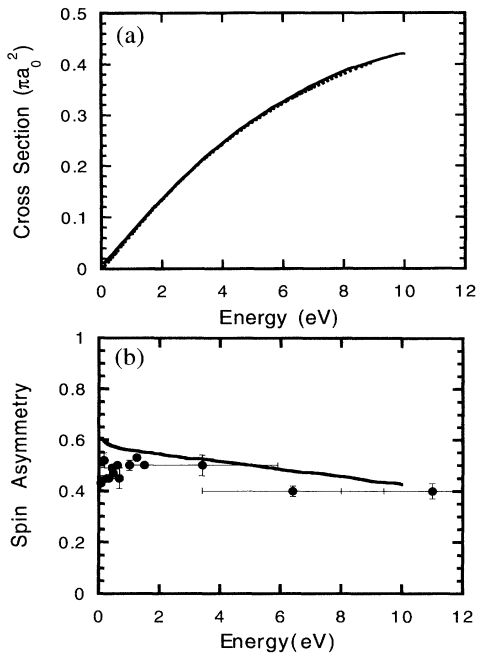

FIG. 3. (a) Cross section for the ionization of atomic hydrogen by electron impact. The solid curve is a calculation based on the hidden crossing theory, and the dots are the experimental data of Ref. [22]. The theory has been multiplied by 0.93 to agree with the measurements at 9 eV in order to show the agreement between the measured and computed energy variation of the cross section. (b) Comparison of the measured spin asymmetry (points with error bars) of Ref. [23] for electron impact on atomic hydrogen with the hidden crossing theory (solid curve).

theory has been multiplied by a factor of 0.93 in order to show the agreement in shape over the entire energy range. Figure 3(b) compares the computed spin asymmetry with the spin asymmetry measured by Lubell and co-workers [23]. The computed value of 0.6 at threshold is not in good agreement with the measured value of 0.4, but for energies of 1 to 10 eV the agreement is good. Our results confirm a rapid variation of the spin asymmetry [24] between threshold and 1 eV, but quantitative agreement is lacking. The rapid variation can be traced to anharmonic corrections for the ^3P state. For all other states the anharmonic corrections are small. In this connection note that integration around the first top-of-barrier branch point also gives the probability for excitation to states with principal quantum number $n = 2$, and this probability has been computed essentially exactly for $E = 0.405$ au [25]. Our calculations using the hidden crossing theory agree with these more conventional results within 10%. Despite the imperfect agreement at threshold, these first *ab initio* calculations of the Wannier threshold show that theory can accurately describe the electron-electron correlations for two electrons when both electrons are in continuum states.

Our quantitative results using the hidden crossing theory resolve several issues concerning the Wannier threshold law. Firstly, absolute cross sections and spin asymmetry in good agreement measurements over an extended energy range are obtained. Secondly, the Wannier factor $E^{\zeta w}$ is seen to be the first term in an asymptotic series, the higher terms of which include nonanalytic factors. Thirdly, we confirm [26] the importance of nonzero L even for $E = 0$. Finally, only the lowest harmonic oscillator mode is used for each partial wave. Higher modes enter only through the matching of adiabatic to diabatic functions at R_Q. These contributions are negligible for neutral atoms. The angular distribution in θ is Gaussian for each partial wave, but, since each Gaussian is different for the several partial waves, the final angular distribution is not Gaussian. The hidden crossing theory appears to get the main features of threshold ionization correct. It can be further developed to include small contributions from more remote branch points, higher anharmonic corrections, and diabatic corrections to analyze departures from the simple Wannier predictions. Previously, these small corrections have mainly been investigated classically.

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