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Wave propagation and diffraction on a potential ridge

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The drastic perturbation of high Rydberg levels in a magnetic field is interpreted as a prototype effect of wave propagation on a ridge with formation of standing waves and with diffraction from radial into angular excitation modes. Analogs of this phenomenon include two-electron excitations into continuum or high Rydberg levels and may well be quite numerous since ridges occur generally on molecular potential surfaces. The Wannier-Peterkop-Rau theory of two-electron detachment at threshold is shown to provide the essential mathematical model for the description of these phenomena in terms of a base set of two eigenmodes that mediate the diffraction process. The apparent limitation of the original theory to an infinitesimal range of coordinates straddling the ridge is lifted. The problem remains of utilizing the eigenmodes as mediators of the coupling among the complete sets of adiabatic modes that seem to afford an adequate description of phenomena away from the ridges, that is, in potential valleys.

I. INTRODUCTION

In 1953 Wannier[1] made a key remark on the process of molecular ionization by electron collision at energies E barely in excess of the threshold I. He pointed out that the incident and the ejected electron can simultaneously escape the molecular field only by moving in their joint phase space along classical trajectories within a certain narrow bundle. The useful width of this bundle shrinks as E decreases causing the ionization cross section to become proportional to $(E-I)^{\zeta}$, where $\zeta = 1.127$ (for a neutral molecule) is a root of a second-degree equation referred to in the following as the "Wannier equation." The limit of the shrinking bundle represents the two electrons as maintaining equal distances from the residual ion during their escape. Thus it consists of configurations in unstable equilibrium, because either electron that may lag behind the other remains more exposed to the ionic field and will fail to escape.

Wannier's conclusion met with resistance, partly because of its reliance on classical mechanics for low speed electrons and partly because it was disconnected from other aspects of the ionization process. This lack of connection was in fact modeled after the formulation of Wigner's threshold law for single particle ejection in zero field. Wannier's analysis has since been successfully duplicated in a wave mechanical Wentzel-Kramers-Brillouin (WKB) approximation by Peterkop[2] and Rau[3] in 1970 and its conclusion has been strikingly verified in a 1973 experiment by Cvejanovic and Read.[4]

Several considerations have enlarged the role of Wannier's analysis in the wake of its experimental verification. On the experimental side it was suggested that the ionization threshold law implies a corresponding law for the threshold excitation of high Rydberg states.[5] On the theoretical side it became apparent that both of these threshold laws should evetually be incorporated in an extended Macek-Lin treatment of doubly excited helium.[6] All these studies were formulated in hyperspherical coordinates but the threshold law analysis was confined to an infinitesimal cone of the hyperspace; removal of this restriction should help their consolidation.

The main point raised in this paper is that the essence of the Wannier-Peterkop-Rau analysis transcends its application to collision threshold laws. The analysis actually bears on the classical or wave mechanical motion of any system along the ridge of a rounded potential barrier represented by

$$a(x) - b^2(x)y^2 , \tag{1}$$

with the x axis lying along the ridge. This potential will depend, in general, on additional coordinates, but the pair (x, y) is singled out here because motion along the x axis is of primary interest in the examples to be considered and because the potential decreases as y departs from $y=0$ in either direction. Thereby the x axis represents a locus of points of *unstable equilibrium*. The Wannier analysis is now seen to identify eigenmodes of motion that remain quasistationary in spite of this instability while propagating along x. The ridge is also viewed as the locus of breakdown of quasi-adiabatic approximations that have been successful for treating nonseparable systems such as the pair of electrons in doubly excited helium.[6,7] Indeed, motion along the ridge may provide the main mechanism for a massive transfer of excitation between degrees of freedom (x, y) whose coupling can be treated as an adiabatic perturbation in other regions of configuration space. The occurrence

of this set of properties will be called the "Wannier phenomenon."

A prototype for an extended Wannier analysis is afforded by the motion of a single Rydberg electron in a magnetic field, a phenomenon that displays remarkable "quasi-Landau" resonances extending into the continuum.[8-11] Here the sum of the Coulomb and diamagnetic potentials

$$V(r,\theta) = -1/r + \tfrac{1}{2}\alpha^2 r^2 \sin^2\theta$$
$$= (-1/r + \tfrac{1}{2}\alpha^2 r^3) - \tfrac{1}{2}\alpha^2 r^2 \cos^2\theta\,, \qquad (2)$$

has a ridge along $\theta = \frac{1}{2}\pi$ in a meridian plane; that is, $\theta = \frac{1}{2}\pi$ in Eq. (2) corresponds to $y = 0$ in Eq. (1). This potential rises to infinity as r increases along the ridge, where $\sin^2\theta = 1$, in contrast to Wannier's application to a pair of electrons in a Coulomb field where the potential flattens out as indicated by $a(\infty) = 0$ in Eq. (1). (The quasi-Landau resonances arise from formation of standing waves along this ridge.) That notable phenomena result from propagation along potential ridges with different asymptotic behavior suggests that the essential features of the Wannier phenomenon relate to *local* properties of the potential field (1) or (2) along the ridge rather than to its asymptotic behavior. Accordingly we shall not specify the functions $a(x)$ and $b(x)$ in Eq. (1), in contrast to Refs. 1–3, except by requiring them to vary slowly over a wavelength of propagation as one would do in WKB procedures.

We aim then at disentangling the general aspects of the Wannier phenomenon by an adaptation of Peterkop's[2] treatment. The magnetic-Rydberg problem will serve as the main context for our treatment because it involves a minimum of extraneous elements; this context will be described in Sec. II, reviewing and extending the approach of Refs. 9 and 10. Section III will present the new development while the concluding comments of Sec. IV will introduce the remaining problem of utilizing the Wannier approach to remedy the localized breakdown of adiabatic treatments.

II. THE MAGNETIC-RYDBERG PROBLEM

The Schrödinger equation for an electron in the potential field (2), with orbital magnetic quantum number m, is represented in a.u. by

$$\left(\frac{d^2}{dr^2} + 2E_m + \frac{2}{r} - \frac{\Lambda_m^2}{r^2}\right) f_m(r,\theta) = 0\,, \qquad (3)$$

$$\Lambda_m^2 = -\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{m^2}{\sin^2\theta} + \alpha^2 r^4 \sin^2\theta\,, \qquad (4)$$

[Eqs. (5) and (6) of Ref. 10]. Here α indicates the frequency of Larmor rotation ($\alpha/B = 2.13\times10^{-10}$ a.u./gauss) and the energy eigenvalue E_m excludes the Paschen-Back contribution of spin and orbit. The operator Λ_m^2 is the sum of the squared orbital momentum $\vec{l}^2$, for a given value of m, and of the diamagnetic potential energy $\alpha^2 r^2 \sin^2\theta$ multiplied by r^2. It will be regarded as a function of the parameter αr^2. For each value of αr^2, Λ_m^2 has a complete set of eigenfunctions called the oblate-spheroidal functions g_{lm},[12]

$$\Lambda_m^2 g_{lm}(\alpha r^2;\theta) = [\lambda_{lm}(\alpha r^2) + \alpha^2 r^4] g_{lm}(\alpha r^2;\theta)\,. \qquad (5)$$

The eigenvalue of this equation has been separated into λ_{lm} and $\alpha^2 r^4$ according to a standard practice[12] which will prove convenient. Equation (5) reduces to that of associated Legendre polynomials in the limit of $\alpha r^2 \to 0$ (i.e., for zero value of the magnetic field and/or radial distance) in which case the ordering label $l \geq |m| = 0, 1, 2, \ldots$, coincides with the orbital quantum number, $\lambda_{lm} \to l(l+1)$.

The spectral effects of the diamagnetic term $\alpha^2 r^4 \sin^2\theta$ in Eq. (4) remain extremely small for low Rydberg levels and for laboratory fields. For higher excitations, as the mean value $\langle \alpha r^2 \rangle$ increases, each spectral level begins to rise above its zero-field value reflecting an increase of the corresponding eigenvalue of Λ_m^2 (Fig. 1). Simultaneously each node or antinode of $g_{lm}(\alpha r^2;\theta)$ at $\theta < \frac{1}{2}\pi$ shifts progressively toward $\theta = 0$, while those at $\theta > \frac{1}{2}\pi$ shift toward $\theta = \pi$ (Fig. 2). This shift results from the field hindering any electron motion orthogonal to the coordinate axis. However, symmetry requires the antinode (or node) that lies at $\theta = \frac{1}{2}\pi$ for even (odd) value of $l - m$ to remain fixed; this circumstance will prove important.

Note also that the diamagnetic term $\alpha^2 r^4 \sin^2\theta$ in Eq. (4) represents a potential barrier separating two valleys at $\theta \lessgtr \frac{1}{2}\pi$. The parameter λ_{lm} in Eq. (5)—more properly $\lambda_{lm} - m^2$—measures the *excess* of the eigenvalue of Λ_m^2 *over the ridge* of this barrier, $\alpha^2 r^4 + m^2$. Hence an eigenfunction $g_{lm}(\theta)$ oscillates in the barrier region as well as over both valleys if $\lambda_{lm} > m^2$, but it tunnels through the barrier and oscillates only in each valley for $\lambda_{lm} < m^2$. Figure 1 shows how each $\lambda_{lm}(\alpha r^2) - m^2$ is positive for low αr^2 but becomes negative at large r; the transition between these two regimes is critical for our problem. In the limit of $r \to \infty$ each spheroidal function g_{lm} reduces to a pair of oscillator functions of the variable $r\sin\theta$, one centered at $\theta = 0$ and one at $\theta = \pi$.

An adiabatic approximation[10] considers approximate solutions of Eq. (3), $f_m \sim h_{lm}(r) g_{lm}(\alpha r^2;\theta)$,

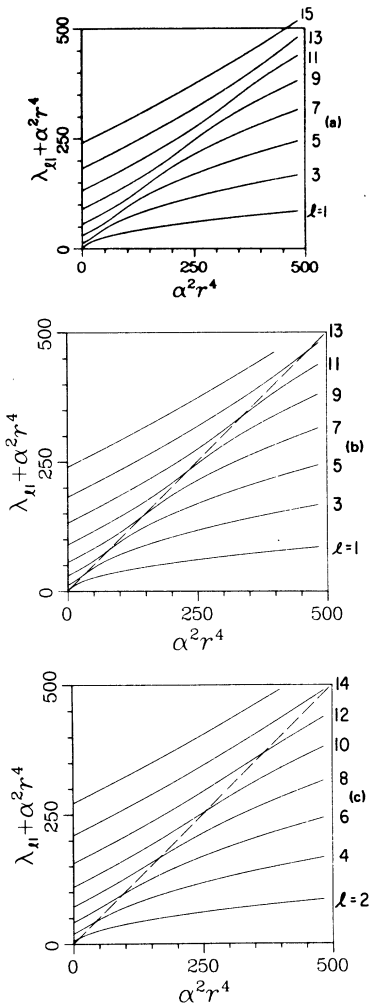

FIG. 1. Eigenvalues of the oblate spheroidal Eq. (5) versus α^2r^4: (a) $m=1$ and $l-m$ even, showing sequence of avoided crossings; (b) same as (a), with line representing the locus of avoided crossings, Eq. (8a); (c) same as (b) for $l-m$ odd, showing weak effect of avoided crossings. [The contrast of curves in (b) and (c) is analogous to that of solid and dashed curves in Fig. 6 of Ref. 6]. (Courtesy of G. L. Webster.)

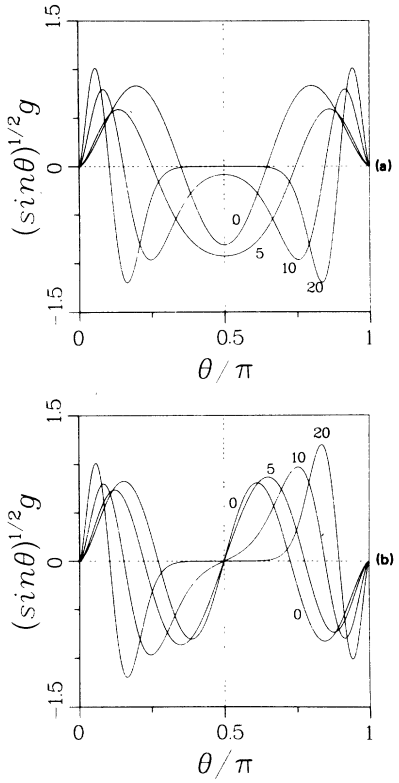

FIG. 2. Eigenfunctions of the oblate spheroidal Eq. (5) for different values of the parameter αr^2: (a) $l=3$, $m=1$; (b) $l=4$, $m=1$. Curves in (a) and (b) show contrasting dependence on αr^2 near $\theta/\pi=0.5$ (courtesy of G. L. Webster).

disregarding derivatives $\partial g_{lm}/\partial r$. This approach becomes inadequate as αr^2 increases and affects the g_{lm} at an increasing rate. Exact solutions of Eq. (3) have the expansion

$$f_m(r,\theta)=\sum_l{}' h_{lm}(r)\,g_{lm}(\alpha r^2;\theta), \tag{6}$$

which reduces Eq. (3) to the system of coupled ordinary equations

$$\left(\frac{d^2}{dr^2}+2E_m+\frac{2}{r}-\frac{\lambda_{lm}(\alpha r^2)+\alpha^2r^4}{r^2}\right)h_{lm}(r)+\sum_{l'}{}'\left[2\left(g_{lm}\left|\frac{dg_{l'm}}{dr}\right.\right)d/dr+\left(g_{lm}\left|\frac{d^2g_{l'm}}{dr^2}\right.\right)\right]h_{l'm}(r)=0\,. \tag{7}$$

The $\sum'$ in (6) and (7) indicates summation over *even* values of $l'-l$ *only*, as appropriate to the symmetry of (3) under $\theta\to\pi-\theta$. Equation (7) shows how the diamagnetic potential affects the motion of the electron at two separate levels of approximation. At the adiabatic level it merely replaces each eigenvalue $l(l+1)$ of $\vec{l}^2$ by the eigenvalue $\lambda_{lm}+\alpha^2r^4$ of Λ_m^2. This level of approximation is represented by disregarding the second line of Eq. (7), whereby $h_{lm}(r)$ is determined by a radial equation with the potential $-2/r+(\lambda_{lm}+\alpha^2r^4)/r^2$ and each spectral line is shifted to shorter wavelengths as shown on the right-hand side of Fig. 3. At a higher level one considers that the factor $\sin^2\theta$ of the diamagnetic potential has matrix elements off-diagonal in l. This effect introduces the terms in the second line of Eq. (7) which couple the equations for different radial amplitudes h_{lm} and

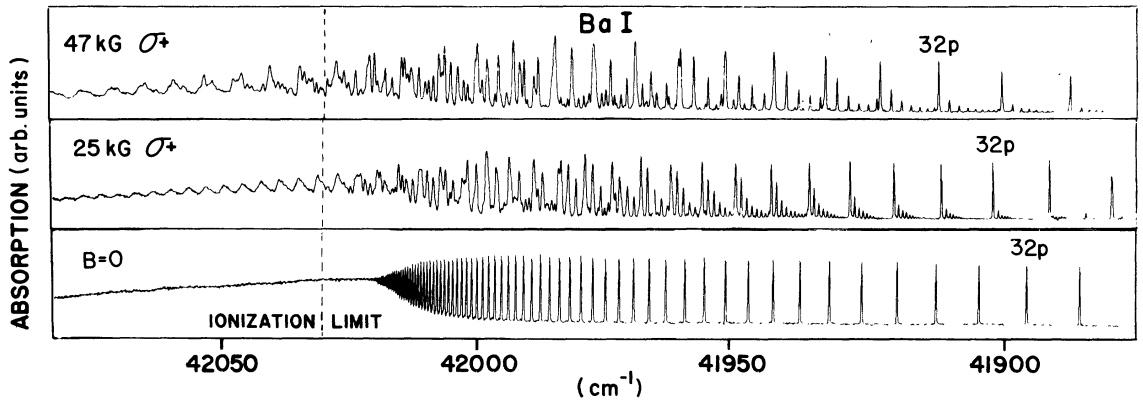

FIG. 3. Absorption spectrum of barium near the ionization limit in fields of different strengths. Values of $l-m$ are even for initial and final levels of $\sigma+$ transitions (from Ref. 8).

$h_{l'm}$. These coupling terms remain small for moderate values of αr^2, where they can be treated as perturbations (*quasiadiabatic approximation*).

The effects of the coupling terms manifest themselves in the spectra as the principal quantum number n increases along a spectral series with a concurrent increase of $\langle \alpha r^2 \rangle$. First, they break down the optical selection rules which restrict the values of the orbital number l, thus causing the appearance of additional lines. Figure 3 shows satellite lines appearing in the absorption spectrum at increasing values of n; these lines can be labelled initially with values of l' different from the single l observed at lower n. As n increases further, the intensity of the satellites increases rapidly and their classification becomes uncertain. We witness here a breakdown of the quasiadiabatic approximation. The further appearance of a periodic "quasi-Landau" modulation of the spectrum near and beyond the ionization threshold is totally foreign to the adiabatic approach; its quantitative interpretation is a goal pursued here.

Breakdowns of adiabaticity generally result from "avoided crossings" of adiabatic eigenvalues—i.e., in our case, of the curves $\lambda_{lm}(\alpha r^2)+\alpha^2 r^4$ versus $\alpha^2 r^4$—which imply rapid variations of the channel eigenfunctions g_{lm}. Figure 1 displays a striking sequence of avoided crossings along the line $\lambda_{lm} = m^2$. Several circumstances indicate strongly that these avoided crossings originate from a phenomenon occurring along the ridge of the diamagnetic potential, at $\theta = \frac{1}{2}\pi$:

(a) The condition $\lambda_{lm} = m^2$ marks the transition of the wave functions $g_{lm}(\theta)$ from oscillatory to tunnelling behavior at $\theta = \frac{1}{2}\pi$.

(b) The avoided crossing behavior in Fig. 1 is far more apparent for even than for odd values of $l-m$, which are distinguished by the occurrence of antinodes rather than of nodes of $g_{lm}(\theta)$ at $\theta = \frac{1}{2}\pi$.

(c) The transition from oscillatory to tunnelling behavior of a wave function is indeed far sharper at an antinode than at a node (Fig. 2). As αr^2 increases but $\lambda_{lm}(\alpha r^2)$ still remains $> m^2$, the amplitude of $g_{lm}(\theta)$ *increases* at the antinode $\theta = \frac{1}{2}\pi$, in proportion to $(\lambda_{lm} - m^2)^{-1/4}$, as long as a WKB approximation remains valid; when WKB fails the drop of $g_{lm}(\alpha r^2; \frac{1}{2}\pi)$ toward its small values characteristic of the tunnelling regime is thus dramatic.

(d) The quasi-Landau modulation of the absorption spectrum of Fig. 3, in the high Rydberg range and beyond the ionization threshold, has been accounted for in terms of standing waves forming along the ridge, $\theta = \frac{1}{2}\pi$, by a one-dimensional model that sets $\theta = \frac{1}{2}\pi$ and disregards $\partial/\partial\theta$ in Eqs. (3) and (4).[11]

Qualitatively the breakdown of adiabaticity at $\theta = \frac{1}{2}\pi$ becomes apparent by considering the symmetry under reflection of $\theta - \frac{1}{2}\pi$. As a wave function propagates outward from the low r range, the diamagnetic potential tends to deflect it toward $\theta = 0$ or $\theta = \pi$. This deflection can proceed adiabatically for $\theta \neq \frac{1}{2}\pi$ but is hindered by symmetry which keeps an antinode or node locked at $\theta \sim \frac{1}{2}\pi$ (Fig. 2). As a result the wave keeps propagating along the potential ridge until it is stopped by the rising level of the potential along the ridge, $\alpha^2 r^2$. The breaking of the wave is reflected in the appearance of spectral lines with higher values of l. Indeed the excitation of higher-l components of the wave field (6) represents a *transfer of energy away from the radial motion* whose wave number is reduced by the increased value of λ_{lm} in Eq. (7).

In conclusion the *locus of the breakdown* of the quasiadiabatic approximation is identified by the pair of conditions

$$\lambda_{lm}(\alpha r^2) \sim m^2, \tag{8a}$$

$$\theta \sim \tfrac{1}{2}\pi, \tag{8b}$$

in our magnetic-Rydberg example. References 6 and 7 yield an analogous pair of conditions for the motion of a pair of electrons in a central field. In that second example the breakdown of adiabaticity is responsible for double excitations by photoabsorption and for all excitations by slow-electron impact. Similar effects will presumably occur for any wave propagating along a potential ridge, typically along the ridges of molecular potential surfaces.

Two steps will be required to remedy this breakdown:

(1) To develop a solution of Eq. (3), or analogous equation, that describes the Wannier phenomenon of propagation along the ridge. Such a specialized solution need not hold far outside the range of Eqs. (8a) and (8b) but it must permit matching to solutions valid in other regions. This development forms the subject of Sec. III. (2) To combine the Wannier solution with quasiadiabatic procedures that may hold in other ranges.

III. PROPAGATION ALONG THE RIDGE

Equation (3), which governs the Wannier phenomenon in the region identified by the conditions (8a) and (8b), will be considered here as a special case of the wave equation

$$(\nabla^2 + k^2)\psi = 0\,, \tag{9}$$

with a certain dependence of the wave number k on the space variables. It will be adequate to consider initially a two-dimensional space, as in Eq. (3), because only two space variables play a critical role here as in the two-electron six-dimensional problem considered by Wannier; indeed the determination of the Wannier parameter ζ hinges only on variations of the potential within the plane of radial variables (r_1, r_2).

To recast Eq. (3) in the form (9), the condition (8b) suggests using the pair of coordinates $(r, \theta - \frac{1}{2}\pi)$. Setting

$$\xi = \theta - \tfrac{1}{2}\pi\,, \tag{10}$$

Eqs. (3)–(5) yield

$$k^2(r,\xi) = k_0^2(r) + \tfrac{1}{2}k_1^2(r)\xi^2\left(1 + 2\sum_{n=1}^{\infty}\frac{(-4\xi^2)^n}{(2n+2)!}\right) + O\left(\frac{m^2}{r^2}\right), \tag{11}$$

$$k_0^2 = 2E_m + 2/r - \alpha^2 r^2\,, \quad k_1^2 = 2\alpha^2 r^2\,, \tag{12}$$

where the terms $O(m^2/r^2)$ are negligible in practice. The quadratic dependence of k^2 on ξ is central to the Wannier phenomenon.

Consider now the condition (8a). It implies that the kinetic energy of the electron stems *entirely* from motion *along* the ridge $\xi = 0$. Indeed the solution of Eq. (5) for $\lambda_{lm} = m^2$ coincides for $\theta \sim \frac{1}{2}\pi$ with a parabolic cylinder function[13] of order zero whose expansion $1 - c\xi^4 + \cdots$ lacks the term $\propto \xi^2$. (The alternative solution odd in ξ has the expansion $\xi - c'\xi^5 + \cdots$.) The Starace calculation (item d above) amounted to integrating Eq. (9) by WKB method along the r axis—i.e., on the ridge—considering only the k_0^2 term of Eq. (11). The phase of the Peterkop-Rau wave function *on* the ridge can be derived in the same manner. Thus we characterize the solution of interest of Eq. (9) as *oscillating along the ridge* according to

$$\psi(r, 0) \propto \sin \int^r k_0(r')\,dr'\,. \tag{13}$$

A. The Wannier phenomenon

Further guidance is provided by reviewing the substance of Wannier's original analysis.[1] The r axis in our present context corresponds in Wannier's problem to the line $r_1 = r_2$ which constitutes the axis of the bundle of trajectories mentioned at the outset of this paper. Other trajectories of that bundle are deflected by a force, $-\partial V/d\xi \propto \xi$ in our coordinates, which increases linearly with ξ and whose effect is governed by $(d/dt)(mr^2 d\xi/dt) = -\partial V/\partial\xi$. Wannier transforms this equation of motion into an equation for the trajectories, $\xi = \bar{\xi}(r)$, by eliminating the time variable through the relation $d\xi/dt = (d\bar{\xi}/dr)(dr/dt)$ and applying an approximation linear in $\bar{\xi}$ and $d\bar{\xi}/dr$. Using then $md^2r/dt^2 = -\partial V/\partial r$ and the kinetic energy expression $T = E - V(r, \xi)$, Wannier's equation for the trajectories reduces to

$$2T\left(r^2\frac{d^2\bar{\xi}}{dr^2} + 2r\frac{d\bar{\xi}}{dr}\right) + \frac{\partial T}{\partial r}r^2\frac{d\bar{\xi}}{dr} = \frac{\partial T}{\partial\xi} \propto \bar{\xi}\,. \tag{14}$$

In our context T is represented by $\frac{1}{2}k^2(r, \xi)$, whereby (14) becomes

$$\frac{d^2\bar{\xi}}{dr^2} + \frac{d\ln(k_0 r^2)}{dr}\frac{d\bar{\xi}}{dr} - \tfrac{1}{2}\frac{k_1^2}{k_0^2 r^2}\bar{\xi} = O(\xi^2); \tag{15}$$

terms of order ξ^2 are to be disregarded in accordance with Wannier's linearization. In Wannier's problem—and within a "Coulomb zone", $|E| \ll |V|$—the coefficients of Eq. (15) can be made constant by taking $\ln r$ as the independent variable. A general trajectory that obeys Eq. (15) with constant coefficients is, of course, a superposition of a base set of two exponential solutions. Each of these exponential solutions is an eigenvector of translations along the potential ridge.

In this paper the coefficients of Eq. (15) will be treated instead as locally constant, that is, as slowly variable in the sense of WKB approximations. This approach was anticipated by the remark at the end of Sec. I about the Wannier phenomenon relating to local properties of the potential

field along the ridge. General solutions of Eq. (15) with slowly variable coefficients are superpositions of a base set of two exponential WKB solutions.

That WKB approaches are relevant to our class of problems is manifested by the large quantum numbers of the relevant states. (Variational approaches are instead appropriate for low quantum numbers.) For the Wannier problem the specific WKB condition $|d\chi/dr| \ll 1$ is demonstrated to hold explicitly for $r \gg 1$ in Footnote 19 of Ref. 3. This condition holds also in the magnetic-Rydberg problem, except at large-r turning points which will require a special treatment. Wannier himself has discussed the validity of a classical treatment extensively.[1]

On this basis I identify the Wannier phenomenon as the existence of particular bundles of solutions of the trajectory Eq. (15) that converge (or diverge) exponentially to (from) the ridge $\xi = 0$. The rate of convergence (divergence) is a root ζ of the second-degree algebraic equation with coefficients equal to the local value of the coefficients of Eq. (15). These special bundles of trajectories constitute *eigenmodes* of motion of a particle—or system of particles—in the region about a potential ridge. These eigenmodes are characterized by a distribution in ξ whose profile remains *translationally invariant along the ridge* to within the slow variation of the coefficients of Eq. (15). The goal of this section is to describe the wave mechanical analog of the Wannier eigenbundles of trajectories.

The Wannier law for threshold ionization results from arguing that the pair of incident and ejected electrons escapes at near-threshold energies through the eigenbundle of diverging trajectories. The root ζ for the diverging eigenbundle represents its rate of attenuation along the potential ridge. The divergence itself implies that a part of the bundle feeds into highly excited but bound states rather than into ionization; this process has only been outlined qualitatively thus far[6] as its further description will require a wave mechanical representation. Completing this description is an eventual goal of the development initiated in the present paper. In the magnetic-Rydberg phenomenon the trajectory eigenbundles cannot escape the atom along the ridge $\xi = 0$, where the potential rises as $\alpha^2 r^2$. There results reflection at a turning point r_1; in a wave mechanical treatment the reflection generates standing waves whose amplitude exhibits the quasi-Landau resonances as a function of energy. The trajectories with $\bar{\xi} \neq 0$ should then diverge eventually away from the ridge i.e., into either of the potential valleys leading to $\theta = 0$ or $\theta = \pi$.

B. General procedure

To construct a solution of Eq. (9) that propagates on the ridge according to Eq. (13), we represent this solution in terms of amplitude and phase functions by setting

$$\psi(r, \xi) = f_m(r, \theta)/r = A(r, \xi) e^{iS(r,\xi)}, \tag{16}$$

with A and S real. Introducing the phase function S serves to identify the direction of motion of the particle because $A^2 \vec{\nabla} S$ represents the current density in our units. Standing wave solutions of Eq. (9) are represented by combining (16) with its complex conjugate. Substitution of (16) transforms Eq. (9) into a system of two equations for A and S (Ref. 14),

$$\nabla^2 A + (k^2 - |\vec{\nabla} S|^2) A = 0, \tag{17}$$

$$2\vec{\nabla} A \cdot \vec{\nabla} S + A \nabla^2 S = 0. \tag{18}$$

Equation (18) is equivalent to the continuity equation of the particle flux for a stationary state

$$\vec{\nabla} \cdot A^2 \vec{\nabla} S = 0, \tag{18'}$$

for $A \neq 0$.

A WKB approximation is often introduced to solve the system of Eqs. (17) and (18) by disregarding the $\nabla^2 A$ term in Eq. (17), inasmuch as geometrical optics relies on the amplitude of a wave varying much more slowly than its phase. Equation (17) reduces then to the Hamilton-Jacobi equation

$$|\vec{\nabla} S|^2 = k^2(r, \xi), \tag{19}$$

whose solution identifies classical trajectories as the streamlines of $\vec{\nabla} S$. The amplitude function $A(r, \xi)$ is determined in a second step from the continuity Eqs. (18') or (18). This approach originates from the familiar applications to one-dimensional systems: Setting ξ at 0, Eq. (19) would yield $S = \int^r k_0(r')\, dr'$—as in Eq. (13)—and Eq. (18) would then yield $A = k_0^{-1/2}$. Equation (17) is then satisfied only to the extent that $\nabla^2 A = d^2 A/dr^2 = d^2(k_0^{-1/2})/dr^2$ is negligible; therein lies the WKB approximation.

A lesser resort to approximation is, however, required when following the same approach in the presence of two, or more, independent variables as shown below. We shall in fact proceed through the following steps.

(1) Introduce Eq. (19) as a subsidiary condition to Eq. (17) designed to *select* a particular solution that behaves in accordance with Eq. (13). A concurrent boundary condition is also imposed, namely, that $\vec{\nabla} S$ be parallel to the r axis at $\xi = 0$. This condition identifies the phase function to be constructed in Sec. III C by integrating Eq. (19) away from $\xi = 0$.

(2) Solve the continuity Eq. (18), thereby determining the variation of the amplitude function $A(r,x)$ along each streamline of $\vec{\nabla}S$ (Sec. III D).

(3) Solve the equation

$$\nabla^2 A = \frac{1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial A}{\partial r} + \frac{1}{r^2}\frac{\partial^2 A}{\partial \xi^2} = 0 , \tag{20}$$

that is, the residue of Eq. (17) after having solved (19) (Sec. III E).

Here we see how the problem of solving the system (17) and (18) depends critically on the number of independent variables. Equation (20) consists of two terms in our problem with the coordinates (r, ξ); in general it consists of one term per independent variable. The solution of Eq. (18) amounts to fixing one of these terms corresponding to the variation of A in the direction of $\vec{\nabla}S$; hence it determines $\nabla^2 A$ completely in a one-dimensional system, whereby Eq. (20) can be satisfied only in a WKB approximation. This structure is reduced in the presence of additional variables, since previous solution of Eqs. (18) and (19) no longer fixes the value of $\nabla^2 A$. Equation (20) will thus be regarded in Sec. III E as the wave equation governing the variations of A in directions orthogonal to $\vec{\nabla}S$. This equation is nevertheless not altogether independent of Eqs. (18) and (19); it will be made compatible with them only by treating its coefficients as independent of S, thus introducing an attenuated form of WKB approximation. Its integration will yield slow variations of A in directions orthogonal to $\vec{\nabla}S$, as expected for a WKB amplitude, but these variations are essential to multivariable wave propagation.

The succession of steps outlined here will be carried out explicitly for our prototype two-variable (r, ξ) system, with complementary remarks on the extension to multivariable problems. Two alternative parametrizations will be utilized:

(a) Expansion of $S(r, \xi)$ and $A(r, \xi)$ into powers of ξ^2, following the procedure of Peterkop.[2] Peterkop's truncation of the expansion, disregarding terms of $O(\xi^4)$, will be seen to give adequate consideration to the essential features of the problem.

(b) Replacement of the ordinary coordinates (r, ξ) with an intrinsic pair of orthogonal coordinates (S, T), such that $S = \text{const}$ represents a line of constant phase and $T = \text{const}$ represents a classical trajectory. The wave propagation properties will be embodied in the metric for these coordinates, as described in the following.

C. The Hamilton-Jacobi equation

Consider the expansions

$$S(r, \xi) = \sum_{n=0}^{\infty} S_n(r) \frac{\xi^{2n}}{(2n)!} = S_0(r) + \tfrac{1}{2} S_1(r)\xi^2 + O(\xi^4) , \tag{21}$$

$$\vec{\nabla}S(r, \xi) = \left(\sum_{n=0}^{\infty} \frac{dS_n}{dr}\frac{\xi^{2n}}{(2n)!} , \ \frac{1}{r}\sum_{n=1}^{\infty} S_n(r)\frac{\xi^{2n-1}}{(2n-1)!} \right) = \left(\frac{dS_0}{dr} + \tfrac{1}{2}\frac{dS_1}{dr}\xi^2 + \cdots , \ S_1(r)\frac{\xi}{r} + \cdots \right) , \tag{22}$$

$$|\vec{\nabla}S|^2 = \sum_{n=0}^{\infty} \left[\sum_{\nu=0}^{n} \binom{2n}{2\nu} \frac{dS_\nu}{dr}\frac{dS_{n-\nu}}{dr} + \frac{1}{r^2}\sum_{\nu=1}^{n} \binom{2n}{2\nu-1} S_\nu S_{n-\nu+1} \right] \frac{\xi^{2n}}{(2n)!} = \left(\frac{dS_0}{dr}\right)^2 + \left(\frac{dS_0}{dr}\frac{dS_1}{dr} + \frac{S_1^2}{r^2} \right)\xi^2 + O(\xi^4) . \tag{23}$$

Since the squared wave number $k^2(r, \xi)$ has been introduced in Eq. (11) through an analogous expansion in powers of ξ^2, the equation $|\vec{\nabla}S|^2 = k^2$ may be treated by equating the corresponding coefficients of the expansions (23) and (11).

The zeroth order equation obtained in this manner,

$$dS_0/dr = k_0(r) , \tag{24}$$

ensures that our procedure satisfies the condition (13). [The sign of $S_0(r)$ is irrelevant for our purposes.] The next equation,

$$k_0(r)\frac{dS_1}{dr} + \frac{S_1^2}{r^2} = \tfrac{1}{2}k_1^2(r) , \tag{25}$$

is central to our procedure. [Replacement of k_0 and k_1 by their expressions appropriate to Wannier's two-electron problem would turn Eqs. (24) and (25) into Eqs. (14) and (15) of Ref. 2.] Equation (25) constitutes the wave mechanical form of Wannier's linearized trajectory equation (15), since the slope of a trajectory, $r d\bar{\xi}/dr$, must equal the ratio of the components of $\vec{\nabla}S$ in Eq. (22). Indeed, setting $r d\bar{\xi}/dr = [S_1(r)\bar{\xi}/r]/k_0(r)$ gives

$$S_1(r) = k_0(r) r^2 d\ln\bar{\xi}(r)/dr + O(\xi^2) , \tag{26}$$

a standard type of formula that transforms the first-order nonlinear Riccati equation (25) into the second-order linear equation (15). [See Eqs. (28)–(30) and (18) of Ref. 2.]

Equation (15) has been solved analytically in Refs. 2 and 3 for the two-electron problem, both in the Coulomb zone and in the farther region

where $E \gg Ze^2/r$. Numerical solutions will be required in other cases including the magnetic-Rydberg problem. To this end we generalize the Wannier parameter ζ by setting

$$\zeta(r)=\frac{d\ln\bar{\xi}}{d\ln r}=\frac{S_1(r)}{k_0(r)r}. \tag{27}$$

Substitution of this expression transforms Eq. (25) into

$$\zeta^2(r)+\frac{d\ln[k_0(r)r]}{d\ln r}\,\zeta(r)+\frac{d\zeta}{d\ln r}-\frac{\frac{1}{2}k_1^2(r)}{k_0^2(r)}=0. \tag{28}$$

For the two-electron problem in its Coulomb region this equation reduces to the Wannier equation for ζ with constant coefficients and with $d\zeta/dr=0$. In general, one may nevertheless solve (28) as though $d\zeta/dr\sim 0$, or at least by treating $d\zeta/d\ln r$ as a constant to be fitted by iteration. Thus we write

$$\zeta(r)=-\frac{d\ln[k_0(r)r]^{1/2}}{d\ln r}\pm\left[\left(\frac{d\ln[k_0(r)r]^{1/2}}{d\ln r}\right)^2+\frac{\frac{1}{2}k_1^2}{k_0^2}-\frac{d\zeta}{d\ln r}\right]^{1/2}. \tag{29}$$

The two roots $\zeta(r)$ thus obtained determine the curvatures of the alternative eigenparabolas of constant phase

$$S(r,\xi)=S_0(r)+\tfrac{1}{2}rk_0(r)\zeta(r)\xi^2+O(\xi^4). \tag{30}$$

[Note that the factor r in Eqs. (27) and (30) stems from the coefficient of $d\xi^2$ in the differential line element; it would reduce to unity for Cartesian coordinates.]

The expression (29) of ζ in terms of the "local" values of k_0 and k_1 determines the Wannier parameter independently of any further specification of the potential function (11), as anticipated in Sec. I. Equations (29) and (27) provide the solution of the Eq. (25) for $S_1(r)$ and the equivalent solution of the trajectory Eq. (15),

$$\bar{\xi}(r)=\exp\int_{r_0}^{r}\zeta(r)\frac{dr}{r}=\left(\frac{r}{r_0}\right)^{\zeta}\left[1+O\left(\frac{d\zeta}{d\ln r}\right)\right], \tag{31}$$

where r_0 is a normalization constant. Recalling that Eq. (15) holds within an approximation linear in $\bar{\xi}$, we note that r_0 should have a value intermediate between 0 and ∞ which makes $\bar{\xi}$ appropriately small at small r for $\zeta>0$ (divergent trajectories) or small at large r for $\zeta<0$ (convergent trajectories). These two alternatives correspond to the alternative signs in the root (29). The following treatment pertains to either one of these alternatives unless otherwise stated.

Extension to larger ξ. Consider now how successive coefficients $S_n(r)$ of the expansion (21), with $n\geq 2$, may be obtained by recursion from the $S_\nu(r)$ with $\nu<n$. Equating the coefficients of ξ^{2n} in the expansions (23) and (11), for $n\geq 2$, yields

$$\sum_{\nu=0}^{n}\binom{2n}{2\nu}\frac{dS_\nu}{dr}\frac{dS_{n-\nu}}{dr}+\frac{1}{r^2}\sum_{\nu=1}^{n}\binom{2n}{2\nu-1}S_\nu(r)S_{n-\nu+1}(r)=(-2)^{n-1}k_1^2(r). \tag{32}$$

The key point is now this: The coefficients dS_ν/dr and $S_\nu(r)$ of highest order ν in Eqs. (32) have $\nu=n>1$ and appear only *linearly*, in contrast to Eq. (25) which contains $S_1(r)$ quadratically. Therefore Eq. (32) determines $S_n(r)$ by quadratures, uniquely, in terms of the $S_\nu(r)$ with $\nu<n$; the latter are determined in turn by earlier steps of the recursion. We conclude that the quadratic equation (25), solved in Refs. (2) and (3), constitutes an exceptional element of the recursion process, namely, the one that identifies two alternative eigenmodes.

The recursion proceeds uneventfully thereafter enabling one to construct the function $S(r,\xi)$ without any restriction to the infinitesimal range of ξ considered by Peterkop and Rau. Singular points of the constant phase surfaces may well be encountered at a finite distance from the ridge, corresponding to intersections within a bundle of trajectories. Such singular points would limit the range of the special solutions considered in this paper. The Wannier-Peterkop-Rau analysis thus appears to have already identified the essential aspects of propagation along the ridge. The construction of $S(r,\xi)$ will thus be regarded as accomplished throughout a finite range of (r,ξ), even though our present purposes do not require its explicit calculation.

The intrinsic frame and its metric. At each point (r,ξ) the axis $\vec{\nabla}S$ of the coordinate frame (S,T) and the axis $\hat{r}$ of the frame (r,ξ) form an angle α defined by

$$\tan\alpha(r,\xi)=\frac{r^{-1}(\partial S/\partial\xi)_r}{(\partial S/\partial r)_\xi}=\zeta(r)\xi+O(\xi^3). \tag{33}$$

The second coordinate T may be introduced as a normalization constant for the representation of a particular trajectory of our bundle in terms of the standard trajectory $\bar{\xi}(r)$, i.e., by writing $\xi=T\bar{\xi}(r)$. However the solution $\bar{\xi}(r)$ provided by Eq. (31) holds only over an infinitesimal range of ξ. Beyond the linear approximation represented by Eq. (15), the trajectories of our bundle no longer differ only by a scale factor T. We write then the more general trajectory equation

$$\xi=T\bar{\xi}(r,T)\underset{T=0}{\longrightarrow}T\bar{\xi}(r). \tag{34}$$

For larger T, the function $\bar{\xi}(r,T)$ is determined

by extending the Eqs. (26) or (27) which require the trajectory to be parallel to $\vec{\nabla}S$ and hence to have the slope (33),

$$r\left(\frac{\partial\xi}{\partial r}\right)_{T(r,\xi)=\text{const}} = \left(\frac{\partial \ln\bar{\xi}}{\partial \ln r}\right)_T \xi = \tan\alpha(r,\xi) = \zeta(r)\xi + O(\xi^3). \tag{35}$$

The differential metric elements for both frames (r, ξ) and (S, T), are expressed in standard form; they shall include here the third coordinate, φ, for the sake of later applications. Thus we write

$$ds^2 = dr^2 + r^2 d\xi^2 + r^2 \sin^2\theta\, d\varphi^2 = h_S^2 dS^2 + h_T^2 dT^2 + h_\varphi^2 d\varphi^2, \tag{36}$$

with

$$h_S(r,\xi) = |\vec{\nabla}S|^{-1} = k(r,\xi)^{-1},$$
$$h_T(r,\xi) = |\vec{\nabla}T|^{-1}, \tag{37}$$
$$h_\varphi(r,\xi) = r\cos\xi.$$

To calculate $|\vec{\nabla}T|$ note that the orthogonality of $\vec{\nabla}T$ and $\vec{\nabla}S$ complements Eq. (33) with

$$\tan\alpha(r,\xi) = \frac{-(\partial T/\partial r)_\xi}{r^{-1}(\partial T/\partial\xi)_r}. \tag{33'}$$

It follows that

$$|\vec{\nabla}T|^2 = \left(\frac{\partial T}{\partial r}\right)_\xi^2 + \frac{1}{r^2}\left(\frac{\partial T}{\partial \xi}\right)_r^2 = \left[\frac{1}{r}\left(\frac{\partial T}{\partial \xi}\right)_r \frac{1}{\cos\alpha}\right]^2, \tag{38}$$

and further, from Eq. (34),

$$\left(\frac{\partial T}{\partial \xi}\right)_r^{-1} = \left(\frac{\partial \xi}{\partial T}\right)_r = \bar{\xi}(r,T) + T\left(\frac{\partial \bar{\xi}}{\partial T}\right)_r = \bar{\xi}(r,T)\left[1 + \left(\frac{\partial \ln\bar{\xi}}{\partial \ln T}\right)_r\right]. \tag{39}$$

Finally we obtain, with reference also to Eq. (31),

$$h_T(r,\xi) = |\vec{\nabla}T|^{-1} = r\bar{\xi}(r,T)\left[1 + \left(\frac{\partial \ln\bar{\xi}}{\partial \ln T}\right)_r\right]\cos\alpha = r\left(\frac{r}{r_0}\right)^\zeta\left[1 + O\left(\frac{d\zeta}{d\ln r}\right) + O(\xi^2)\right]. \tag{40}$$

Additional variables. In an N-dimensional space the expansion (11) of the squared wave number of the wave equation about the ridge takes the form

$$k^2(r,\xi_1,\xi_2,\ldots) = k_0^2(r) + \tfrac{1}{2}\sum_{i=1}^{N}\sigma_i k_i^2(r)\xi_i^2\left(1 + \sum_{n=2}^{\infty} a_n^{(i)}\xi_i^{2(n-1)}\right), \tag{41}$$

where $\sigma_i = \pm 1$ for different values of i and k_i^2 may vanish. In our magnetic-Rydberg problem we have $N=3$, $\sigma_i = 1$, and $k_2^2(r) = 0$, since the axial symmetry of the problem makes k^2 independent of the third coordinate, $\xi_2 \equiv \varphi$. The Wannier two-electron problem has $N=6$, the k_i vanish for $i>2$ and $\sigma_2 = -1$, implying stable equilibrium about $\xi_2 = 0$. References 2 and 3 have treated ξ_2 on an equal footing with ξ_1, introducing two parameters $\zeta_1(r)$ and $\zeta_2(r)$. However, the expression (29) of ζ_2 has a factor $\sigma_2 = -1$ in front of $k_2^2(r)$ which makes the discriminant negative and ζ_2 and $S(r, \xi_1, \xi_2)$ complex. We had defined S initially as a real phase function; according to Eq. (16) an imaginary dependence of S on ξ_2 is equivalent to an exponential variation of the real amplitude function A. An alternative, but equivalent, procedure would avoid complex values of S by removing all terms of the expansion (41) with $\sigma_i = -1$ from the k^2 term of the Hamilton-Jacobi equation (19), and combine them instead with the residue $\nabla^2 A$ of Eq. (17); these terms, which represent a potential well, would thus contribute to variations of the amplitude function A directly rather than through a complex S.

D. The equation $\operatorname{div} A^2\vec{\nabla}S = 0$

This equation requires the probability density of the Rydberg electron in our problem—or of the corresponding system in other problems—to vary in proportion to the local condensation of the streamlines $\vec{\nabla}S$. Accordingly its solution has a main role in determining the threshold law in Wannier's problem and the intensity distribution within the manifold of excited states in the magnetic-Rydberg problem.

Let us start from the equation in its form (18), linear in $A(r, \xi)$, entering in it the expansion

$$\vec{\nabla}S \equiv \{k_0(r), k_0(r)\zeta\xi\} + O(\xi^2) \tag{42}$$

from Eqs. (22), (23), and (27). The equation is then

$$2\frac{\partial A}{\partial r}k_0(r) + \frac{2}{r}\frac{\partial A}{\partial \xi}k_0(r)\zeta\xi + A\left(\frac{1}{r^2}\frac{d}{dr}r^2 k_0 + \frac{1}{r}k_0\zeta\right) + O(\xi^2) = 0. \tag{43}$$

Multiplication by r/Ak_0 and grouping of terms reduce this equation to

$$\frac{\partial \ln[A^2 k_0(r) r^2]}{\partial \ln r} + 2\frac{\partial \ln A}{\partial \ln \xi}\zeta + \zeta + O(\xi^2) = 0 . \quad (43')$$

To proceed further we should now also expand $A(r, \xi)$ into powers of ξ^2, but this step requires a discussion of symmetry.

The equations of our problem are invariant under reflection on the ridge, that is, under the coordinate transformation $\xi \to -\xi$. This implies occurrence of eigenfunctions of Eq. (9) of alternative parity, even or odd under this reflection. It is the amplitude function $A(r, \xi)$ which has alternative parity, since the phase function may not vanish identically at $\xi = 0$ and has in fact been taken as even. The essential point now is that the factor $\partial \ln A / \partial \ln \xi$ in the second term of Eq. (43′) has quite different expansions depending on the parity of $A(r, \xi)$. It is of $O(\xi^2)$ for even parity but it equals $1 + O(\xi^2)$ for odd parity, i.e., when $A = A_1 \xi[1 + O(\xi^2)]$. Equation (43′) yields thus the alternative solutions, expressed in terms of the trajectory function (31),

$$A(r, \xi) = A_0(r) + O(\xi^2), \quad A_0^2 k_0 r^2 \propto \bar{\xi}(r)^{-1} \propto r^{-\zeta} \quad \text{(even)} \quad (44a)$$

$$A(r, \xi) = A_1(r)\xi + O(\xi^3), \quad A_1^2 k_0 r^2 \propto \bar{\xi}(r)^{-3} \propto r^{-3\zeta} . \quad \text{(odd)} \quad (44b)$$

We see here that odd-parity eigensolutions with positive ζ and divergent streamlines decrease in amplitude with increasing r far more rapidly than even solutions do. This result agrees with the remark in Sec. II that quasi-Landau resonances occur only for σ polarization, i.e., for even values of $l-m$ and even parity under ξ reflection. For the Wannier two-electron problem, Refs. 1–3 have considered only even-parity solutions. On the other hand Klar and Schlecht have obtained the result (44) for both types of state using coordinates for which even (odd) parity in ξ_2 corresponds to singlet (triplet) states of the electron pair.[15]

The sharper dependence on r of odd-parity eigenmodes is analogous to phenomena familiar in other processes of field propagation. Thus, e.g., the field of an electric 2^k pole lying in the (x, y) plane decreases in the z direction far more sharply for high than for low values of k, even though it is governed by the same equation, $\vec{\nabla} \cdot \vec{E} = 0$. The difference stems from the requirement of k-fold symmetry about the z axis. The role of symmetry will be more directly apparent in our problem when formulated in the intrinsic coordinates (S, T, φ), introduced in Eq. (36), ff., and thus extended to a finite range of ξ.

In the intrinsic system $\vec{\nabla} S$ has a single nonzero component,

$$\vec{\nabla} S \equiv (k, 0, 0) . \quad (45)$$

The continuity equation (18′) takes then the simple form

$$\frac{1}{h_S h_T h_\varphi}\frac{\partial}{\partial S} A^2 h_T h_\varphi k = 0 , \quad (46)$$

whose general solution is represented by

$$A(S, T) = (h_T h_\varphi k)^{-1/2} F(T) \quad (47)$$

in terms of an integration factor $F(T)$. Equation (47) holds in this form regardless of symmetry, but solutions of even or odd parity have distinctly different behavior of $F(T)$, represented by

$$F_{\text{even}}(0) = F_0 \neq 0 , \quad \left(\frac{dF_{\text{even}}}{dT}\right)_{T=0} = 0 \quad \text{(even)} \quad (48a)$$

$$F_{\text{odd}}(T) = TF_1(T) , \quad F_1(0) = F_{10} \neq 0 , \quad \left(\frac{dF_1}{dT}\right)_{T=0} = 0 \quad \text{(odd)} . \quad (48b)$$

Here F_0 or F_{10} serves as a normalization constant, while the further variations of $F_{\text{even}}(T)$ or $F_1(T)$ remain to be determined by integrating $\nabla^2 A = 0$ along T.

The consistency of Eqs. (47) and (48a) (even) with the small-ξ expansion (44a) (even) is apparent from the expressions of h_T and h_φ, Eqs. (37) and (40). For the odd-parity case notice firstly that the dependence of $A(S, T)$ on S, i.e., its variation *along each streamline*, is represented in Eq. (47) through the factor $(h_T h_\varphi k)^{-1/2}$ regardless of parity. Odd parity is represented by the factor T in Eq. (48b) (odd), which represents the main variation of $F_{\text{odd}}(T)$, since $F_1(T)$ will be seen to vary slowly. Comparison with Eq. (44b) (odd) involves expressing this factor in terms of (r, ξ), by means of the trajectory Eq. (34), i.e., writing Eq. (48) as

$$A(r, \xi) = (h_T h_S k)^{-1/2} T F_1(T) = \xi[h_T \bar{\xi}(r, T)^2 h_\varphi k]^{-1/2} F_1(T) \quad \text{(odd)} . \quad (49)$$

Consistency with Eq. (44b) (odd) is now apparent since the factor $\bar{\xi}^2$ in this equation combines with the factor $\bar{\xi}$ in h_T to yield a contribution of $(\bar{\xi}^3)^{-1/2}$.

E. The equation $\nabla^2 A = 0$

Consider finally the Eq. (20), $\nabla^2 A = 0$, which follows from Eqs. (17) and (19) in our approach. The dependence of A upon the coordinate S has already been expressed in Eq. (47) through the parameters h_T, h_φ, and k, but we should see now how to determine the factor $F(T)$. Expressing Eq. (20) in the coordinates (S, T, φ), with A in its form (47), yields

$$\frac{1}{h_S h_T h_\varphi}\left(\frac{\partial}{\partial S} h_T h_\varphi k \frac{\partial}{\partial S} + \frac{\partial}{\partial T} h_S h_\varphi h_T^{-1} \frac{\partial}{\partial T}\right) \times [h_T h_\varphi k]^{-1/2} F(T) = 0 . \quad (50)$$

The derivatives with respect to S operate only on $(h_T h_\varphi k)^{-1/2}$; accordingly they contribute to Eq. (50) a term that acts as a squared wave number for the propagation of $F(T)$ along T. Setting $b(S,T) = [h_T h_S k]^{1/2}$, the resulting equation reduces thus in effect to the ordinary differential equation in T,

$$\left\{\frac{\partial}{\partial T} h_S h_\varphi h_T^{-1} \frac{\partial}{\partial T} \frac{1}{b(S,T)} - b(S,T)\left[\frac{\partial^2 \ln b}{\partial S^2} + \left(\frac{\partial \ln b}{\partial S}\right)^2\right]\right\} \times F(T) = 0, \quad (51)$$

which can be solved numerically starting from the boundary conditions (48). Equation (51) shows the effective wave number of the propagation along T to be small, since it depends on second variations of $\ln b$ along the streamlines.

Note here that the dependence on S of $b(S,T)$ and of the other metric coefficients makes Eq. (51) appear incompatible with our procedure of solving Eqs. (18), (19), and (20) sequentially, because it makes $F(T)$ itself a function of S in contrast to its role in Eq. (47). Disregarding this dependence on S constitutes a WKB-type approximation which is introduced here as anticipated in Sec. II B. This approximation appears consistent with our initial understanding that the coefficient $k^2(r,\xi)$ of Eq. (9), and hence the resulting metric coefficients, Eq. (37), vary slowly along the ridge. Equation (51) can still be integrated along T for any given value of S. What is, in fact, disregarded is the contribution to Eq. (46) that would result upon substitution of Eq. (47) with an S-dependent factor $F(T)$.

Problems with several independent variables, with a wave number represented by Eq. (41) in terms of several ξ_i, introduce a set of intrinsic variables $T_i = \xi_i/\bar{\xi}_i(r, T_1, T_2, \ldots)$. Each classical trajectory is then defined as the intersection of several surfaces $T_i = \text{const}$. The function $F(T)$ depends on several T_i and belongs to one of several possible species of the symmetry group of the ridge $T_i = 0$. Equation (51) would then include additional terms with derivatives $\partial/\partial T_i$; it may also include wave number terms originating from terms of the expansion (41) with $\sigma_i = -1$ as indicated at the end of Sec. III C. This consideration points up that our procedure amounts in fact to dealing explicitly with a single variable of the wave equation (9), namely, with the pathlength along the bundle of trajectories orthogonal to the surfaces of constant phase S. The wave propagation over these surfaces remains to be treated by Eq. (51).

Actual performance of explicit calculations of $S(r,\xi)$ and $F(T)$ does not seem relevant until methods will have been developed for incorporating the wave propagation along the potential ridge into solutions that satisfy conditions at distant boundaries.

IV. DISCUSSION

Section III substantiates the main point of this paper, namely, that the Wannier-Peterkop-Rau analysis of the ionization threshold law enables us to construct a base set of eigenmodes of wave propagation along a potential ridge. The curvature of the wavefront of each eigenmode represents a progressive diffraction of the wave away from (or into) the direction of the ridge. The construction procedure extends transversally from the ridge over a finite domain. The alternative roots of the Wannier equation (28) characterize the different properties of two eigenmodes of wave propagation, particularly by appearing as exponents of the radial coordinate in Eqs. (31) and (44). A further characterization of eigenmodes according to symmetry about the ridge has emerged in Sec. III D.

The next main task facing us is to utilize these results to compensate the breakdown of the adiabatic approach to nonseparable wave propagation, which is localized on a ridge as described in Sec. II. Recall from Sec. II that Eq. (6) represents the expansion of an exact wave function into a *complete* system of angular functions, and that the resulting system of coupled radial equations, Eq. (7), is *exact*. The breakdown to be remedied is that the effects of channel coupling in Eq. (7) become increasingly large and nontransparent at large radii. These effects obscure the origin of the quasi-Landau resonances in the spectrum near the ionization threshold in Fig. 3. Formation of standing waves along the ridge presumably accounts for the resonances but we do not yet see how to fit this interpretation within the context of the coupled Eq. (7). Recall also that the magnetic-Rydberg example of Sec. II was introduced as the prototype of a class of phenomena which may prove very broad.

A further characteristic feature emerges from Sec. II. The locus of the breakdown of the quasi-adiabatic approach, as defined by Eq. (8a), $\lambda_{lm}(\alpha r^2) \sim m^2$, is seen in Fig. 1 to *cut across* the entire spectrum of potential energy curves $\lambda_{lm}(\alpha r^2) + \alpha^2 r^4$, in the very region of the avoided crossings. This picture suggests that the eigenmodes of propagation on the ridge play the following role in the context of the quasiadiabatic approach. In Fig. 1 the diagonal line $\lambda_{lm}(\alpha r^2) + \alpha^2 r^4 = m^2 + \alpha^2 r^4$ may be viewed as representing the adiabatic potential level of the eigenmodes of propagation on the ridge. Incorporation of these eigenmodes into the coupled system, Eq. (7), would introduce a strong coupling between

either eigenmode and each adiabatic channel near the intersection of their respective levels. This coupling might then *replace* much of the direct coupling between the several channel pairs (l, l') in Eq. (7). The eigenmodes are thus viewed in the role of mediators of the coupling among the adiabatic channels, whose *strength and complexity* obscure the interpretation of Eq. (7). [While the diagram of Fig. 1 may suggest that the coupling affects primarily pairs of adjacent channels (l, l'), with $l' = l \pm 2$, its extension to larger values of $\alpha^2 r^4$ would show the range of an avoided crossing to spread over channels with $|l' - l| \geq 2$.]

A pattern of quasiadiabatic approximation where one level crosses a manifold of other levels has been treated by Demkov and Komarov.[16] In that case, however, the crossing level and the manifold were understood to belong to the same system of orthogonal channels whereas the $g_{lm}(\theta)$ of Sec. II (or the corresponding adiabatic channels of Refs. 5 and 6) form a complete set which becomes *overcomplete* upon inclusion of the eigenmodes of the ridge. The eigenmodes have thus the character of collective coordinates whose introduction serves to interpret properties of a system without being orthogonal to its standard coordinates. Extension of the Demkov-Komarov treatment to this different circumstance is a remaining task.

A further separate task consists of extending the treatment of Sec. III to the turning point at large r in the magnetic-Rydberg problem, where $k_0(r)$ vanishes. The two-dimensional nature of our problem with curved lines of constant phase, $S(r, \xi) = \text{const}$, prevents a simple application of the usual Airy function procedure that complements the WKB approximation. The boundary at $k(r, \xi) = 0$ will presumably couple the two eigenmodes with effects that are not yet foreseen.

Note added. A description of the turning point phenomena, developed after submission of the present paper, is being published separately.[17]

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