Multichannel quantum mechanics as a Hamiltonian phase flow

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We cast the quantum mechanics of multichannel systems in the broader mathematical framework of Hamiltonian phase-space flow. This flow results from symplectic transformations that preserve antisymmetric products, namely, metric relations among alternative solutions with the same dynamics. This viewpoint affords new insight into recent successful phase-amplitude methods.

I. INTRODUCTION

The fragmentation of atoms and molecules proceeds through "channels" characterized by alternative distributions of constituents, of energy, and of angular momentum among the fragments. Chemical reactions proceed generally by combining reactants into a complex which then fragments. An initial framework, encompassing all fragmentation processes, was outlined by one of us in 1981 for atoms and molecules [1] on the following basis:

(a) Each configuration of a system with N constituents (electrons and nuclei) can be represented by a single point of a $3(N-1)$-dimensional space, whose axes consist of the constituents' coordinates in their center-of-mass frame. Polar coordinates in this space, with origin at the system's center of mass, consist of a "hyperradius"— the system's radius of inertia $R = \sqrt{\sum_i m_i r_i^2 / M}$, where $M = \sum_i m_i$—and of $(3N - 4)$ hyperangles $\{\Omega\}$ representing the $2(N-1)$ directions $\hat{r}_i$ of the constituents and the $(N-2)$ independent ratios $\alpha_i = \tan^{-1}(r_i/r_{i+1})$.

(b) The Schrödinger equation for atoms or molecules, governed by Coulomb forces, takes in hyperspherical coordinates the general form

$$\left\{ -\frac{1}{2M} \left[\frac{\partial^2}{\partial R^2} - \frac{\Lambda^2}{R^2} \right] - \frac{C(\Omega)}{R} \right\} \Psi(R, \Omega) = E\Psi(R, \Omega),$$

(1)

where Λ represents a "grand angular momentum" operator [2] and $C(\Omega)$ an effective "squared electric charge" operator. The system's dynamics centers on the nonzero commutator of Λ and $C(\Omega)$. [Differences among the particle masses are incorporated in $C(\Omega)$.]

(c) A complete set of eigenfunctions of (1) is identified by a *set* of quantum numbers β (one for each angle in the set Ω) appropriate to the $R \to 0$ limit where the centrifugal potential in (1) dwarfs the Coulomb interaction. The set β includes the index λ labeling the eigenvalues of Λ^2 and specifying radial boundary conditions,

$$\Psi_\beta \propto R^\lambda \quad \text{as} \quad R \to 0.$$

(2)

Further elements of $\{\beta\}$ distinguish eigenfunctions of Λ^2 degenerate in λ. All but a finite subset of this infinite set has negligible amplitude at any finite value of R; as R in-

creases, the gradual expansion of the significant subset of $\{\beta\}$ affords an opportunity for visualizing and organizing the full set.

(d) At the opposite "fragmentation" limit, $R \to \infty$, each eigenfunction Ψ_β resolves into a superposition of components fragmenting through alternative channels i,

$$\Psi_\beta \overset{R \to \infty}{\to} \sum_i \phi_{i\infty}(\Omega) \left[\exp(ik_i R) R^{\zeta_i} J_{i\beta}^+ \right.$$
$$\left. + \exp(-ik_i R) R^{-\zeta_i} J_{i\beta}^- \right].$$

(3)

Here, the angular functions $\phi_{i\infty}(\Omega)$ exhibit narrow localizations on the hypersphere, focused on fragmentation "directions" (actually configurations of the system) which embody the result of shorter-range correlations among the constituents. Further propagation into the true fragmentation channels involves a transformation to different coordinates incorporating the distance between the (weakly interacting) fragments and the internal coordinates of each fragment. The significant particle correlations manifest themselves in the smooth evolution from short-range channels β to the "prefragmentation" channels i via the Jost matrices $J_{i\beta}^+$ and $J_{i\beta}^-$. The study of Eq. (1) aims at constructing these matrices.

(e) At any given total energy E, some of the $\{i\}$ channels are "closed," meaning that E does not prove sufficient to carry the system to complete fragmentation in that channel. The k_i values of this subset are imaginary, whereby one of the exponentials in (3) diverges; the divergence is then removed by considering only superpositions $\sum_\beta A_\beta \Psi_\beta$ whose coefficients of divergent terms vanish [3].

On this basis, Ref. [1] contemplated a partial separation of hyperradial and hyperangular motions through approximate "adiabatic" functions

$$\Psi_\mu^{\text{ad}}(R, \Omega) = F_\mu(R)\Phi_\mu(R; \Omega).$$

(4)

Each angular function Φ_μ represents a mode of correlation in the hyperangular degrees of freedom (depending parametrically on R) that arises by disregarding the radial kinetic energy in (1). Each Φ_μ thus describes an eigenchannel of the balance between centrifugal and

Coulomb potentials, satisfying the $(3N - 4)$-dimensional equation

$$\frac{1}{R^2}\left[\frac{\mathbf{\Lambda}^2}{2M} - RC(\Omega)\right]\Phi_\mu(R;\Omega) = U_\mu(R)\Phi_\mu(R;\Omega); \quad (5a)$$

each eigenvalue $U_\mu(R)$ serves as a potential for the complementary radial equation

$$\left[-\frac{1}{2M}\frac{d^2}{dR^2} + U_\mu(R)\right]F_\mu(R) = EF_\mu(R). \quad (5b)$$

This approximation, patterned after the familiar Born-Oppenheimer approach to molecular physics, implies (incorrectly in this case) that the motions in Ω governed by (5a) are much faster than the motion in R governed by (5b); it also disregards all correlations between these motions altogether. These correlations are instead accounted for in separate steps that mix different adiabatic channels; for example, the recent "diabatic by sector" method has proven successful in reproducing the spectra of moderate excitations [4].

The adiabatic procedure (5) has nevertheless yielded valuable results, long before as well as after its formulation in Ref. [1], particularly by classifying multiply excited states [5]. On the other hand, it has failed altogether to encompass the simultaneous escape of two electrons from an atom, near its energy threshold, outlined semi-classically by Wannier in 1953 [6]. Recently a transparent semianalytic procedure has been developed in our group displaying a progressive superposition of base channels—whether adiabatic or not—of the full Hamiltonian of (1) and steering its solution toward fragmentation channels of type (3) [7,8].

At this point, a seminal remark has been introduced by V. Aquilanti et al. [9] which places all treatments of multichannel processes within the framework of the Hamiltonian mechanics of phase-space trajectories. Hamilton's canonical transformations are "symplectic" [10,11], meaning that they conserve antisymmetric products of the form $q_1p_2 - q_2p_1$. This product establishes a relationship between pairs of states $(1,2)$ governed by the same dynamics but differing in their initial distributions of potential and kinetic energies. Analogous symplectic transformations occur in the evolution of pairs of Schrödinger wave functions $\{\psi_1(x), \psi_2(x)\}$, an evolution that preserves their antisymmetric Wronskian $\psi_1 d\psi_2/dx - \psi_2 d\psi_1/dx$, which vanishes when $\psi_1 = \psi_2$ but peaks when their phase difference reaches $90°$. Section II will detail how this relationship emerges from replacing Schrödinger's second order equation by a pair of first order equations, much as Lagrange's equations are replaced by Hamilton's [12].

The connection between wave-mechanical multichannel treatments and Hamiltonian phase-space trajectories emerging from Ref. [9] will be developed here in greater detail. We view the oscillations of single-channel wave functions, propagating radially from an origin toward infinity, as the counterparts of a variable-frequency oscillator's behavior in the course of time. This correspondence, to be developed in Sec. II, will lead naturally to wave-

mechanical phase-amplitude formalisms. By the same token Sec. III will show the radial propagation of multichannel wave functions as corresponding to the long-time evolution of coupled-oscillator systems. The long-term behavior of *generic* coupled oscillators may appear more complicated than the corresponding fragmentations of molecules into constituent species. Yet critical and highly specific structures are known to emerge, e.g., from the collective vibrations of large biochemical entities, a correspondence that might be worth pursuing.

We are thus outlining a correspondence between the *flow* of trajectories in a classical phase space and the *evolution* of a multichannel quantum system as it develops outward from its center of mass or inward from its fragmentation axes. The transition from short- to long-range behavior, i.e., from $\{\beta\}$ to $\{i\}$ channels, therefore proceeds smoothly, as envisioned in Refs. [7,8]. These developments are not basically new; they have been collected here to cast multichannel quantum physics in a fuller light.

II. SINGLE-CHANNEL FORMULATION

The most familiar connection between classical and quantum mechanics arises in the semiclassical limit, where the WKB approximation applies. In this case, for potentials varying slowly over a wavelength, the quantum mechanical phase corresponds to Hamilton's principal function S for classical motion in the *same* potential [13]. This is the best-known example of an (approximate) phase-amplitude (PA) method.

We focus here instead on alternative classical-quantum correspondences, also connected to Hamilton-Jacobi theory, leading to *exact* PA methods. Our classical system will always consist of an oscillator, or set of oscillators, for any quantum Hamiltonian. For simplicity, we begin with a single space dimension x. The stationary-state wave function $\psi(x)$ for a particle in a potential $V(x)$ satisfies the time-independent Schrödinger equation

$$\left(\frac{d}{dx}\right)^2\psi = -k^2(x)\psi, \quad (6)$$

where $k^2(x) = 2[E - V(x)]$ denotes twice the kinetic energy of the particle in units with $\hbar = m = 1$. The minus sign in (6) stems from the imaginary unit i in the momentum operator $p = -i(d/dx)$, whose sign indicates the direction of motion. Specializing first to a plane wave, i.e., to a constant $V(x)$, (6) yields two linearly independent solutions $\psi^\pm = \exp(\pm ikx)$, whose flow is represented by the flux operator

$$\mathcal{F}(\psi) = -\frac{i}{2}\left(\psi^*\frac{d\psi}{dx} - \frac{d\psi^*}{dx}\psi\right), \quad (7)$$

namely,

$$\mathcal{F}(\psi^\pm) = \pm k. \quad (8)$$

Alternatively, we may write solutions to (6) in terms

of real-valued functions $f = \sin kx$ and $g = \cos kx$ representing standing waves and leading directly to an analogy with a classical Hamiltonian phase flow. Standard procedures [14,15] reduce second-order equations like (6) to pairs of first-order equations, treating the wave function and its derivative as a pair of independent functions to be determined. In this context, we denote the wave function f and its derivative df/dx by the suggestive labels q and p, reducing (6) to the system

$$\frac{dq}{dx} = p, \qquad \frac{dp}{dx} = -k^2 q. \qquad (9)$$

Identifying the coordinate x with time, Eqs. (9) represent Hamilton's equations of motion for a harmonic oscillator with the Hamiltonian

$$H = \frac{1}{2}p^2 + \frac{1}{2}k^2 q^2. \qquad (10)$$

The propagation in x of the wave function f thus corresponds to the flow in time of the oscillating q. At each phase-space point (q,p), the right-hand sides of (9) determine an infinitesimal symplectic transformation—depending on q, p, and on the time—which tells the solution where to flow next. Distinct flows (q_1, p_1), (q_2, p_2) remain independent. In the language of symplectic geometry, this independence conserves the antisymmetric bilinear form

$$q_1 p_2 - q_2 p_1 = \text{const.} \qquad (11)$$

Recalling that p represents here the derivative of q, Eq. (11) expresses the well-known conservation of the Wronskian of two independent solutions q_1 and q_2 of Eq. (6). Still treating k^2 as a constant, we write the plane wave solutions $\psi^\pm$ in terms of the independent real functions f and g: $\psi^\pm = f \pm ig$. The flux (7) then becomes

$$\mathcal{F}(\psi^\pm) = W(f, g). \qquad (12)$$

Conservation of the flux, of the Wronskian, and of the symplectic form (11) are thus equivalent.

Classical mechanics capitalizes on conserved quantities through the Hamilton-Jacobi theory, i.e., by a time-dependent symplectic transformation—with a generating function $S(q, P, t)$—from the original phase-space coordinates (q, p) to a new pair (Q, P) that are constants of the motion (Chap. 10 of [16]). When $k(x)$ is constant, the conserved momentum P is identified with the total energy E of the oscillator,

$$E = \frac{1}{2}p^2 + \frac{1}{2}k^2 q^2 = \frac{1}{2}(k \cos kx)^2 + \frac{1}{2}k^2(\sin kx)^2 = \frac{1}{2}k^2, \qquad (13)$$

i.e., with half the squared flux. The conjugate position coordinate Q, also conserved, turns out to be a shift x_0 in the x coordinate. In terms of these constants, the position coordinate q (i.e., the real wave function f) reads [cf. Eqs. (10)–(21) of [16]]

$$q = \sqrt{\frac{2E}{k^2}} \sin k(x + x_0). \qquad (14)$$

The Hamilton-Jacobi procedure thus diverts the focus of the problem from ordinary position and momentum coordinates to coordinates that emphasize the overall *phase shift* $\delta = kx_0$ and *size* (identified by the total energy) of the oscillator's displacement. This change of emphasis foreshadows the Hamiltonian generation of phase-amplitude methods.

Both E and x_0 become functions of x in the presence of a potential $V(x)$, with motion generated by adding $\Delta H = -V(x)q^2$ to the oscillator's Hamiltonian. The Hamilton-Jacobi theory then determines equations of motion for x_0 and E (Chap. 11 of [16])

$$\frac{dx_0}{dx} = \frac{\partial \Delta H}{\partial E} = -2k^{-2}V(x)\sin^2 k(x + x_0), \qquad (15a)$$

$$\frac{dE}{dx} = -\frac{\partial \Delta H}{\partial x_0} = 2k^{-1}EV(x)\sin 2k(x + x_0). \qquad (15b)$$

Equations (15) establish x_0 and E as evolving according to their own Hamiltonian flow, which expresses the progressive *deviation* of the wave function from the plane wave (14) as it encounters more and more of the potential. Translating (15) in terms of the phase shift via the scale transformation $\delta = kx_0$ yields

$$\frac{d\delta}{dx} = -2k^{-1}V(x)\sin^2(kx + \delta), \qquad (16a)$$

$$\frac{dE}{dx} = 2k^{-1}EV(x)\sin 2(kx + \delta), \qquad (16b)$$

reminiscent of Calogero's variable phase approach to the radial equations of scattering theory [17,18], wherein $\delta(x)$ represents the scattering phase shift due to a potential that vanishes beyond x. The flow of $\delta(x)$ steers δ toward the correct value of the phase shift in the limit $R \to \infty$.

An alternative and very useful single-channel PA method results from a deeper examination of the classical oscillator. Lewis [19] observed that the time-dependent oscillator exhibits a constant of the motion, to which Eliezer and Gray [20] gave a geometrical interpretation by embedding the one-dimensional oscillator in a plane. Consider in addition to the oscillator's motion along one direction q an independent motion along an orthogonal space axis q'. The oscillator then orbits in the (q, q') plane, with Hamiltonian

$$H_r = \frac{1}{2}\left[\left(\frac{dr}{dt}\right)^2 + r^2\left(\frac{d\theta}{dt}\right)^2 + k^2(t)r^2\right] \qquad (17)$$

in the polar coordinates $r = \sqrt{q^2 + q'^2}$, $\tan\theta = q'/q$. Because H_r does not depend explicitly on θ, the angular momentum $l = r^2(d\theta/dt)$ is conserved; this is Lewis' invariant. Lewis and Leach [21] exploit this invariant by a canonical transformation to the phase-space coordinates $(Q, P) = (\theta, l)$, subject to a Hamiltonian flow

$$\frac{d\theta}{dt} = \frac{\partial K}{\partial l} = \frac{l}{r^2}, \quad \frac{dl}{dt} = -\frac{\partial K}{\partial \theta} = 0. \tag{18}$$

The Hamiltonian for this flow,

$$K = \frac{l^2}{2r^2}, \tag{19}$$

depends on the solution r to the radial equation of motion (termed the "auxiliary equation" by Lewis)

$$\frac{d^2 r}{dt^2} + k^2(t)r - \frac{l^2}{r^3} = 0. \tag{20}$$

Any solution of (20), together with the angle θ from (18), determine the general solution to the original time-dependent oscillator,

$$q(t) = r(t)\sin[\theta(t) + \theta_0]. \tag{21}$$

Following our classical-quantum correspondence, (21) leads to the PA form for two independent (indeed, out of phase) solutions to the wave equation (6):

$$f(x) = \alpha(x)\sin[\phi(x)], \quad g(x) = \alpha(x)\cos[\phi(x)], \tag{22}$$

whose amplitude α and phase ϕ satisfy

$$\frac{d^2\alpha}{dx^2} + k^2(x)\alpha - \frac{l^2}{\alpha^3} = 0, \quad \frac{d\phi}{dx} = \frac{l}{\alpha^2}, \tag{23}$$

respectively. Here the Hamiltonian flow of θ around the fictitious (q, q') plane has reproduced the PA method of Milne [22] (also developed independently by Young [23]). In this case, the conserved quantity l denotes the conserved Wronskian of f and g (or equivalently the flux of $f + ig$) rather than the angular momentum. The Milne phase $\phi(x)$ [with boundary condition $\phi(0) = 0$] flows toward the *total phase* as $R \to \infty$, facilitating the identification of bound states, and the construction of phase shifts due to channel mixing, as described in the next section.

[The form (23) seems to have made the problem needlessly difficult, by replacing a linear second-order equation (6) with a nonlinear second-order equation. However, Korsch and Laurent [24] emphasized that both the phase and amplitude are smooth functions of the dependent variable, an idea later refined by Robicheaux *et al.* [25]. The Milne formalism thus replaces oscillating wave functions with smooth monotonic functions better suited to numerical evaluation.]

III. MULTICHANNEL TREATMENT

A. Symplectic transformations of basis channels

The multichannel PA treatment of Eq. (1) (Chap. 19 of Calogero [17]) follows the single-channel treatment fairly closely, with certain refinements to be described in this section, beginning with the selection of basis channels. Following remark (c) of the introduction, we select a complete set of "hyperspherical harmonics" $\{Y_\beta\}$. We expand the full wave function Ψ in terms of this complete set with R-dependent coefficients denoted by q_β, anticipating their identification with classical coordinates:

$$\Psi = \sum_\beta q_\beta(R)Y_\beta(\Omega). \tag{24}$$

This expansion reduces the partial differential equation (1) to a set of coupled ordinary differential equations in R,

$$\frac{d^2 q_\beta}{dR^2} = -\sum_{\beta'} k_{\beta\beta'}^2 q_{\beta'}, \tag{25a}$$

where

$$k_{\beta\beta'}^2(R) = \int d\Omega Y_\beta(\Omega)\left[2ME - \frac{\Lambda^2}{R^2} + 2M\frac{C(\Omega)}{R}\right]Y_{\beta'}^*(\Omega) \tag{25b}$$

plays the role of a coupling matrix.

Expansion into the harmonics Y_β advances the solution to (1) in two ways: first, it shifts the focus from continuous variables Ω to discrete variables β, and therefore from partial to ordinary differential equations; second, it introduces pairs of harmonics, in the form $|\beta\rangle\langle\beta'|$, forming a basis of operators whose superpositions represent observables that *embody all particle correlations* [26].

Exploiting the Hamilton-Jacobi theory we reduce (25a) to Hamiltonian form, just as in the single-channel case, defining for each channel "position" q_β a conjugate "momentum" $p_\beta = dq_\beta/dR$, yielding the analog of Eqs. (9) and (10),

$$\frac{dq_\beta}{dR} = \frac{\partial H}{\partial p_\beta}, \quad \frac{dp_\beta}{dR} = -\frac{\partial H}{\partial q_\beta}, \tag{26}$$

with the Hamiltonian

$$H(q_\beta, p_\beta, R) = \frac{1}{2}\sum_\beta p_\beta^2 + \frac{1}{2}\sum_{\beta\beta'} q_\beta k_{\beta\beta'}^2(R)q_{\beta'}. \tag{27}$$

Each channel β thus maps in the classical analogy to one degree of freedom in a collection of coupled harmonic oscillators with time-dependent spring constants.

This analogy may not help us immediately to visualize the quantum dynamics, for coupled oscillator systems generally exhibit their own complicated behavior. Nevertheless, we stress here that the motion of the oscillator system unfolds in time, just as the interactions among channels manifest themselves as R grows, both driven by the same underlying symplectic structure. Specifically, in the $2n$-dimensional phase space $(\vec{q}, \vec{p})$ of a classical system with n degrees of freedom, symplectic transformations are generated by first-order equations of the form

$$\begin{pmatrix} \dot{\vec{q}} \\ \dot{\vec{p}} \end{pmatrix} = \begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & -\mathbf{A}^t \end{pmatrix}\begin{pmatrix} \vec{q} \\ \vec{p} \end{pmatrix}, \tag{28}$$

where $\mathbf{A}, \mathbf{B}, \mathbf{C}$ are $n \times n$ matrices, with $\mathbf{B}$ and $\mathbf{C}$ symmetric. The $2n \times 2n$ matrix in (28) is termed "Hamiltonian" or "infinitesimally symplectic" [11].

Thus far we have not specified the choice of the channels β. Many such choices exist, corresponding to alternative ways of parceling out the total radius of inertia

R among groups of constituents. These alternatives—indexed by "Jacobi trees" [27]—yield equivalent results in the end, but should be chosen for ease of interpretation in any given application. Transformations between sets of Jacobi coordinates imply changing the angles $\{\Omega\}$ on the hypersphere and therefore the quantum numbers $\{\beta\}$. Nevertheless, expansion into a new set of harmonics $\{\tilde{\beta}\}$ yields the same close-coupling equations (26) and (27). Transformations between Jacobi trees thus also entail symplectic transformations, since they leave the form of Hamilton's equations invariant. Indeed, the separation of (27) into two terms involving q_β's and p_β's separately suggests viewing such a transformation as a point transformation, i.e., as a change of coordinates alone. An example would be any orthogonal (or unitary) transformation in a space with axes labeled by different sets β.

Transformation to adiabatic channels, mentioned in the introduction, amounts to a slightly less trivial coordinate transformation. The adiabatic approximation transforms from β channels to μ channels that reduce k^2 to its diagonal form k_0^2 at each R, thereby continually seeking "normal mode" coordinates. This transformation is also symplectic, as pointed out in Ref. [9]. A straightforward calculation shows the residual nonadiabatic coupling to be taken into account via equations of the form (26), but with the Hamiltonian

$$H = \frac{1}{2} \sum_\mu p_\mu^2 - \sum_{\mu\mu'} p_\mu P_{\mu\mu'} q_{\mu'} + \frac{1}{2} \sum_\mu q_\mu \left(k_0^2\right)_{\mu\mu} q_\mu,$$

(29)

representing coupling via elements of the first derivative operator in the adiabatic basis, $P_{\mu\mu'} = \langle \mu | \partial/\partial R | \mu' \rangle$, familiar from the Born-Oppenheimer theory. Reference [9] introduces further a sequence of symplectic transformations to "post-adiabatic" bases, aimed at minimizing channel coupling. We stress here that all these bases are *formally* equivalent; their choice is largely a matter of preference, governed by their ability to display the coupling meaningfully. Thus spherical harmonics have proven useful in applying the PA method to the diamagnetic Kepler problem [7], while an adiabatic basis has proven more relevant to studying two-electron excitations in helium [8].

B. Flow from short- to long-range behavior

Turning now to the dynamic evolution of the multichannel system (26) and (27) in a basis of hyperspherical harmonics β, we may as a first approximation reduce the system to uncoupled channels by ignoring off-diagonal elements of k^2. Each channel β, with squared wave number $k_{\beta\beta}^2$, possesses two linearly independent solutions, regular and irregular at $R = 0$, denoted by f_β and g_β. These are conveniently expressed as the Milne functions $f_\beta = \alpha_\beta \sin \phi_\beta$ and $g_\beta = \alpha_\beta \cos \phi_\beta$, with ϕ_β vanishing at $R = 0$. As indicated in Sec. II, each Wronskian $W(f_\beta, g_\beta)$ is conserved, representing the conserved channel flux. However, we actually identify two constants

of the motion in the coefficients of f_β and g_β of an arbitrary channel wave function

$$q_\beta = f_\beta a_\beta + g_\beta b_\beta,$$

(30)

corresponding to the two constants of integration of the second-order Schrödinger equation in channel β.

The multichannel PA results are now almost trivial. In the presence of $(k_1^2)_{\beta\beta'}$—the remaining off-diagonal portion of k^2—the former constants a_β and b_β become functions of R, governed by the additional Hamiltonian

$$\Delta H = \frac{1}{2} \sum_{\beta\beta'} q_\beta \left(k_1^2\right)_{\beta\beta'} q_{\beta'},$$

(31)

representing formally the coupling between the classical oscillators. The explicit equations of motion, analogous to (16), work out to

$$\frac{da_\beta}{dR} = \sum_{\beta'} \left(L_{\beta\beta'}^{(aa)} a_{\beta'} + L_{\beta\beta'}^{(ab)} b_{\beta'}\right),$$

(32a)

$$\frac{db_\beta}{dR} = \sum_{\beta'} \left(L_{\beta\beta'}^{(ba)} a_{\beta'} + L_{\beta\beta'}^{(bb)} b_{\beta'}\right),$$

(32b)

$$L_{\beta\beta'}^{(aa)} = g_\beta \left(k_1^2\right)_{\beta\beta'} f_{\beta'}, \qquad L_{\beta\beta'}^{(ab)} = g_\beta \left(k_1^2\right)_{\beta\beta'} g_{\beta'}, \quad \text{(32c)}$$

$$L_{\beta\beta'}^{(ba)} = -f_\beta \left(k_1^2\right)_{\beta\beta'} f_{\beta'}, \qquad L_{\beta\beta'}^{(bb)} = -f_\beta \left(k_1^2\right)_{\beta\beta'} g_{\beta'},$$

(32d)

identical with the PA equations (14) of Ref. [7]. The coupling matrix L in (32) has the form of an infinitesimally symplectic matrix (28). Once the "hard" part, i.e., construction of the single-channel Milne functions, is complete, the problem reduces to the linear, first-order system (32).

A final step, relevant to interpretation and described in detail in Ref. [7], rearranges various solutions q_β into eigenchannels of constant phase shift. Owing to separability at $R = 0$, the wave functions (24) may originate in any channel β_0. Our notation reflects this fact by appending the index β_0 to all relevant quantities:

$$q_{\beta\beta_0} = f_\beta a_{\beta\beta_0} + g_\beta b_{\beta\beta_0}.$$

(33)

Recognizing $a_{\beta\beta_0}$ and $b_{\beta\beta_0}$ as coefficients of the sinelike and cosinelike Milne functions, Ref. [7] constructs their ratio, the "short-range reaction matrix" [3]

$$K_{\beta\beta'}(R) = \sum_{\beta_0} b_{\beta\beta_0} \left(a^{-1}\right)_{\beta_0\beta'}.$$

(34)

In a single channel, K would represent the tangent of the channel's phase shift δ, relative to the regular solution. In the multichannel context we diagonalize $K_{\beta\beta'}$, producing R-dependent eigenchannels $|p(R)\rangle$. Each of these channels accumulates a phase shift $\delta_p(R)$, defined as the

inverse tangent of the pth eigenvalue of $K_{\beta\beta'}$.

Preliminary applications of the PA formalism have shown, in the simple systems of Refs. [7] and [8], that the eigenchannels $|p\rangle$ do evolve in a physically meaningful way. In the diamagnetic Kepler problem, the $|p\rangle$'s display alternative localizations in "Landau" and "quasi-Landau" regions of configuration space, that is, along and across the magnetic field axis, respectively [7]. In the analysis of two-electron excitations in helium, the evolution of each phase shift has revealed coupling between adiabatic channels beyond the expected coupling at avoided crossings of the relevant potential curves [8,28]. These additional interactions reflect the dressing of the squared wave number $(k_1^2)_{\beta\beta'}$ by Milne functions in Eq. (32). Channel interactions are enhanced whenever the phases of two channels become nearly degenerate. Efforts are in progress to identify phenomena in which these interactions manifest themselves. A further step in the PA program, also being developed, seeks eigenchannels of total phase rather than of phase shifts, thus eliminating the need for radial basis functions f and g.

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