Magnetically Quantized Continuum Distorted Waves

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A new derivation of continuum distorted-wave theory is presented. It is generalized to magnetically quantized continuum distorted waves. The context is analytic continuation of hydrogenic-state wave functions from below to above threshold, using parabolic coordinates and quantum numbers including m the magnetic quantum number. This continuation applies to excitation, charge transfer, ionization, and double and hybrid events for both light- and heavy-particle collisions. It is applied to the calculation of double-differential cross sections for the single ionization of the hydrogen atom and for a hydrogen molecule by a proton for electrons ejected in the forward direction at a collision energy of 50 keV and 100 keV respectively.

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A continuum distorted wave (CDW) [1] theory for charge transfer in ion-atom collisions was first presented by Cheshire [2]. It proved to be a remarkably successful, flexible, and pragmatic theory [3]. Many improvements have since been made. Crothers [4] showed that CDW bound states are in general unnormalized (and proposed CDW for light-particle collisions). The use of a gauge transformation in the impact parameter (ρ) time-dependent treatment leads to a ρ-dependent phase factor [5] with the internuclear potential eliminated. An on-shell derivation of CDW is more physically understandable and avoids artificial logarithmic potentials and spurious nonlocal operators [6]. The net perturbation is the nonorthogonal kinetic energy —$\partial_{\boldsymbol{r_T}}.\partial_{\boldsymbol{r_P}}$ where the electron has position vectors $\boldsymbol{r_P}$, $\boldsymbol{r_T}$ with respect to the projectile (P) and target (T) nucleus. Elastic-divergence free CDW Neumann-Born series may be derived [7], with connected kernel.

Thomas double scattering is a second-order event leading to electron capture [8,9]. Fortunately CDW2 resolves the matter, with only one Thomas resonance, and including all strong and intermediate coupling. Moreover, consideration of CDW3 [10] shows that the Thomas CDW series has converged. In the case of capture/excitation, variational coupled equations may be formulated and applied [11,12].

For ionization, following the CDW final state of Belkič [13], Crothers and McCann [14] introduced CDW-EIS (eikonal-initial state). Some of the major advantages are that both the initial and final states are normalized, all long-range Coulomb boundary conditions are satisfied, and the full two-center final state is a product of two CDWs, one T and one P based, so that most of the post-collision interaction is included. A dynamic molecular theory, CDW-EIS has been generalized to electron impact [15,16] and to R (relativistic) CDW-EIS [17].

O'Rourke *et al.* [18] have described the application of CDW-EIS to doubly differential cross sections (DDCS) including complete longitudinal momentum distributions (electron, recoil, and projectile ion). They also considered DDCS 2D plots against k/v at forward scattering and 3D plots against k/v and θ_k (where $\boldsymbol{v}$ is the impact velocity, $\boldsymbol{k}$ is the ejected electron velocity, and θ_k is the polar angle of the ejected electron).

However, no evidence was found, by our experimental and theoretical group [19], for saddle points for collisions of 40 keV protons with either He or H_2. Moreover, for 100 keV proton collisions with H_2 CDW-EIS calculations predict saddle points in contradiction with our experimental group [20]. This was puzzling, since saddle-point electrons are normally associated with lower impact energies. We were therefore moved to reconsider the very basis of CDW-EIS. Accordingly, a new derivation of continuum distorted-wave theory is presented. It is generalized to magnetically quantized continuum distorted waves. The context is analytic continuation of hydrogenic-state wave functions from below to above threshold, using parabolic coordinates and quantum numbers including m the magnetic quantum number.

In the time-independent distorted-wave formalism, the exact transition amplitude is given in the post-interaction formulation [21] by

$$T_{fi} = \langle \psi_f^- | (H - E)^\dagger | \Psi_i^+ \rangle + \langle \psi_f^- | H - H^\dagger | \psi_i^+ \rangle . \quad (1)$$

Here Ψ_i^+ is the exact total scattering wave function satisfying $(H - E)\Psi_i^+ = 0$ and outgoing-wave boundary conditions. The total Hamiltonian is H, the total energy is E, and dagger means complex conjugate and operating to the left. The distorted initial- and final-state CDW wave functions are ψ_i^+ and ψ_f^- given by

$$\psi_i^+ = \phi_i(\boldsymbol{r_T}) \exp\left(-\frac{1}{2} i \boldsymbol{v} \cdot \boldsymbol{r} + i \boldsymbol{K_i} \cdot \boldsymbol{R}\right) \times {}^{m_i}D_{\boldsymbol{v}}^+(\boldsymbol{r_P}, Z_P) \exp\left[\frac{iZ_P Z_T}{v} \ln(vR - \boldsymbol{v} \cdot \boldsymbol{R})\right], \quad (2)$$

$$\psi_f^- = (2\pi)^{-(3/2)} \exp\left(-\frac{1}{2} i \boldsymbol{v} \cdot \boldsymbol{r} + i \boldsymbol{K_F} \cdot \boldsymbol{R} + i \boldsymbol{k} \cdot \boldsymbol{r_T}\right) \times {}^{m_T}D_{\boldsymbol{k}}^-(\boldsymbol{r_T}, Z_T) {}^{m_P}D_{\boldsymbol{k}-\boldsymbol{v}}^-(\boldsymbol{r_P}, Z_P) \times \exp\left[-\frac{iZ_P Z_T}{v} \ln(vR + \boldsymbol{v} \cdot \boldsymbol{R})\right], \quad (3)$$

having included the internuclear eikonal phases [5]. The plane waves of the nuclear motion are parametrized by the initial ($\boldsymbol{K_i}$) and final ($\boldsymbol{K_f}$) relative momentum of the nuclei, with $\boldsymbol{R}$ the position vector of P with respect to T. The electron translation factor is $\exp(-\frac{1}{2}i\boldsymbol{v}\cdot\boldsymbol{r})$, where $\boldsymbol{r}$ is the electron position vector relative to the midpoint of the nuclei. Z_T and Z_P are the target and projectile charges, and $\phi_i(\boldsymbol{r_T})$ the initial stationary bound state. m_T, m_P, and m_i are the magnetic quantum numbers of the target, projectile, and the initial state, respectively, and without any loss of generality we can set $m_i = 0$.

Here we define the CDW given by

$$\begin{aligned} {}^mD_{\boldsymbol{v}}^+(\boldsymbol{r};Z) &= \exp\left(im\phi + \frac{\pi\nu}{2}\right)(vr - \boldsymbol{v}\cdot\boldsymbol{r})^{|m|/2}(vr + \boldsymbol{v}\cdot\boldsymbol{r})^{|m|/2}\frac{\Gamma(1+\frac{1}{2}|m| - i\nu)\Gamma(1+\frac{1}{2}|m|)}{\Gamma^2(1+|m|)} \\ &\quad\times M\left(i\nu + \frac{1}{2}|m|, 1+|m|, ivr - i\boldsymbol{v}\cdot\boldsymbol{r}\right)M\left(\frac{1}{2}|m|, 1+|m|, -ivr - i\boldsymbol{v}\cdot\boldsymbol{r}\right) \\ &\simeq \exp(im\phi)(vr - \boldsymbol{v}\cdot\boldsymbol{r})^{-i\nu} \qquad r\to\infty, \end{aligned} \tag{4}$$

where $\nu = \frac{Z}{v} = \frac{\mu Z}{k}$, μ is the reduced mass, M is the regular Kummer function, and

$${}^mD_{\boldsymbol{v}}^-(\boldsymbol{r};Z) = [{}^mD_{-\boldsymbol{v}}^+(\boldsymbol{r};Z)]^*, \tag{5}$$

which distorted waves satisfy the correct asymptotic boundary conditions. The results (4), (5) indicate that the three two-body phases accumulating asymptotically in Eq. (3) are correct [22]. The exact Ψ_i^+ is approximated by ψ_i^+ with the CDW taken in its eikonal form [Eq. (4)]: hence G/CDW-EIS (eikonal-initial state).

We note $\boldsymbol{p}$ is the momentum of the ejected electron relative to the projectile. ϕ_T is the angle between the planes $(\boldsymbol{r_T}, \boldsymbol{k})$ and $(\boldsymbol{v}, \boldsymbol{k})$ and ϕ_P is the angle between the planes $(\boldsymbol{r_P}, \boldsymbol{p})$ and $(\boldsymbol{v}, \boldsymbol{p})$. We note also that, although $\boldsymbol{p} = \boldsymbol{k} - \boldsymbol{v}$, $\boldsymbol{p}$ and $\boldsymbol{k}$ are skew vectors.

Equations (2) to (5) represent a generalization of previous CDWs [6,14], following the introduction of three magnetic quantum numbers. They afford the inclusion of a rapidly convergent complete set of CDWs, which permits (especially target) continuum rotational coupling, an important physical mechanism. We shall present details elsewhere, while only mentioning here that, in Schiff [23] [Eq. (16.36) and (37)] we interchange η and ξ for convenience, and set

$$\lambda_1 = \frac{1}{2} - i\nu \text{ and } n_1 = -\frac{1}{2}|m| - i\nu \quad \left(\nu = \frac{Z}{v}\right),$$

$$\lambda_2 = \frac{1}{2} \text{ and } n_2 = -\frac{1}{2}|m|, \tag{6}$$

where λ_1 and λ_2 are separation constants and n_1 and n_2 are the standard parabolic quantum numbers.

The uniform two-center nature of ψ_f^- may be confirmed by noting that

$$\begin{aligned}\exp(i\boldsymbol{k}\cdot\boldsymbol{r_T})E_{\boldsymbol{k},-(1/2)\boldsymbol{v}}(\boldsymbol{r},t) &= \exp(i\boldsymbol{p}\cdot\boldsymbol{r_P} + i\boldsymbol{p}\cdot\boldsymbol{k}) \\ &\quad\times E_{\boldsymbol{p},(1/2)\boldsymbol{v}}(\boldsymbol{r},t),\end{aligned} \tag{7}$$

where in the impact parameter treatment

$$E_{\boldsymbol{k},\boldsymbol{u}}(\boldsymbol{r},t) = \exp\left(i\boldsymbol{u}\cdot\boldsymbol{r} - i\frac{u^2t}{2} - i\frac{k^2t}{2}\right). \tag{8}$$

It may also be noted that in ${}^mD_{\boldsymbol{v}}^+(\boldsymbol{r};Z)$, the first M function is outgoing, whereas the second is ingoing and vice versa for ${}^mD_{\boldsymbol{v}}^-(\boldsymbol{r};Z)$.

Since $H^\dagger\psi_f^{-*}$ and $H\psi_i^+$ both contain the nonorthogonal kinetic energy $-\partial\boldsymbol{r_T}\cdot\partial\boldsymbol{r_P}$, the second term in Eq. (1) may be neglected, and the generalized (G)CDW in Eq. (2) may assume its asymptotic eikonal form, for all but the smallest partial-wave azimuthal angular momentum quantum numbers. Thus we have derived GCDW-EIS.

In Fig. 1 we present DDCS for proton hydrogen-atom 50 keV collisions for forward scattering. We plot $\frac{d^2\sigma}{d\Omega_k dE_k}$ versus E_k, the ejected electron energy and where Ω_k is the solid angle $\sin\theta_k d\theta_k d\phi_k$. The dashed line corresponds to $m_P = 0 = m_T$ [14]. The solid line corresponds to the inclusion of $m_P = -1, 0, +1$ and $m_T = -1, 0, +1$, making 9 contributions, to our new G (generalized) CDW-EIS theory for DDCS. There is a shallow minimum implying a saddle point. In Fig. 2, we show that for $m_T = 0$, $m_P = 0$ dominates $m_P = \pm1$, which dominates $m_P = \pm2$.

In Fig. 3, we show that for $m_P = 0$, $m_T = \pm1$ dominates $m_T = \pm2$, except very close to the cusp. However,

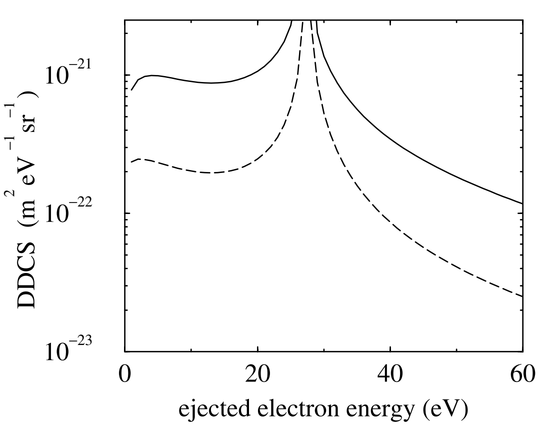

FIG. 1. The DDCS for the collision of 50 keV proton with a hydrogen-atom at an electron emission angle of 0°. Dashed line: GCDW-EIS with $m_P = m_T = 0$ (= CDW-EIS); solid line: GCDW-EIS with double summation over m_P and m_T from -1 to $+1$.

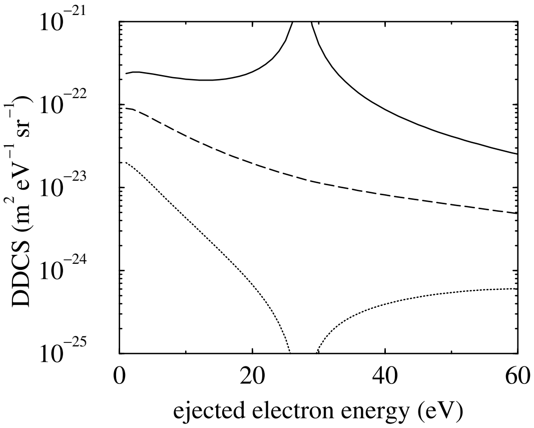

FIG. 2. The DDCS for the collision of 50 keV proton with a hydrogen atom at an electron emission angle of 0°. Solid line: GCDW-EIS with $m_P = m_T = 0$ (= CDW-EIS); dashed line: GCDW-EIS with $m_T = 0$ and $m_P = \pm 1$; dotted line: GCDW-EIS with $m_T = 0$ and $m_P = \pm 2$.

to the left down to 10 eV, $m_T = \pm 1$ dominates $m_T = 0$. Results not shown for $m_P = \pm 2$, with $m_T = 0, \pm 1, \pm 2$, for $m_P = \pm 3$, with $m_T = 0, \pm 1, \pm 2, \pm 3$, and for $m_P = \pm 4$, with $m_T = 0, \pm 1, \pm 2, \pm 3, \pm 4$, all show DDCS orders of magnitude less and with strong anticusps.

In Figs. 4 and 5 we illustrate proton hydrogen-molecule 100 keV forward scattering DDCS, namely $\frac{kd^2\sigma}{dE_k d\cos\theta_k}$ plotted against k/v. In Fig. 4, we include only $m_P = 0 = m_T$ in the lower curve [14], whereas in the upper curve we sum the DDCS over m_P and m_T, each from -2 through 0 to $+2$. The minimum at $k/v = 0.5$ is so shallow as to be almost indistinguishable from a horizontal point of inflexion. This implies a shelf rather than a saddle.

In Fig. 5, the DDCS of the upper curve in Fig. 4 (summed over m_P and m_T each from -2 to $+2$) are plotted against our relative experimental results [20] suitably scaled. The agreement is much improved compared to our basic $m_P = 0 = m_T$ theory [20]. From Fig. 4, we note that for $k < v$, the DDCS are increased and the cusp is broadened, compared to the original $m_P = 0 = m_T$ theory. This makes physical sense because slower electrons will have more time to experience rotational coupling out of their azimuthal plane. For $k > v$, the cusp is not broadened per se but for the highest values of k, the DDCS are increased.

In conclusion, CDW, CDW-EIS, and GCDW-EIS theories have been shown to be remarkably robust in rising to the experimental challenges, both theory and experiment being generated within our own group.

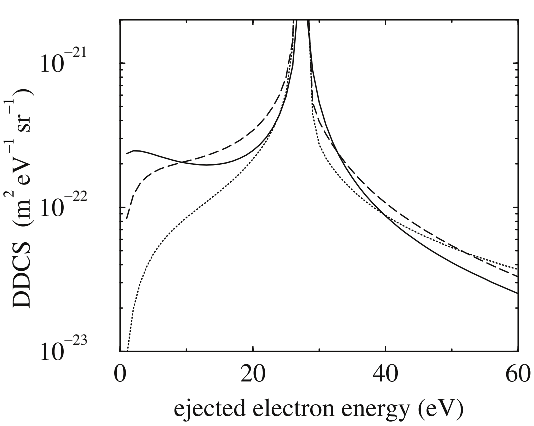

FIG. 3. The DDCS for the collision of 50 keV proton with a hydrogen-atom at an electron emission angle of 0°. Solid line: GCDW-EIS with $m_P = m_T = 0$ (= CDW-EIS); dashed line: GCDW-EIS with $m_P = 0$ and $m_T = \pm 1$; dotted line: GCDW-EIS with $m_P = 0$ and $m_T = \pm 2$.

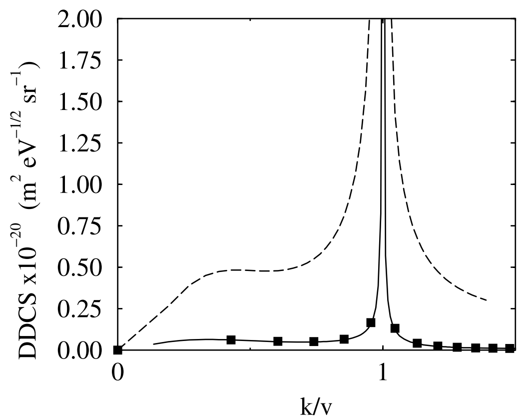

FIG. 4. The DDCS for the collision of 100 keV proton with H_2 at an electron emission angle of 0°. Solid line: CDW-EIS; squares: GCDW-EIS with $m_P = m_T = 0$ showing it reduces down to original CDW-EIS theory; dashed line: GCDW-EIS with double summation over m_P and m_T from -2 to $+2$.

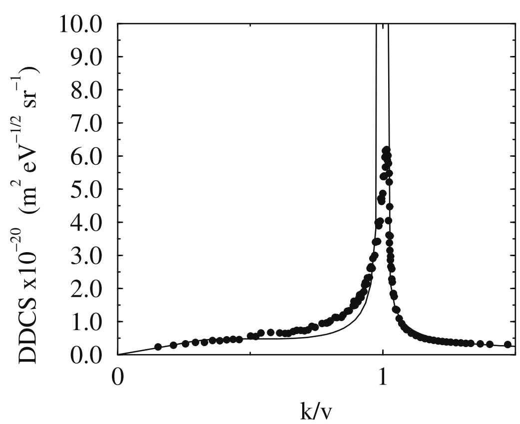

FIG. 5. The DDCS for the collision of 100 keV proton with H_2 at an electron emission angle of 0°. Solid line: GCDW-EIS with double summation over m_P and m_T from -2 to $+2$. Circles: experimental results of [20].

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