Loss of wave-packet coherence in stationary scattering experiments

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We consider the cross section for a scattering reaction averaged over a statistical ensemble of incident beam wave packets. We generalize a result known from neutron diffraction that static experiments involving stationary scattering via conservative interactions and steady beam currents cannot distinguish the wave-packet nature of the incident beam. Thus we interpret the results of recent experiments on the loss of interference effects in proton scattering from molecular hydrogen as due to the weak collimation of the incident beam rather than alterations to beam wave packets.

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I. INTRODUCTION

A nice example of the *van Cittert–Zernike theorem* of transverse coherence from an extended, incoherent source is an estimation of the *area of coherence* of sunlight around a point on a screen at the Earth's surface [1]. The theorem yields a *transverse coherence length*, viz. the diameter of the area of coherence, proportional to λ/α, where α is the angular diameter the sun's disk subtends at the Earth's surface. With a mean wavelength of 550 nm and $\alpha \simeq 9.3$ mrad, one has a transverse coherence length of 0.06 mm. To observe for example double-slit interference with sunlight, one has to introduce slits closely spaced by less than this amount [2].

Egodapitiya *et al.* [3] have measured in a precision experiment the transverse coherence length of a nearly monochromatic beam of protons, de Broglie wavelength λ, passing through a collimator aperture and scattered by a crossed beam of molecular hydrogen. The two-center nature of the molecular scattering gives rise to a well-established "double-slit interference" effect [4], which the authors were able to suppress by reducing the distance L of the reaction volume to the collimator aperture. A decrease in L increases the angular width $\alpha \simeq a/L$ the collimator aperture subtends at the target, where $a \ll L$ is the aperture width in the scattering plane. They found that the corresponding decrease in the transverse coherence length λ/α of the scattered protons relative to the two-center molecular bond length suppresses as expected the observed interference effects in the scattering cross section.

A sampling of their results is shown in Fig. 1 along with the theoretical cross sections of Chowdury, Schulz, and Madison [5]. The measurements involved 75 keV incident protons, monochromatic to less than 1 eV, scattered at extraordinarily small angles of less than 1 mrad in 0.1 mrad bins. With an aperture width of $a = 0.15$ mm in the scattering plane, they varied the distance to the reaction volume from $L = 50$ cm down to $L = 6.5$ cm and thereby increased the collimator angular width from $\alpha = 0.30$ mrad to $\alpha = 2.3$ mrad. Thus, with a de Broglie wavelength of $\lambda = 0.10$ pm, they reported a corresponding decrease in the transverse coherence length of the incident beam from $\lambda/\alpha \simeq 6.6$ a.u. at $L = 50$ cm to $\lambda/\alpha \simeq 0.86$ a.u. at $L = 6.5$ cm, and therefore a change in λ/α from greater to smaller than the "two-slit" intermolecular separation $D = 1.6$ a.u. of the molecular hydrogen. They thus accounted for their observed loss at $L = 6.5$ cm of the interference dip evident in the cross section around 0.8 mrad for large L. They have recently extended their studies of coherence to electron capture by protons colliding with molecular hydrogen [6].

While we feel these experiments demonstrate the role of transverse coherence in establishing interference effects, we disagree with the conclusions of Egodapitiya *et al.* [3] that the variable collimation somehow affects the incident beam in a fundamental quantum way. In the next section, we use an S-matrix momentum formulation of scattering theory to average the cross section in a general way over a statistical ensemble of rather arbitrary incident-beam *wave packets*. We follow an approach given long ago by Wichmann [7] but generalize it somewhat to allow for poorly collimated incident wave packets with mean centroid momenta off axis relative to

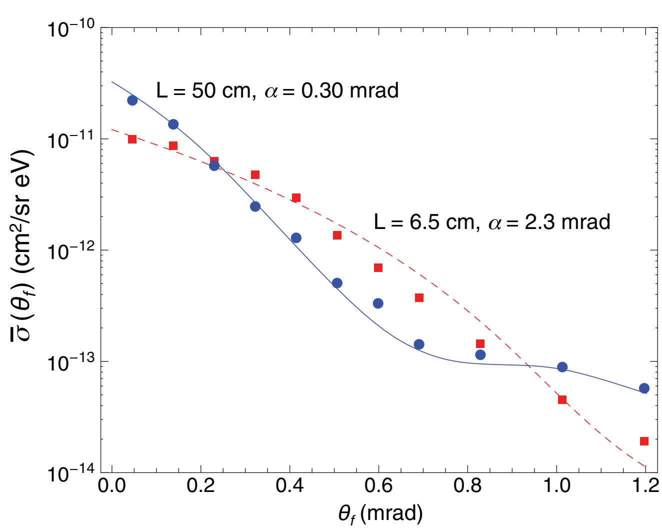

FIG. 1. (Color online) Proton-scattering cross section for ionization of H_2 as a function of the proton-scattering angle as in Fig. 1 of Egodapitiya *et al.* [3]. The round (blue) and square (red) points are the $L = 50$ cm and $L = 6.5$ cm measurements, respectively, while the solid (blue) and the dashed (red) curves show the calculated cross section from Ref. [5] *averaged* according to Eq. (14). The size of the data points corresponds roughly to the error bars in the data, and differences in the blue and red measurements are well outside the statistical error.

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the incident-beam axis. Thus we show that the static energy-conserving scattering reactions with steady beam currents considered here will distinguish neither wave-packet structure nor coherence in the incident beam. Instead, we account for the loss of interference observed by Egodapitiya *et al.* as simply an incoherent average over the poorly collimated ensemble of incident-beam momenta.

Our conclusions are analogous to ones derived some time ago by Bernstein and Low [8] (see also [9]) in connection with the notion of lost wave-packet coherence in neutron diffraction, although they assumed strong collimation throughout. Our approach uses the density matrix to describe the incident beam and is similar to the derivation of the cross-section average given by Gottfried [10] (we found the reference to Wichmann there), except Gottfried also assumes strong collimation throughout. Zeilinger and co-workers have thoroughly studied the effects of beam preparation and collimation on wave-packet coherence while compiling a long and well-documented record of work on matter-wave interferometry beginning with precision neutron-diffraction experiments back in the 1980s. See for example [11,12] and references therein.

We stress that our results here are not new. No fundamental changes to familiar quantum scattering descriptions are required to explain the observations of Egodapitiya *et al.*, contrary to their claims. Wichmann's approach is based on asymptotic momentum wave packets, removing from the discussion the shape and spread in time of the corresponding *coordinate* wave packets. In the popular text on scattering theory, Taylor closely follows Wichmann but neglects to reference him [13]. However, neither Wichmann, nor Taylor, nor the conventional scattering references that we know of make any reference to transverse coherence. Here, we attempt to connect with Egodapitiya *et al.*'s experiments throughout our presentation. We employ a density-matrix derivation to facilitate the averaging over the incident-beam statistical ensemble. The density matrix also sets the stage for generalizing our discussion to measurement interferometry, as advanced in the rich literature on neutron-diffraction experiments, although the cross sections considered here involving a single detector-entrance channel trace just the diagonal elements of the scattered-state density matrix.

II. SCATTERING OF WAVE PACKETS

One is inclined customarily to start with the free-particle coordinate wave packet,

$$\psi_i(\boldsymbol{r},t) = \int \phi_i(\boldsymbol{p}) \frac{e^{i\,\boldsymbol{p}\cdot\boldsymbol{r}}}{(2\pi)^{3/2}} e^{-ip^2t/2m}\, d\,\boldsymbol{p}, \tag{1}$$

to describe the *incident* beam as it passes through the last collimator slit on its way to the reaction volume. Here $\phi_i(\boldsymbol{p}) = \langle \boldsymbol{p}|i\rangle$ is a free-particle *momentum* wave packet and $\langle \boldsymbol{r}|\boldsymbol{p}\rangle = e^{i\,\boldsymbol{p}\cdot\boldsymbol{r}}/(2\pi)^{3/2}$ is a plane-wave momentum eigenstate. (We adopt a system of units in which $\hbar \equiv 1$, unless we state explicitly otherwise.) A 75 keV proton moves at 3.8×10^6 m/s, so that incident beams with currents in the range 1 μA to 1 nA used by Egodapitiya *et al.* [3] have a mean spacing between protons of some 0.6 mm to 6 cm. Electron beams at 13.6 eV with similar currents have roughly half these spacings between electrons. Thus there is generally only one incident-beam particle at a time passing through the last collimator and hence through the reaction volume. Egodapitiya *et al.* also routinely achieve incident beams monochromatic to 1 eV at 75 keV and therefore with sharp *momentum* distributions $|\phi_i(\boldsymbol{p})|^2$ with widths on the order of $\Delta p_i/p \simeq \sqrt{1\text{ eV}/75\text{ keV}} \simeq 0.004$.

The plane-wave contributions $e^{i\,\boldsymbol{p}\cdot\boldsymbol{r}}$ to (1) will image through the last collimator aperture as overlapping diffraction patterns near the target molecules in the reaction volume a distance L away. (We ignore any small fraction of particles that might scatter microscopically off the slit edge.) Two contributions $e^{i\,\boldsymbol{p}\cdot\boldsymbol{r}}$ and $e^{i\,\boldsymbol{p}'\cdot\boldsymbol{r}}$ are considered coherent [2] if their overlapping patterns are not displaced by more than the angular width $\sim \lambda/a$ of their central maxima in the scattering plane and thus not by more than the distance $\sim\lambda L/a \equiv \lambda/\alpha$, where α is the angular width of the collimator as before. This idea forms the basis of the van Cittert–Zernike theorem.

Accordingly, one might presume that wave-packet coherence could be modulated and the resulting effect observed by changes in the angular width of the last collimator, as the experiments of Egodapitiya *et al.* [3] might seem to suggest. As we shall see, however, this conclusion is flawed in the case of static scattering reactions considered here that conserve energy and therefore the magnitude of the momentum. When energy is conserved and the incident beam is mostly forward moving, the scattering reaction effectively selects a random plane-wave contribution $e^{i\,\boldsymbol{p}\cdot\boldsymbol{r}}$ from the incident wave packet, thereby collapsing all wave-packet coherence. The resulting cross section becomes a fully incoherent average over the corresponding momentum distribution $|\phi_i(\boldsymbol{p})|^2$ of the incident beam.

To see how this comes about, we turn to a general description of wave-packet scattering. The microscopic process of scattering of an incident-beam particle with a target molecule is described broadly by the S matrix [7,14] according to $|f\rangle = S|i\rangle$, where we will assume $\langle \boldsymbol{p}|f\rangle = \phi_f(\boldsymbol{p})$ is the free-particle momentum wave packet of the scattered particle. If we work in the momentum representation, this description is time independent and remarkably straightforward.

To generalize to a mixed state characterizing a statistical ensemble of incident-beam wave packets, we introduce the density operator for the microscopic scattering reaction

$$\rho_f = |f\rangle\langle f| = S|i\rangle\langle i|S^\dagger = S\rho_i S^\dagger. \tag{2}$$

The diagonal elements of the resulting density matrix define the probabilities for detection of a momentum eigenstate $|\boldsymbol{p}_f\rangle$ according to $P(\boldsymbol{p}_f) = \langle \boldsymbol{p}_f|\rho_f|\boldsymbol{p}_f\rangle$. Then

$$P(\hat{\boldsymbol{p}}_f) = \int p_f^2 dp_f\, P(\boldsymbol{p}_f) = \int p_f^2 dp_f \langle \boldsymbol{p}_f|S\rho_i S^\dagger|\boldsymbol{p}_f\rangle \tag{3}$$

describes the likelihood of scattering into the element of solid angle $d\,\hat{\boldsymbol{p}}_f = d\Omega_f$ around $\boldsymbol{p}_f$ defined by the detector.

The spatial range of the microscopic scattering reaction is typically tens of atomic units, so generally less than 1 nm. We take $\mathcal{A}$ as the area of the last slit and assume it defines roughly the cross section of the incident beam and hence of its intersection with the reaction volume. As we have seen, the width of $\mathcal{A}$ in the scattering plane is a macroscopic dimension generally on the order of 0.1 to 1 mm.

One recognizes energy conservation in the microscopic scattering reactions with the introduction of the familiar *on-shell* transition matrix T_{fi} according to $S_{fi} = -2\pi i \delta(E_f - E_i) T_{fi}$ [14], so that for transitions between momentum eigenstates $\langle \boldsymbol{p}_f|$ and $|\boldsymbol{q}\rangle$

$$S(\boldsymbol{p}_f,\boldsymbol{q}) = -2\pi i \frac{m}{q}\delta(p_f - q)T(\boldsymbol{p}_f,\boldsymbol{q}). \tag{4}$$

Then the integral over p_f in Eq. (3) becomes effortless and one obtains for the scattering probability into $d\hat{\boldsymbol{p}}_f$ (using $\int d\boldsymbol{q}|\boldsymbol{q}\rangle\langle\boldsymbol{q}| = 1$)

$$P(\hat{\boldsymbol{p}}_f) = \int d\boldsymbol{q}\, d\boldsymbol{q}'\delta(q-q') \times (2\pi m)^2 T(\boldsymbol{p}_f,\boldsymbol{q})\langle\boldsymbol{q}|\rho_i|\boldsymbol{q}'\rangle T^*(\boldsymbol{p}_f,\boldsymbol{q}'). \tag{5}$$

Here $\delta(q-q')$ ensures that the intermediate momentum *magnitudes* are conserved. (The subscripts f,i on S_{fi} and T_{fi} could include additional internal variables to generalize the development here to an arbitrary inelastic or rearrangement collision.)

Following Wichmann [7], we generalize now the initial state of the incident beam $\langle\boldsymbol{q}|\rho_i|\boldsymbol{q}'\rangle$ to an ensemble of free-particle momentum wave packets,

$$\langle\boldsymbol{q}|\rho_i|\boldsymbol{q}'\rangle = e^{-i(\boldsymbol{q}-\boldsymbol{q}')\cdot\boldsymbol{x}_i}\phi_i(\boldsymbol{q};\boldsymbol{p}_i')\,\phi_i(\boldsymbol{q}';\boldsymbol{p}_i')^*, \tag{6}$$

defined by the momenta $\boldsymbol{p}_i'$ and offsets $\boldsymbol{x}_i$ of the classical straight-line trajectories of the particles in the beam as they pass through the last collimator slit. Thus the phase $e^{-i\boldsymbol{q}\cdot\boldsymbol{x}_i}$ displaces the centroid of the wave packet $\phi_i(\boldsymbol{q};\boldsymbol{p}_i')$ by $\boldsymbol{x}_i$ with respect to our z axis along the beam axis through the center of the last collimator to the pass-through point of the packet's trajectory inside the slit. Here $\boldsymbol{p}_i' = \boldsymbol{p}_i + \boldsymbol{p}_{i\perp}'$ is the mean *centroid* momentum of the wave packet with respect to the beam axis, and $\boldsymbol{p}_i \equiv p_i\hat{\boldsymbol{z}}$ with $\boldsymbol{p}_{i\perp}'$ in the plane of the collimator slit with $\boldsymbol{p}_i\cdot\boldsymbol{p}_{i\perp}' \equiv 0$. Note we suppress an explicit *shape parameter* for the packet, which Wichmann introduced and labeled. It is already implied by the function ϕ_i.

Thus we generalize Wichmann somewhat to include off-axis incident momenta $\boldsymbol{p}_i'$, albeit with $p_i \gg p_{i\perp}'$ so that $p_i'^2 = p_i^2 + p_{i\perp}'^2 \simeq p_i^2$. We require only that the source and incident-beam optics along with the overall collimation have sufficiently shaped and directed these wave-packets along the general direction of the beam axis so that $\phi_i(\boldsymbol{q};\boldsymbol{p}_i')\phi_i(\boldsymbol{q}';\boldsymbol{p}_i')^* \simeq 0$ unless $q_z \simeq q_z' \simeq p_i > 0$. This is a fairly weak constraint that collimation is at least sufficient to ensure the wave packets are all moving mostly forward, albeit each with its own narrow intrinsic width (quantum dispersion) $\Delta q_i \ll p_i$.

The mixed state describing the incident beam is obtained by averaging over a statistical ensemble of incident wave packets from Eq. (6) according to

$$\overline{\langle\boldsymbol{q}|\rho_i|\boldsymbol{q}'\rangle} = \int\frac{d\boldsymbol{p}_{i\perp}'}{\Delta\boldsymbol{p}_\perp}\int\frac{d\boldsymbol{x}_i}{\mathcal{A}}\langle\boldsymbol{q}|\rho_i|\boldsymbol{q}'\rangle. \tag{7}$$

We assume a uniform distribution in $\boldsymbol{x}_i$ of incident wave packets normalized over the last collimator slit area $\mathcal{A}$, and a uniform distribution in $\boldsymbol{p}_{i\perp}'$ of incident momenta also normalized over the last slit with total effective spread $\Delta\boldsymbol{p}_\perp$. That is, we assume a uniform bundle of slightly diverging wave-packet trajectories such that a distance L away at the reaction volume $\Delta\boldsymbol{p}_\perp' \simeq p_i\alpha$ in the scattering plane, where $\alpha \simeq a/L$ is the collimator angular width.

As Wichmann points out, our averaging over the lateral offsets $\boldsymbol{x}_i$ of wave packets in the beam is equivalent to averaging over lateral offsets of the target molecules across the reaction volume. The procedure amounts to describing the target as a random distribution of single scattering centers, which is physically realistic with the low-intensity beams and rarified gas targets of interest here.

A key advantage of the momentum representation is evident immediately. Introducing the $\boldsymbol{x}_i$ dependence from Eq. (6), the ensemble average over $\boldsymbol{x}_i$ is straightforward and gives

$$\int\frac{d\boldsymbol{x}_i}{\mathcal{A}}\langle\boldsymbol{q}|\rho_i|\boldsymbol{q}'\rangle = \frac{(2\pi)^2}{\mathcal{A}}\delta(\boldsymbol{q}_\perp - \boldsymbol{q}_\perp')\phi_i(\boldsymbol{q};\boldsymbol{p}_i')\phi_i^*(\boldsymbol{q}';\boldsymbol{p}_i'), \tag{8}$$

where the area of integration has been extended to infinity with impunity since the macroscopic cross-sectional area $\mathcal{A}$ is already large compared to any dimension characterizing the microscopic scattering event. Here $\boldsymbol{q}_\perp,\boldsymbol{q}_\perp'$ are momentum components perpendicular to the beam axis along z. With the cofactor $\delta(\boldsymbol{q}_\perp - \boldsymbol{q}_\perp')$ and noting that $q^2 = q_z^2 + q_\perp^2$, one readily establishes for the momentum-conserving factor from Eq. (5) the identity

$$\delta(q-q') \equiv \frac{q}{|q_z|}\{\delta(q_z - q_z') + \delta(q_z + q_z')\}. \tag{9}$$

However, as we noted above Eq. (7), we assume the fairly weak collimation condition that $\phi_i(\boldsymbol{q};\boldsymbol{p}_i')\phi_i(\boldsymbol{q}';\boldsymbol{p}_i')^* \simeq 0$ unless $q_z \simeq q_z' \simeq p_i > 0$, so that here $\delta(q_z + q_z') = 0$.

Then with $\delta(q_z - q_z')\delta(\boldsymbol{q}_\perp - \boldsymbol{q}_\perp') = \delta(\boldsymbol{q} - \boldsymbol{q}')$, the double integral over $\boldsymbol{q}$ and $\boldsymbol{q}'$ in Eq. (5) collapses, and we obtain for the scattering probability averaged over $\boldsymbol{x}_i$, setting aside the average over $\boldsymbol{p}_{i\perp}'$ for the moment,

$$\overline{P}(\hat{\boldsymbol{p}}_f)\mathcal{A} = \int d\boldsymbol{q}\frac{q}{|q_z|}\sigma(\boldsymbol{p}_f,\boldsymbol{q})|\phi_i(\boldsymbol{q};\boldsymbol{p}_i')|^2. \tag{10}$$

Here $\sigma(\boldsymbol{p}_f,\boldsymbol{q}) \equiv (2\pi)^4 m^2|T(\boldsymbol{p}_f,\boldsymbol{q})|^2$ is the microscopic cross section [14] for ideal scattering between the (plane-wave) momentum eigenstates $\langle\boldsymbol{p}_f|$ and $|\boldsymbol{q}\rangle$. Again following Wichmann, we note that $\overline{P}(\hat{\boldsymbol{p}}_f)\mathcal{A}\,d\hat{\boldsymbol{p}}_f$ is the effective cross-sectional area that the exit channel defined by $d\hat{\boldsymbol{p}}_f$ presents to the incident beam, so that $\overline{\sigma}(\boldsymbol{p}_f,\boldsymbol{p}_i') = \overline{P}(\hat{\boldsymbol{p}}_f)\mathcal{A}$ is the effective differential cross section for microscopic scattering averaged over wave-packet displacements $\boldsymbol{x}_i$ in the incident beam.

Equation (10) is a key result [and equivalent to Eq. (21) in Wichmann [7] and Eq. (3.22) in Taylor [13]]. It demonstrates that the effective cross section $\overline{\sigma}(\boldsymbol{p}_f,\boldsymbol{p}_i') = \overline{P}(\hat{\boldsymbol{p}}_f)\mathcal{A}$ depends only on the square of the incident-beam momentum distribution $|\phi_i(\boldsymbol{q};\boldsymbol{p}_i')|^2$ and thus is independent of any wave-packet coherence. Changes in the collimator distance L will not alter this conclusion. *Therefore, experiments with even weakly collimated beams incident on stationary targets cannot distinguish coherent wave-packet structure* (cf. also [8], and [11], Sec. III). This conclusion is readily generalized to inelastic and exchange reactions.

As long as we are not scattering in the vicinity of a resonance, we may assume further, as is usually done, that the microscopic cross section $\sigma(\boldsymbol{p}_f,\boldsymbol{q})$ varies little over the short interval $\Delta q_i \ll p_i$ near $\boldsymbol{q} \simeq \boldsymbol{p}_i'$ where $\phi_i(\boldsymbol{q};\boldsymbol{p}_i')$ is nonvanishing. Then, $\sigma(\boldsymbol{p}_f,\boldsymbol{p}_i')$ can be safely removed from the integral over $\boldsymbol{q}$ in Eq. (10). Invoking the normalization of the incident wave packets $\int d\boldsymbol{q}|\phi_i(\boldsymbol{q};\boldsymbol{p}_i')|^2 = 1$, we then obtain

$$\overline{\sigma}(\boldsymbol{p}_f,\boldsymbol{p}_i') = \frac{p_i'}{p_i}\sigma(\boldsymbol{p}_f,\boldsymbol{p}_i') \tag{11}$$

fully independent of the shape and coherence of the incident wave packets. In the strong collimation limit $\boldsymbol{p}_i' \to \boldsymbol{p}_i$, one obtains the result widely adopted in analyzing scattering experiments. Namely, the measured cross section from a well collimated beam of incident particles, albeit averaged over a statistical ensemble, remains a good representation of the ideal microscopic cross section between momentum eigenstates [10].

Finally, restoring the ensemble average over the $\boldsymbol{p}_{i\perp}'$ in the incident beam, we have in the case of weak collimation

$$\overline{\sigma}(\boldsymbol{p}_f,\boldsymbol{p}_i) \simeq \int \frac{d\,\boldsymbol{p}_{i\perp}'}{\Delta\,\boldsymbol{p}_\perp}\frac{p_i'}{p_i}\sigma(\boldsymbol{p}_f,\boldsymbol{p}_i'). \tag{12}$$

We will use this result in the next section to analyze the data in Fig. 1.

III. EFFECTIVE CROSS SECTIONS

We return now to a comparison of the data in Fig. 1 with the beam-averaged cross section in Eq. (12). Let $\sigma(\boldsymbol{p}_f,\boldsymbol{p}_i) = \sigma(\theta_f)$ be the microscopic cross section expressed in terms of a proton scattering angle θ_f relative to the incident-beam z axis. A poorly collimated projectile proton incident somewhat off axis along $\boldsymbol{p}_i' = \boldsymbol{p}_i + \boldsymbol{p}_{i\perp}'$ can be thought of as simply shifting this scattering cross section according to $\sigma(\boldsymbol{p}_f,\boldsymbol{p}_i) \to \sigma(\boldsymbol{p}_f,\boldsymbol{p}_i') = \sigma(\theta_f + \theta_i')$, where θ_i' is the angle of incidence relative to the incident-beam axis. Because we assume the collimation is nevertheless good enough so that $p_i'^2 = p_i^2 + p_{i\perp}'^2 \simeq p_i^2$, we take $d\,\boldsymbol{p}_{i\perp}' \simeq p_i' d\theta_i'$ and $\Delta\,\boldsymbol{p}_\perp' \simeq p_i\alpha$, where $\alpha \simeq a/L$ is the angular width of the last collimator slit. Thus, in Eq. (12), we take

$$\int \frac{d\,\boldsymbol{p}_{i\perp}'}{\Delta\,\boldsymbol{p}_\perp}\frac{p_i'}{p_i} \simeq \int \frac{d\theta_i'}{\alpha}\frac{p_i'^2}{p_i^2} \sim \int \frac{d\theta_i'}{\alpha}, \tag{13}$$

so that

$$\overline{\sigma}(\theta_f) \simeq \int_{-\alpha/2}^{\alpha/2} \frac{d\theta_i'}{\alpha}\sigma(\theta_f + \theta_i'). \tag{14}$$

Figure 1 compares this collimator-averaged cross section with the data of Egodapitiya *et al.* [3] for two angular widths α. At $L = 50$ cm with $a = 0.15$ mm, we have $\alpha = 0.3$ mrad and the beam-averaged cross section $\overline{\sigma}(\theta_f)$ is virtually indistinguishable from the theoretical cross section $\sigma(\theta_f)$ calculated by Chowdhury, Schulz, and Madison [5], the $L \to \infty$ limit. At $L = 6.5$ cm, we have $\alpha = 2.3$ mrad so that the integration range in Eq. (14) now covers the entire plot range and the interference dip around 0.8 mrad washes out completely. We conclude it is the weakened beam collimation at $L = 6.5$ cm and the consequent bundle of off-axis incident-wave-packet trajectories that averages out the two-center interference in the molecular scattering.

IV. DISCUSSION

It is natural to debate the size and coherences of supposed wave packets of particles in the incident beam. Such debates, however, will remain unresolved when extracting cross sections from the results of familiar static (energy-conserving) experiments with steady beam currents. One can consider each particle to be emitted as (i) a wave packet with an energy spread equal to the energy spread of the beam ensemble or (ii) a free-particle plane wave with an energy that varies from one plane wave to the next. Both of these rather disparate beam profiles lead to the same ensemble-averaged cross sections. In the end, all that one can say is that a static scattering reaction selects effectively a random (plane-wave) momentum eigenstate of the incident beam, and the usual theoretical cross sections between momentum eigenstates of the incident and target particles will account for experimental results.

If the collimation is weak, the cross section must be further averaged incoherently over off-axis incident-beam directions. These off-axis contributions to the beam ensemble can be regarded as incoherent—while defining a transverse coherence. Each individual scattering distribution produced by a particular incident direction combines incoherently with the other distributions, and each distribution is slightly shifted in scattering angle by the angle of incidence θ_i'. Overall, observable interference effects will be diminished to some degree depending on the degree to which the beam is uncollimated. The transverse coherence gives a rule of thumb for estimating the degree to which an interference effect is washed out.

In the ionization experiment of Egodapitiya *et al.* [3], $p + \mathrm{H}_2 \to p + \mathrm{H}_2^+ + e$, the ionized electron was not detected, although the ionization energy was fixed by selecting a fixed proton energy loss of 30 eV where a pronounced molecular interference effect is observed. (The cross section shown in Fig. 1 is therefore integrated over outgoing electron directions.) One could in principle, however, detect all of the reaction fragments in coincidence with multihit imaging (COLTRIMS) and thus invoke overall momentum conservation for the reaction $\boldsymbol{p}_i + \boldsymbol{P}_i = \boldsymbol{p}_f + \boldsymbol{P}_f + \boldsymbol{p}_e$ with $\boldsymbol{p}_e$ the ionized electron momentum and $\boldsymbol{P}_f$ the recoil-ion H_2^+ momentum. Here we take $\boldsymbol{P}_i = 0$ since the experiment involved cold H_2 target molecules with vanishing initial effective momentum. One could then postselect the coincidence data to filter those events with vanishing total momenta perpendicular to the beam axis and therefore with $\boldsymbol{p}_{i\perp}' = \boldsymbol{p}_{f\perp} + \boldsymbol{P}_{f\perp}' + \boldsymbol{p}_{e\perp}' \equiv 0$, i.e., with $\boldsymbol{p}_i' \equiv p_i\hat{\boldsymbol{z}} = \boldsymbol{p}_i$. Such constrained data sorting would avoid the averaging introduced in Eq. (12), and it is difficult to imagine the result to have much dependence on collimator angular width $\alpha \simeq a/L$.

This idea simplifies considerably in the case of the recent electron-*capture* experiments of Sharma *et al.*, $p + \mathrm{H}_2 \to \mathrm{H} + \mathrm{H}_2^+$ [6]. Using the same 75 eV protons as in their ionization experiment, they established a two-center molecular interference effect in the capture cross section at the large collimator distance $L = 50$ cm, which again washes out at the shorter distance $L = 6.5$ cm. For this two-body scattering reaction, momentum conservation with $\boldsymbol{P}_i = 0$ gives simply $\boldsymbol{p}_i = \boldsymbol{p}_f + \boldsymbol{P}_f$. Since these are also energetic collisions compared to the capture threshold, not only do the scattering angles remain extremely small but also the initial proton and final hydrogen-atom wave numbers are essentially equal, $\Delta p_i/p_i \simeq 1/3200$. Thus momentum conservation and collision kinematics dictate that $\boldsymbol{P}_f$ is essentially orthogonal to $\boldsymbol{p}_i$ (and $\boldsymbol{p}_f$ as well) with magnitude $P_f \simeq p_i\theta_f$. That is, the component of recoil momentum along $\boldsymbol{p}_i$ (or $\boldsymbol{p}_f$) remains extremely small, viz. $\boldsymbol{P}_f \cdot \hat{\boldsymbol{p}}_i \simeq P_f^2/2p_i \ll P_f$.

The upshot is, given an off-axis ensemble of incident protons along $\boldsymbol{p}_i'$, there corresponds a mirror ensemble of recoil ions with each recoil $\boldsymbol{P}'_f$ perpendicular to the corresponding incident $\boldsymbol{p}_i'$, requiring the capture cross section $\sigma(\boldsymbol{p}_f, \boldsymbol{P}'_f, \boldsymbol{p}_i')$ to be averaged incoherently over the cone of $\boldsymbol{p}_i'$ defined by the collimator, analogous to the average in Eq. (12). The two-particle angular distribution defined by $P(\hat{\boldsymbol{p}}_f, \hat{\boldsymbol{P}}'_f) = \sigma(\boldsymbol{p}_f, \boldsymbol{P}'_f, \boldsymbol{p}_i')/\mathcal{A}$ suggests that one could extract a beam-profile distribution $P(\hat{\boldsymbol{p}}_i') \equiv \sigma(\boldsymbol{p}_f, \boldsymbol{p}_i' - \boldsymbol{p}_f, \boldsymbol{p}_i')/\mathcal{A}$ and thus provide a strong check on the effects of collimation on the beam. Alternatively, as we suggested above for an ideal ionization experiment, one might postselect on the recoil ions with say $\boldsymbol{P}'_f \equiv P_f\hat{\boldsymbol{x}}$ perpendicular to the beam axis and therefore with $\boldsymbol{p}_i' \equiv p_i\hat{\boldsymbol{z}} = \boldsymbol{p}_i$ and thus extract $\sigma(\boldsymbol{p}_f, P_f\hat{\boldsymbol{x}}, p_i\hat{\boldsymbol{z}})$. Again, such data sorting would avoid the averaging introduced in Eq. (12).

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