Photoionization of a quantum grating formed by a single atom

S F Zhang\textsuperscript{1,2,3}, B Najjari\textsuperscript{1,3} and X Ma\textsuperscript{1,2,\ast}

\textsuperscript{1} Institute of Modern Physics, Chinese Academy of Sciences, Lanzhou 730000, People’s Republic of China
\textsuperscript{2} University of Chinese Academy of Sciences, Beijing 100049, People’s Republic of China

\textsuperscript{\ast} Author to whom any correspondence should be addressed.

Received 18 April 2021, revised 4 August 2021
Accepted for publication 9 August 2021
Published 25 August 2021

Abstract

When an atom passes through a macroscopic diffraction grating its wave function acquires a regular space structure and its collision by another particle can be thought of as scattering, of the latter, on a grating composed of a single atom (hereafter termed as ‘quantum-grating’). Photoionization of such a ‘quantum grating’ unveils interference features and in particular a striking difference in the photoelectron and recoil ion spectra which no longer ‘mirroring’ each other as in the case of photoionization of atoms or molecules. We show that complete information about the macroscopic diffraction grating is directly contained in the recoil ion spectra while only partly exhibited in the spectra of the electron.

Keywords: quantum-grating, photoionization, interference, allowed and forbidden momentum regions, basic atomic collision

Recent explorations in matter-wave interferometry promise the test of quantum superposition principle at the large scales of massive objects [1, 2]. In collision physics, processes involving a molecular target compared to an atom can unveil different features due to the nature of their corresponding electronic wave functions. For instance, in the ionization processes, the electron is emitted from the multi-sites of the molecule and the coherent contributions of the corresponding indistinguishable pathways lead to interference phenomena. Thus, significant efforts have been employed to explore various interference phenomena arising when particles (including photons) interact with molecules (see the pioneering works of [3, 4] and the recent followings of [5–8], including references therein). However, research works performed in this field dealt exclusively with ionization of atomic targets including molecules and clusters. Yet, none of these studies have considered the breakup of an atom passed through a diffraction grating induced in collision with charged particles nor by absorption of photons. Because of the uncontrolled exchanged momentum between the atom and the diffraction grating, the wave function of such an atom will acquire a wave-packet property due to the uncertainty principle. When such an atom is taken to interact with a charged particle, or a photon, the result can be viewed as scattering of the latter on an object which can be thought as a diffraction grating and will be referred to as ‘quantum grating’. Like its macroscopic analogous this quantum grating (QG) possesses a periodic spacial structure, which consists of stronger and weaker interacting parts in space corresponding to respectively larger and smaller values of the atomic probability density but constructed only from a single atom. This can be viewed as ‘splitting’ the atom into a set of...
identical atomic ‘copies’ at equidistant separation from each other. Such an atomic QG qualitatively differs from a molecular object where the ‘multi-site’ structure of the electron wavefunction is due to the presence of ‘real’ nuclei. Therefore, there are all ingredients to expect that the process of ionization of an atomic QG will strongly differ from ionization of not only a ‘normal’ atom but also a molecule.

In this letter we examine photoionization of a helium atom passed through a diffraction grating. Due to the spacial ‘multi-sites’ structure of the atomic QG one might expect to observe interference pattern in the spectra of resulting fragments from the ionizing reactions which are clearly different from those spectra of photo ionization of ‘normal’ atomic targets.

In particular, it will be shown that interference patterns in the spectra of the emitted electrons and recoil ions are different in nature compared to the known interference in photoionization of ‘normal’ atomic targets. For instance, the interference effects in the QG can manifest only under certain conditions, and will disappear for instance in the electron spectrum if the electron is detected individually. Atomic units (\(\hbar = -e = 1\)) are used throughout the text unless otherwise stated. Where \(m_e\) is the electron mass, \(\hbar\) is Planck constant divided by \(2\pi\) and \(e\) is the electron charge.

Let a helium atom with an initial momentum \(P_i = (0, 0, P_i)\) be launched through a macroscopic diffraction-grating. The latter is located in \((x-y)\) plane perpendicular to \(P_i\) and consists of \(N_0\) slits along \(x\)-direction (as illustrated in figure 1). The dimensions, along the \(x\)- and \(y\)-directions, of each slit are denoted by \(a\) and \(b\), respectively. The separation between the neighboring slits (the grating constant) is \(d(>a)\). After the passage through the grating the wave function of the helium atom at large distances can be approximated using Huygens–Fresnel principle [9] and in single-active-electron (SAE) approach reads [10]

\[
\Psi_f(R, r, t) \sim A \exp(iP_{\perp} \cdot R - iE_i t) \\
\times \sin(\alpha x) \sin(N_0 \gamma x) \sin(\beta y) \sqrt{\phi(r)},
\]

where \(A\) is the normalization constant and depends only on the diffraction grating parameters and the incident momentum of the helium atom. \(R = (x, y, z)\) is the position vector of the atomic center-of-mass (CM) with respect to the center of the interaction region, taken here as the origin of the coordinate system. \(r\) is the electron position vector with respect to the atomic nucleus, \(D\) is the distance from the macroscopic slits to the interaction region of the QG and the photon, \(\alpha = Pa/2D\) and \(\beta = Pb/2D\) are parameters related to Fraunhofer diffraction along \(x\)- and \(y\)-directions respectively, and \(\gamma = Pd/2D\) is the parameter related to multi-slits. Furthermore, \(\phi(r)\) is the initial internal electronic state of the helium atom, \(E_i = \frac{P_i^2}{2M_e} + \epsilon_i\) is the total initial energy of the atom with \(\epsilon_i\) being its internal binding energy and \(M_e\) its total mass. The linear dimensions of the interaction region are assumed to be much smaller than the distance \(D\) between this region and the diffraction grating. In the interaction region the atomic QG is ionized by absorbing a photon from an electromagnetic radiation whose central frequency and energy-width are \(\omega_e\) and \(\Delta \omega_e\), respectively. The momentum and polarization vectors of the radiation are \(\kappa\) and \(\epsilon_e\) with \((\kappa \cdot \epsilon_e = 0)\). Assuming that the momenta of the resulting fragments after the ionization are measured, we take the final state of the whole atom as a product of a plane wave, which describes the motion of its CM, and an internal state describing the motion of the ionized electron. The latter is denoted by the continuum state \(\varphi_{\kappa_e}\) with an energy \(\kappa^2_e/2\) where \(\kappa_e\) is the asymptotic momentum of the electron in the rest frame of the atomic nucleus.

Denoting by \(P_f = (P_{f, x}, P_{f, y}, P_{f, z})\) and by \(E_f = \sqrt{\nu^2 + \frac{\kappa^2_e}{2}}\) the final momentum and energy of the atom (electron plus residual ion), respectively, the final state of the system reads [10]

\[
\Psi_f(R, r, t) = \frac{1}{\sqrt{V}} \exp(iP_f \cdot R - iE_ft) \varphi_{\kappa_e}(r).
\]

With \(V\) being a normalization volume of the CM motion. The transition amplitude for absorption of a single photon is then given by

\[
d\sigma_f = -i \int_{-\infty}^{+\infty} dt \left\langle \Psi_f(t) \left| \hat{W}_{EM} \right| \Psi_i(t) \right\rangle,
\]

where \( \hat{W}_{EM} = \frac{i}{\omega} \hat{A}(x, t) \cdot \hat{p} \) describes a single photon interaction, in the radiation gauge, with an electron (lightest particle) at position \(x = R_x + r\) in the laboratory frame with \(R_x\) being the position vector of the nucleus. Furthermore, \(A(x, t) = \sqrt{\frac{2m_e}{\omega^2}} \epsilon_e \omega_e \epsilon(x - \omega t)^\nu\) stands for the three dimension vector potential of the radiation field with a normalization volume \(V_e\), and \(\hat{p}\) is the momentum operator acting on the internal electronic states. Once the transition amplitude is derived, the fully-differential cross section for photoionization reads

\[
\frac{d\sigma_f}{dP_{rec} dP_e} = \lim_{T \to \infty} \frac{|a_f|^2}{T} \phi_{in} \left( \frac{V}{8\pi^4} \right) \left( \frac{V_e}{8\pi^4} \right) \\
\times \left| \left\langle \varphi_{\kappa_e} \right| e^{\omega t} \left( \epsilon_{\kappa_e} \cdot \hat{p} \right) \left| \varphi_i \right\rangle \right|^2 \times G.
\]

\(T\) is the measure time (as long as possible), \(\phi_{in} = c/V_e\) is the flux of the incident photons, \(V_e\) is the normalization volume of the emitted photoelectron and \(c\) is the speed of light. \(G\) is given by

\[
G = \left| F_{\beta}(P_{f, y} - \kappa_\beta) \sum_n F_\alpha(P_{f, x} - \kappa_\alpha + nP_d/D) \right|^2.
\]

The total momentum of the CM of the atom and the momenta of the fragments released in ionization are related by \(P_f = P_{rec} + \hat{p}\) and \(P_{rec} \simeq \hat{k}_e + \nu\) are the momenta, in the laboratory frame, of the recoil ion and the emitted electron, respectively, with \(\nu = \hat{P}_{rec}/M_a\) being the central velocity vector of the wave-packet representing the localized atom. The two \(\delta\)-functions in the expression (4) ensure the momentum conservation along \(z\)-axis (the direction of the incidence of the target on the macroscopic diffraction grating) and the energy conservation, which, after simplifications, are expressed by \(P_{rec} = P_i + \kappa_\beta - \kappa_e\) and \((\hat{p}_e - \nu)^2/2 = \omega_e - \nu \cdot \kappa_\beta + \epsilon_e\), respectively.
The term \( \mathbf{v} \cdot \mathbf{k} \) in the latter equation accounts for the non relativistic Doppler shift. Furthermore, the functions \( F_\eta \) in expression of \( G \) reflect the momentum spread in the \((x - y)\) plane due to the diffraction grating, and given here by

\[
F_\eta(\xi) = \int_{-\infty}^{+\infty} dx \ e^{i(x \sin(\eta x) / x)} = \begin{cases} 
\pi & ; -\eta < \xi < \eta \\
\pi / 2 & ; \xi = \eta \\
0 & ; \text{otherwise},
\end{cases}
\]

where \( \eta = \alpha \) or \( \beta \) and the summation over \( n \) (in \( G \)) accounts for the coherent contributions from different slits. These functions, together with the momentum conservation along the \( z \)-axis and the energy conservation, determine the photoionization kinematics of the QG. The absence of the \( \delta \) functions in the \( x/y \) components of the momenta, is a direct consequence of considering the diffraction grating as an external action on the helium atom. The total momentum of the system consisting of the helium atom, the grating and the photon is conserved leading to a strong entanglement between the first two (the photon momentum can safely be neglected in the dipole approximation). Since, only the degrees of freedom of the atom are taken into consideration and those of grating’s are not, the momentum conservation is abandoned. In contrast, the energy conservation still holds since the macroscopic grating, due to its enormous mass, does not participate in the energy exchange with the atom.

Besides, the expression (1) describes an atom moving with a well defined momentum \( \mathbf{p}_i \) passed through a diffraction grating. If such an atom has a broad momentum in the direction of the incidence (\( z \)-direction in our case) \( p_{iz} = P_{iz,0} \pm \Delta P_{iz} \), one has to perform a coherent sum of the state (1) over all possible values of the momentum component \( P_{iz} \) [11] and modify the cross section given by expression (4) accordingly [12]. This procedure is similar to the standard method used to account for the broadening in the photon energy. Hereafter, without altering all our above discussion, we will consider, instead of plane-wave, an incident wave-packet whose initial momenta \( \mathbf{p}_i = (0, 0, |P_{iz,0} - P_{iz,0}| \leq \Delta P_{iz}) \) launched on a diffraction grating with \( \Delta P_{iz} \leq 10\% \) of \( P_{iz,0} \), with \( P_{iz,0} \) being the central momentum of the incident wave packet.

In figure 2(a) we show the photoelectron spectrum \( d\sigma / d^3\mathbf{p}_i dP_{rec,z} \) which is obtained from the expression (4) integrated over \( P_{rec,y} \) and \( P_{rec,z} \), meanwhile keeping \( P_{rec,x} = 0 \) and \( p_{iz} \approx 0.1 \text{ a.u.} \). It is seen that the spectra exhibit very clear interference structures due to the coherent contributions of different sites of the state (1). The interference is represented by discrete ‘lumps’ on a ring. The features exhibited in the electron spectrum can be summarized in the following items: (i) the photoelectron spectrum lies on a ring whose size is determined from the energy conservation; (ii) the electron prefers to be emitted along the photon polarization due to the dipole selection rules and (iii) the momentum balance along the \( x \)-axis is represented here by the function \( F_\alpha \) which imposes a flexible condition allowing the electron momentum to lie in regions \( |p_{ix} + nP_{a}/2D| \leq P_{a}/2D \) (\( n = 0, \pm 1, \pm 2, \ldots \)), rather than a strict momentum conservation expressed in the ‘standard’ photoionization, resulting thus in alternating broad maxima and minima, as shown in the spectrum, whose size \( \delta p_{ix} = P_{a}/D \).

The point (ii) constitutes a crucial difference in the photoionization of a QG compared to the photoionization of a normal atom or a molecule. Further analysis shows a ‘saturation’ in the electron spectrum, i.e. the number of the maxima and their positions remain unchanged with further increase in the number \( N_0 \) of slits. In the case under consideration the pattern saturates at \( N_0 \geq 5 \).

Figure 2(b) represents the photoelectron spectrum same as in figure 2(a), but for \( P_{rec,z} \approx 0.5 \text{ a.u.} \). Compared to the...
maxima and minima are dictated by the function size and the center of the ring remain unchanged, since they strongly correlate exactly mirroring each other, this similarity on the same ring in the spectrum, but the size and the center of the ring remain unchanged, since they are imposed by the energy conservation. These shifts in the maxima and minima are dictated by the function $F(x)$. 

Similar analysis shows that the interference patterns are also observed in the recoil ion momentum spectra as shown in figure 3. The spectrum shown in the panel (a) displays the momentum distribution of the recoil ions represented by the cross section $\sigma/d\omega$ obtained by integrating expression (4) over the momentum components $p_x$ and $p_y$ of the electron. This cross section was calculated for the same initial momentum $P$, the distance $D$ as well as the parameters of the EM radiation and the diffraction grating. The recoil ion spectrum is given as a function of the recoil ion momentum components $P_{rec,x}$ and $P_{rec,y}$ at $P_{rec,x} \approx 800$ a.u. and $p_{ex} = 0$.

As for the electron spectra shown in figure 2 the recoil ion spectra come in discrete lumps whose number and locations are defined by the functions $F_x$ and $F_y$, namely the inequalities, $|P_{rec,x} + nP_{a}/D| \leq P_{a}/2D$ and $|P_{rec,y} + \sqrt{2(\omega x + \epsilon y)}| \leq P_{b}/2D$. These conditions show that the number of the maxima in the recoil ion spectra is simply equal to the number of slits $N_0$ and, unlike the electron spectra, no ‘saturation’ in the pattern of the spectra of the recoil ion when this number grows. The reason for this is that, due to the large difference in the masses of the electron and nuclear, the recoil ion momenta $P_{rec,x}$ and $P_{rec,y}$ do not take a part in the energy conservation $(p_x - v)^2/2 = \omega x + \epsilon y$, and the allowed values of $P_{rec,x}$ are unrestricted by the energy constraint. In contrast to photoionization of a ‘normal’ atom (or molecule) in which the momentum spectra of electrons and recoil ion would be very strongly correlated exactly mirroring each other, this similarity does not imply such a strong correlation even in the single-slit case ($N_0 = 1$) and further rapidly diminishes when the number of slits increases.

Furthermore, the spectrum shown in the panel (b) of figure 3 represents the cross section $d\sigma/d\omega$ obtained by integrating expression (4) over all possible final states of the emitted electron. The spectrum is plotted as a function of $P_{rec,x}$ and $P_{rec,y}$ for fixed $P_{rec,z} = P_{z,0} - v(\approx 800$ a.u.). The recoil momenta of the ions are in the $(x - y)$-plane and located on multiple rings with mean radius of $\sqrt{2(\omega x + \epsilon y)} \approx 2.6$ a.u. The rings are centered at points defined by $P_{rec,x} = nP_{d}/D$ with $(n = 0, \pm 1, \pm 2 \ldots)$ and $P_{rec,y} = 0$. The two dashed circles shown in the panel (b) of figure 3 are to highlight the ring features and to guide the reader eyes.

The structures shown in this spectrum, represented by the cross section $d\sigma/d\omega$ unveiled an interesting interference pattern which is completely absent in the photoelectron cross section $d\sigma/d\rho$ (not shown here). Indeed, if one considers the electron spectra $d\sigma/d\rho$ by integrating expression (4) over all allowed final states of the recoil ion, one would observe patterns similar to those in photoionization of a ‘normal’ atom. That is, the interference patterns in the electron spectra vanish when the electron is detected individually. Thus, the interference appears only if the momenta of the electron and the recoil ion are measured simultaneously in coincidence. Therefore, the emission pattern in figure 2 represents two-particle interference phenomena arising provided the superposition principle and quantum entanglement of the electron and recoil ion ‘act’ together (see e.g. [13, 14]). In contrast, interference in the recoil ion spectra is present, no matter whether the emitted electron is detected or not. Thus, it remains even if the recoil ions are taken individually and their spectra demonstrate both ‘one-particle’ and ‘two-particle’ interference.

From both photoelectron and recoil spectra one can deduce that the uncertainty in the exchanged momentum between the macroscopic grating and the atom has a substantial effect on the corresponding cross sections. Similar effects may also be produced by any device as ‘nozzle/skimmer’ or ‘collimator’ used in collision experiments. For instance a gas-jet of a target passed throughout a macroscopic nozzle or an ion beam traversing a collimator might acquire a wave packet characteristic. Therefore the uncertainty in exchanged momentum can substantially influence the emitted electron or the recoil ion spectra in collision involving few body breakup problems [15, 16].

For an illustrative comparison, we shall now consider the photoemission from a linear molecule (initially at rest), composed of $N$ equidistant ‘real’ He atoms whose internuclear distance $\rho$ is in the same order as the corresponding Fraunhofer coherence-length $\lambda \approx 2\pi D/P_d$ of the QG. The description is based on a SAE approach as stated in [10]. In this approach, the fully-differential cross section for photoionization of the molecule is similar to expression (4) but where the quantity $\delta(P_{x} - P_{z,0})G$ is replaced by $\sum_{n} e^{i\varphi_{n}p_{x}}/\delta^{3}(\kappa + P_{z} - P_{n})$. The sum runs over all atomic centers and $p_{x}$ stands for the position vector of the nth atomic nucleus. The corresponding electron spectrum $d\sigma/d\varphi$, where the integration is performed over all possible momenta of the residual ion of the molecule, consists of a product of two terms. The first term represents the cross section of a single helium atom (single center) which itself is proportional to $|e_{x} \cdot p_{x}|^{2}$ in the dipole limit. The second term, at fixed internuclear separations and orientation of the molecule, corresponds to the interference term $\sum_{n} e^{i\varphi_{n}p_{x}}/|\delta^{3}(\kappa + P_{z} - P_{n})|^{2}$, which reduces, in case of two atoms, to a well known
term \( \cos^2(p_z \cdot \rho/2) \), where \( \rho = \rho_2 - \rho_1 \) is the internuclear vector.

Figure 4 displays the photoionization cross section of \( \text{He}_2 \) differential in momentum components \( p_x \) and \( p_y \) of the emitted electron at fixed \( p_y = 0 \). The electromagnetic radiation is linearly polarized along the \( y \)-axis propagating along the \( z \)-axis with a central energy \( \omega_c = 120 \text{ eV} \). The \( \text{He}_2 \) molecule is taken parallel to the \( x \)-axis. Are shown, the momentum distributions of the photoelectron for two internuclear separations (a) \( \rho = 1.6 \text{ a.u.} \) (left panel) and (b) \( \rho = 8 \text{ a.u.} \) (right panel, this choice corresponds to the separation distance between the maxima in the QG). At \( \rho = 1.6 \text{ a.u.} \), the cross sections obtained at such photon energy manifest almost no interference. However, for \( \rho = 8 \text{ a.u.} \approx \lambda \), the momentum distribution exhibits a clear interference structures. These interference effects are the results of coherent scattering from the two centers of the molecule which exhibit one-particle interference inherent in the term \( \cos^2(p_z \cdot \rho/2) \) and a sequence of successive maxima and minima in the cross section. These minima and maxima in turn require that at least \( |p_z \cdot \rho| \geq 2\pi \) and no matter whether the recoil ion is detected or not. Besides, it follows from the presence of \( \delta^{(3)}(\mathbf{r} + \mathbf{P} - \mathbf{P}_f) \) in the cross section that the recoil spectra ‘mirror’ the electron ones in particular when the photon momentum is neglected.

In conclusion, we have considered photoionization of an atom passed through a diffraction grating. Due to its diffraction by the grating the atom finds itself in a state whose wave function possesses a periodic spacial structure with alternating maxima and minima. In the momentum space, this results in the appearance of alternating allowed and forbidden momentum regions. All this brings a novel and interesting features in the process of photoionization.

For instance, unlike photoionization of a ‘normal’ atom or molecule, in the case of an atomic QG there is no ‘mirror symmetry’ correspondence between the momentum spectra of the photoelectrons and recoil ions. Moreover, the spectra of recoil ions display both one- and two-particle interference while the electron spectra are sensitive only to the latter. Besides, the recoil-ion spectra contain a direct information about the diffraction grating, however the electron spectra do not in general. The reason for the ‘striking disparities’ between the electron and recoil ion spectra is due to the large difference between the electron and nuclear masses which has a qualitatively different impact on the photoionization process for an atomic QG compared to the ‘normal’ atomic case.

Moreover, the atomic QG can profoundly manifest itself also when it is probed in other basic atomic collision processes (e.g. ionization by charged particles, radiative and non-radiative electron capture to bound/continuum states and projectile-electron loss) as well as in processes involving photo absorption and Compton scattering.

### Acknowledgment

We thank Dr A B Voitkiv for fruitful and constructive discussions and acknowledge the support from the ‘National Key Research and Development Program of China’ (Grant No. 2017YFA0402300) as well as the CAS President’s International Fellowship Initiative.

### Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors.

### ORCID iDs

X Ma [https://orcid.org/0000-0001-9831-0565](https://orcid.org/0000-0001-9831-0565)

### References

[1] Hornberger K, Gerlich S, Haslinger P, Nimmrichter S and Arndt M 2012 Rev. Mod. Phys. 84 157
[2] Dörre N, Rodewald J, Geyer P, von Issendorff B, Haslinger P and Arndt M 2014 Phys. Rev. Lett. 113 233001
[3] Tuan T F and Gerjuoy E 1960 Phys. Rev. 117 756
[4] Cohen H D and Fano U 1966 Phys. Rev. 150 30
[5] Walter M and Briggs J 1999 J. Phys. B: At. Mol. Opt. Phys. 32 2487
[6] Fernández J, Fojo O, Palacios A and Martín F 2007 Phys. Rev. Lett. 98 043005
[7] Alexander J S, Laforge A C, Hasan A, Machavariani Z S, Ciappina M F, Rivarola R D, Madison D H and Schulz M 2008 Phys. Rev. A 78 060701
[8] Guan X, Secor E B, Bartschat K and Schneider B I 2012 Phys. Rev. A 85 043419
[9] Born M and Wolf E 1999 Principles of Optics: Electromagnetic Theory of Propagation, Interference and Diffraction of Light (Cambridge: Cambridge University Press)
[10] In this paper we deal with photo emission of a single electron, therefore among all electrons, only the wave-function of such an ‘active’ electron will be expressed explicitly, while the ‘inactive’ electrons are ‘absorbed’ in the ‘core’. This approach follows from independent-electron-model, where the magnitude of the overlap between the initial and final states of the inactive electrons is nearly \( \sim 1 \)
Accordingly the wavefunction of the expression (1) has to be replaced by

$$\Psi_i(R, r, t) \sim \int_{P_{i0}^{+\Delta P_{i0}}}^{P_{i0}^{-\Delta P_{i0}}} dP_i A(P_i) \exp (iP_i z - iE_it) \times \frac{\sin(GP_i)}{\sin(Gx)} \times \sin(\alpha x) \times \sin(Nx) \times \sin(\gamma x) \times \sin(\beta y) \times \sin(p) \times \phi_i(r),$$

(7) with the condition $\int dp |A(p)|^2 = 1$ and in what follows $|A(p)|^2$ will be chosen as a Gaussian distribution.

The cross section in this case is obtained by calculating the transition amplitude using the above expression (7), where the integration over $dP_i$ is performed with the help of the $\delta(P_i - P_{i0})$. As a result, the obtained cross section is given by

$$\frac{d\sigma}{dp_{rec}|\psi_i|^2} \propto |A(P_{f0}, z)|^2 \times \delta(E_f - \tilde{E}_i - \omega_{\beta 0}) \times \left| \langle \phi_k | e^{i\epsilon \cdot r (\epsilon \cdot \hat{p}_r)} | \phi_i \rangle \right|^2 \times \tilde{G}. \quad \text{(8)}$$

Where we have substituted in expression (4) $\delta(P_i - P_{s0})$ by $|A(P_{f0}, z)|^2$ and $G$ by $\tilde{E}_i$ and $\tilde{G}$, respectively, and replaced $P_i$ by $P_{f0}$ everywhere.

[11] Pan J-W, Chen Z-B, Lu C-Y, Weinfurter H, Zeilinger A and Zukowski M 2012 Rev. Mod. Phys. 84 777
[12] Waitz M et al 2016 Phys. Rev. Lett. 117 083002
[13] Egodapitiya K N, Sharma S, Hasan A, Laforge A C, Madison D H, Moshammer R and Schulz M 2011 Phys. Rev. Lett. 106 153202
[14] Schulz M, Moshammer R, Fischer D, Kollmus H, Madison D H, Jones S and Ulrich J 2003 Nature 422 48