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Possible effects of attosecond quantum entanglement involving protons on fast processes in M–H and other systems

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Abstract

Quantum entanglement (QE) in micro- and mesoscopic systems in condensed matter is very short-lived due to interactions with the environment. However, neutron Compton scattering (NCS) operates in the attosecond time scale, thus allowing to access QE effects of protons with electrons. Our findings revealed a striking shortfall of NCS-intensity from protons of M–H and various molecular systems; in simple terms, about 20–40% of the protons seem to "disappear". This new effect was recently confirmed with a completely independent method: electron Compton scattering from nuclei (ECS). During the scattering process there is no well-defined time-scale separation between protonic and electronic "motions" and thus the Born–Oppenheimer (BO) approximation is not applicable. A theoretical outline of the NCS (and ECS) results is presented. This theory also applies to other fast processes, like H-jumps, formation or breaking of a chemical bond, electron mobility and/or transfer, etc.

Keywords: Scattering theory; Attosecond physics; Entanglement; Decoherence; Neutron scattering; Electron energy loss spectroscopy

1. Introduction

The counter-intuitive phenomenon of quantum entanglement (QE) between two or more quantum systems has emerged as the most emblematic feature of quantum mechanics [1]. Entangled states are often called Schrödinger's cat states. Experiments investigating QE, however, are focused on collection of a small number of simple (two- or three-level) quantum systems thoroughly isolated from their environment (e.g. atoms in high-Q cavities and optical lattices, or trapped ions), or coupled to it by well-known and controlled interaction mechanisms. These conditions are necessary due to the decoherence [2]. On the contrary, QE in condensed and/or molecular matter at ambient conditions is usually assumed to be experimentally inaccessible. However, two new scattering techniques—NCS and ECS—operating in the attosecond time scale provided results indicating that short-lived entangled states may be detectable in condensed matter even at room temperature [3–5].

In this paper we present a theoretical investigation of scattering from "small" open quantum systems in condensed matter, in the "time window" of decoherence of the scattering system. In particular, extending and improving earlier work [6], no energy integration is carried out in the basic equation (1). Consequently the main theoretical results (say, Eqs. (7–9)) concern the double differential cross-section which is directly extracted from experimental data (i.e. measured scattering intensities, see e.g. [7]). The focus is in "fast" scattering processes with a duration (called scattering time, τ_{sc}) of the order to the scatterer's decoherence time, τ_{dec}, i.e. $\tau_{sc} \sim \tau_{dec}$. Our procedure may be considered to represent an "extension" of standard scattering theory—as applied e.g. to neutron physics [7,8] and electron scattering [9]—in which the concepts of QE and decoherence play no role.

To be specific, the derivations deal with NCS explicitly, but they can rather easily be extended to other "fast"

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processes. In accordance with conventional neutron scattering theory, our starting point is given by the standard expression for the double differential cross section, Eq. (1) below, which is based on "Fermi's golden rule"; see [7,8]. The particular case of large momentum transfer and, consequently, incoherent scattering is considered—which simplifies the formalism, makes the essential points more transparent, and also applies to the NCS and ECS processes. Then a reduced *open quantum system* is introduced, i.e. a micro- or mesoscopic system, characterized by a set of preferred states (also called: pointer basis) [10]. This corresponds to the "small" physical system that scatters a neutron (electron, etc.) with a sufficiently large momentum transfer. Its dynamics is described by a simple Lindblad-type master equation [11], thus incorporating the effects of irreversibility and decoherence into the theoretical model explicitly.

The striking result of the derivations is as follows: the irreversible time-evolution is shown to cause a reduction of the transition rate of the system (from its initial to its final state). In "experimental" terms, this is tantamount to an effective reduction of the system's cross-section density and thus a shortfall of scattering intensity; cf. [3–5].

2. Quantum dynamics of scattering

To simplify notations, let us temporarily assume that the condensed system consists of N atoms of the same kind only, say, hydrogen atoms. The starting point [8,7] is to consider the number of neutrons, $I_{\rm sc}$, scattered per second into a small solid angle $\mathrm{d}\Omega$ (in some given direction) with final energy between E_1 and $E_1 + \mathrm{d}E_1$. One has $I_{\rm sc}(E_1, \Omega) \propto \mathrm{d}^2\sigma/\mathrm{d}\Omega\,\mathrm{d}E_1$, i.e., it is proportional to the double differential cross section

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\,\mathrm{d}E_1} = \frac{k_1}{k_0}\sum_{\nu\nu'} W_\nu \left|\sum_j b_j\langle\nu'|V_j(\mathbf{q})|\nu\rangle\right|^2 \times \delta(E_\nu - E_{\nu'} + E_0 - E_1) \qquad (1)$$

b_j is the so-called bound scattering length of atom $j\,(= 1,\ldots N)$ and $|\mathbf{k}|_i = k_i$. $\hbar\mathbf{q}$ and $\hbar\omega$ are the momentum and energy transfers from the neutron to a scattering nucleus, respectively; i.e., $\hbar\mathbf{q} = \hbar\mathbf{k}_0 - \hbar\mathbf{k}_1$, $\hbar\omega = E_0 - E_1$. "0" and "1" refer to neutron quantities "before" and "after" collision, respectively. ν and ν' refer to the initial and final states of the scattering system, respectively, making the transition $|\nu\rangle \to |\nu'\rangle$. W_ν denote the probabilities of the initial states. It holds $V_j(\mathbf{q}) \equiv \exp(i\mathbf{q}\cdot\mathbf{r}_j)$.

In this equation, the sum $\sum_j$ contains N terms. So the square of its absolute value, $|\sum_j|^2$, is the sum of N^2 terms of which a typical member is (defining $V_j \equiv V_j(\mathbf{q})$ for simplicity of notation)

$$\begin{aligned} M_{jj'(\nu\nu')} &\equiv b_j b_{j'}^*\langle\nu'|V_j|\nu\rangle[\langle\nu'|V_{j'}|\nu\rangle]^* \\ &= b_j b_{j'}\langle\nu'|V_j|\nu\rangle\langle\nu|V_{j'}^\dagger|\nu'\rangle \\ &= b_j b_{j'}\,\mathrm{Tr}[\rho_{\nu'}\,V_j|\nu\rangle\langle\nu|V_{j'}^\dagger] \\ &= b_j b_{j'}\,\mathrm{Tr}[\,\rho_{\nu'}\;V_j\;\rho_\nu V_{j'}^\dagger\,] \end{aligned} \qquad (2)$$

where $V_{j'}^\dagger \equiv \exp(-i\mathbf{q}\cdot r_{j'})$. The N-body density operators $\rho_{\nu'} \equiv |\nu'\rangle\langle\nu'|$ and $\rho_\nu \equiv |\nu\rangle\langle\nu|$ correspond to the final and initial states, respectively. $\mathrm{Tr}[\cdots]$ denotes the trace operation. For simplicity, b is assumed to be real.

In the considered physical context of NCS one has $q \gg 2\pi/d$, where d is the nearest-neighbor distance of two scattering nuclei. Hence the spatial scale of the scattering event, represented by $1/q$ (where $q = |\mathbf{q}|$), is too small for one to detect interference effects due to scattering from pairs of different nuclei. This is because the terms with $j \neq j'$ in this equation correspond to fine—spatially oscillating, i.e. constructive and destructive—interference patterns which tend to average to zero due to the finite spatial (and solid angle) resolution of the detector. These physical considerations imply that the terms with $j \neq j'$ do not contribute to the measured scattering intensity, and therefore one obtains from Eq. (2) the "incoherent approximation" [12,13]

$$M_{jj(\nu\nu')} = b_j^2\,\mathrm{Tr}[\,\rho_{\nu'}\;V_j\;\rho_\nu\;V_j^\dagger\,] \qquad (3)$$

Since the quantity $V_j\;\rho_\nu\;V_j^\dagger = |V_j\nu\rangle\langle\nu V_j|$ is a projector (thus having eingenvalues 0 or 1) and $\rho_{\nu'}$ is a density operator (thus having non-negative eigenvalues), the product $\rho_{\nu'}\;V_j\;\rho_\nu\;V_j^\dagger$ must be hermitian and positive semidefinite. Consequently, $\mathrm{Tr}[\,\rho_{\nu'}\;V_j\;\rho_\nu\;V_j^\dagger\,] \geq 0$ and $M_{jj(\nu\nu')} \geq 0$. Thus, in the expression of the scattering intensity, Eq. (1), and for sufficiently large momentum transfers (as in the case of NCS), occur now only non-negative terms.

The pure states $\rho_{\nu'}$ and ρ_ν refer to the complete (macroscopic N-body) system. Each individual neutron scattering process, however, is expected to involve only a much smaller number of "relevant" degrees of freedom, e.g. those of a few number of atoms. The latter can be described by the reduced density operators $\tilde{\rho}_{\nu'}$ and $\tilde{\rho}_\nu$ obtained from $\rho_{\nu'}$ and ρ_ν through partial trace $\mathrm{Tr}_{(\mathrm{env})}$ over the degrees of freedom of the "environment":

$$\tilde{\rho}_{\nu'} = \mathrm{Tr}_{(\mathrm{env})}[\rho_{\nu'}], \qquad \tilde{\rho}_\nu = \mathrm{Tr}_{(\mathrm{env})}[\rho_\nu] \qquad (4)$$

In general, these are not pure states. Thus one obtains

$$M_{jj(\nu\nu')} = b_j^2\,\mathrm{Tr}[\,\rho_{\nu'}\;V_j\;\rho_\nu\;V_j^\dagger\,] = b_j^2\,\mathrm{Tr}_{(\mathrm{rel})}[\,\tilde{\rho}_{\nu'}\;V_j\;\tilde{\rho}_\nu\;V_j^\dagger\,] \qquad (5)$$

where $\mathrm{Tr}_{(\mathrm{rel})}$ denotes the trace over the degrees of freedom of the relevant subsystem.

Until now, the effect of decoherence played no role in the derivations. In the following we investigate possible implications that QE and its decoherence may have for the scattering process. Obviously, the physical context associated with the relation $\tau_{\rm dec} \sim \tau_{\rm sc}$ is relevant here. Let $\{|\xi\rangle\}$ be the *preferred* representation [10] being selected by the decoherence accompanying the dynamics of a scatterer. According to decoherence theory [2] we may write here

$$\langle\xi|\tilde{\rho}_{\nu'}(t)|\xi'\rangle \equiv \langle\xi|\tilde{\rho}_{\nu'}(0)|\xi'\rangle\, \mathrm{e}^{-\Lambda|\xi-\xi'|^2 t} \tag{6}$$

To simplify the following derivations, we temporarily assume the initial state $\tilde{\rho}_\nu$ to be t-independent, and thus not subject to decoherence.

Performing now the trace in Eq. (5) with respect to the basis $\{|\xi\rangle\}$ and noting the closure relation $\int \mathrm{d}\xi' |\xi'\rangle\langle\xi'| = \hat{\mathbf{1}}$, Eq. (5) may be written as

$$\begin{aligned} M_{jj(\nu\nu')}(t) &\equiv b_j^2 \int\int \mathrm{d}\xi\, \mathrm{d}\xi' \langle\xi|\tilde{\rho}_{\nu'}(t)|\xi'\rangle\langle\xi'|V_j\tilde{\rho}_\nu V_j^\dagger|\xi\rangle \\ &= b_j^2 \int\int \mathrm{d}\xi\, \mathrm{d}\xi' \langle\xi|\tilde{\rho}_{\nu'}(0)|\xi'\rangle \\ &\quad \times \langle\xi'|V_j\tilde{\rho}_\nu\, V_j^\dagger|\xi\rangle \mathrm{e}^{-\Lambda|\xi-\xi'|^2 t} \end{aligned} \tag{7}$$

This quantity contains a t-dependence due to the non-diagonal elements of $\tilde{\rho}_{\nu'}(t)$. Obviously, time-resolved details of this (very fast) dependence are not accessible to our experiment. Therefore, comparison with experimental results should be made after taking the time average over the duration of the scattering process, τ_{sc}. The associated experimentally relevant quantity is then

$$\bar{M}_{jj(\nu\nu')} = \frac{1}{\tau_{\mathrm{sc}}}\int_0^{\tau_{\mathrm{sc}}} \mathrm{d}t\, M_{jj(\nu\nu')}(t) \tag{8}$$

As expected, the last formula includes also the cases in which decoherence is absent, since it trivially holds: if $\Lambda = 0$ then $\bar{M}_{jj(\nu\nu')} = M_{jj(\nu\nu')}$. But for the general case $\Lambda > 0$, all contributions to the rhs of Eq. (7) are reduced due to the exponential factors $\exp(-\Lambda|\xi - \xi'|^2 t)$.

Based on physical considerations, one can conclude that this causes a decrease of the complete matrix element $\bar{M}_{jj\nu\nu'}$. To see this, note first that the "diagonal" terms with $\xi = \xi'$ in Eq. (7) are positive, as easily seen:

$$\langle\xi|\tilde{\rho}_{\nu'}(0)|\xi\rangle\langle\xi|\, V_j\ \tilde{\rho}_\nu\ V_j^\dagger\, |\xi\rangle = \langle\xi|\tilde{\rho}_{\nu'}(0)|\xi\rangle\langle\xi V_j^\dagger|\tilde{\rho}_\nu|V_j^\dagger\xi\rangle \geq 0 \tag{9}$$

By continuity, all associated terms with $\xi \approx \xi'$ should be positive, too, which are thus reduced due to the decoherence effect. The further terms with ξ being much different than ξ' can be positive or negative. But they may be approximately neglected, since they decay very fast and thus contribute less significantly to the average equation (8).

Now we may drop the preceding temporary assumption that the initial state $\tilde{\rho}_\nu$ be time-independent. Thus decoherence may affect $\tilde{\rho}_\nu$ of the relevant system too, since it is an open quantum system. Here one easily recognizes that the above procedure of Eqs. (6)–(8) can be straightforwardly generalized, so that the quantity $M_{jj(\nu\nu')}(t)$ contains additional exponential factors due to the decoherence of $\tilde{\rho}_\nu$. The further conclusions remain unchanged.

In summary, the exponential factors $\exp(-\Lambda|\xi - \xi'|^2 t)$ due to decoherence lead to a reduction of the time averages $\bar{M}_{jj\nu\nu'}$ and thus of the scattering intensity, as observed in our NCS and ECS experiments, cf. [3–5,14].

Starting from a general equation of motion of an open quantum system [11]—instead of Eq. (1)—a generalized treatment of the above model and its main result can be provided, which applies to various "fast" processes in condensed and molecular systems [15].

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