Breakdown of the Born-Oppenheimer description explains neutron Compton-scattering anomaly

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Several neutron Compton scattering experiments reveal an apparent drop of the proton cross section when the collision time $\tau_{\mathbf{q}}$ is around 1 fs. Such small $\tau_{\mathbf{q}}$ corresponds to a large energy spread of the proton wave packet after collision, allowing it to access excited electronic levels. This nonadiabatic excitation of electrons leads to a distortion of the shape of the neutron scattering response function with some redistribution of intensity at energies higher than the nuclear recoil energy and a slight shift of the main neutron intensity peak to lower energies.

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I. INTRODUCTION

Several recent experiments have reported anomalies seen in neutron Compton scattering (NCS) from protons in many different materials.[1–7] The observed anomaly is a large shortfall in the number of scattered neutrons (up to 40%) around the proton recoil peak at very high energy and momentum transfers. This is a region where the impulse approximation (IA) is expected to be almost exact.[8,9] Departures from it[10–12] should be very small and certainly not responsible for the reduction of the intensity. Similar experiments with the proton replaced by a deuteron showed little or no anomaly, suggesting a quantum-mechanical effect. Coherence effects between the struck proton and neighboring exchange-correlated protons were thought responsible for the effect.[13–15] A different interpetation involved entanglement with the environment in the neighborhood of the struck proton.[1,16] A common feature of the experimental evidence was that the reduction of the cross section appeared only when a characteristic time $\tau_{\mathbf{q}}$ associated with the scattering event[9] was short, between 10^{-15}–10^{-16} s. In Fig. 1 the data points, taken from Refs. 3 and 4, show the relative proton to metal cross sections for the metal hydrides NbH and PdH, as a function of $\tau_{\mathbf{q}}$. In the IA, $\tau_{\mathbf{q}}$ is defined for fixed transferred momentum $\mathbf{q}$, as the inverse of the root-mean-square spread of the transfered energy $\hbar\omega$ from the neutron to the nucleus

$$\hbar/\tau_{\mathbf{q}} \doteq \sqrt{\langle\hbar^2\omega^2\rangle_S - \langle\hbar\omega\rangle_S^2}, \tag{1}$$

where $\langle\ \rangle_S$ denotes the average over transfered energy for fixed $\mathbf{q}$, using the scattering response function $S(\mathbf{q},\omega)$ as the probability distribution: $\langle\hbar^n\omega^n\rangle_S = \hbar\int d\omega\hbar^n\omega^n S(\mathbf{q},\omega)$, $n=1,2$. The scattering function is given by

$$S(\mathbf{q},\omega) = \int d\mathbf{k}|\phi(\mathbf{k})|^2\delta\left(\hbar\omega - \frac{\hbar^2q^2}{2M} - \frac{\hbar^2\mathbf{q}\cdot\mathbf{k}}{M}\right), \tag{2}$$

where M is the nuclear mass and $\phi(\mathbf{k})$ is the Fourier transform of the initial nuclear wave function before collision $X(\mathbf{R})$, $\phi(\mathbf{k}) = 1/\sqrt{8\pi^3}\int d\mathbf{R}\,\exp(-i\mathbf{k}\cdot\mathbf{R})X(\mathbf{R})$. The scattering time was obtained[17,9]

$$\tau_{\mathbf{q}} = \frac{M}{\hbar q\sqrt{\langle k_{\mathbf{q}}^2\rangle_\phi}}, \tag{3}$$

where $k_{\mathbf{q}}$ is the projection of $\mathbf{k}$ along $\mathbf{q}$ and the expectation value $\langle\ \rangle_\phi$ is over the momentum distribution $\langle k_{\mathbf{q}}^2\rangle_\phi = \int d\mathbf{k}k_{\mathbf{q}}^2|\phi(\mathbf{k})|^2$. If the nucleus lies initially in an isotropic potential, then $\langle k_{\mathbf{q}}^2\rangle_\phi = (1/3)\langle k^2\rangle_\phi$.

The time $\tau_{\mathbf{q}}$ gives a statistical measure of the length of the time interval during which the collision may occur, in the same way that the spatial extent of a particle wave function gives a statistical measure of the extent of the region in which the particle may be found.

In the interpretations, $\tau_{\mathbf{q}}$ was seen as the collision duration, which had to be small because otherwise decoherence effects would set in and destroy the coherence responsible for the apparent reduction of the cross section. Interestingly, Chatzidimitriou-Dreismann and coworkers remarked[7] that for very short $\tau_{\mathbf{q}}$, the time-scale separation between electronic and protonic motions is not well defined and hence the concept of electronic Born-Oppenheimer (BO) surfaces is not applicable.

Recently, the correctness of the interpretations was disputed[18–21] and even the validity of the analysis of the experiment data[18,22–24] was questioned. In addition, independent neutron transmission measurements of the proton cross section with equally energetic neutrons showed no departure of the cross section from its expected value.[23] These measurements are very difficult to explain with the existing interpretations and apparently challenge the NCS experiments. We will present an explanation that is consistent with all the seemingly contradictory experimental evidence.

II. ELECTRONIC EXCITATION IN A NEUTRON-NUCLEAR COLLISION

The value of $\tau_{\mathbf{q}}$ gives us an estimate of the energy scale involved. When $\tau_{\mathbf{q}}$ becomes very short, $\sim 10^{-16}$ s, we obtain $\hbar/\tau_{\mathbf{q}} \sim 6.5$ eV, which is of the order of the separation of the electronic levels. For $\tau_{\mathbf{q}}$ larger, $\hbar/\tau_{\mathbf{q}}$ is less than typical electronic energies. Although it remains to be seen why $\hbar/\tau_{\mathbf{q}}$ is a

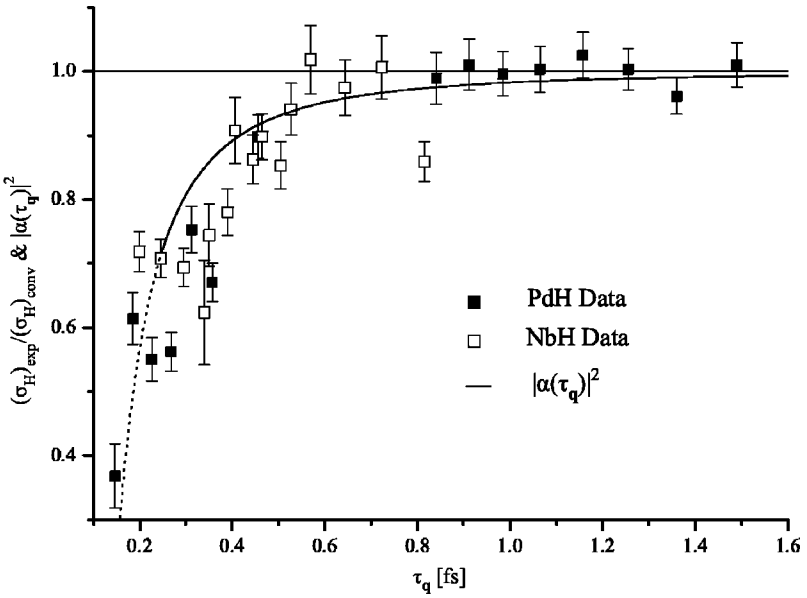

FIG. 1. Squares show relative proton cross-sectional reduction vs $\tau_{\mathbf{q}}$ for PdH (full) and NbH (open), taken from Ref. 3. Line gives the probability that electrons remain in their ground state for a two-level system with $\bar{E}=5$ eV.

relevant energy to the problem, this hints that electronic excitations may be responsible for the anomaly.

The excitation of electronic levels in a neutron-nuclear (NN) collision cannot be described in the BO or adiabatic approximation (in this work we treat the two approximations as one). In the adiabatic approximation, the nuclear motion, rapid or slow, is decoupled from the electronic system. So, when the neutron imparts momentum $\mathbf{q}$ to the nucleus, the motion of the nucleus is always on the same potential surface without affecting the electrons.

More technically, the wave functions for the electron-nuclear system have the product form $\psi_{j,\mathbf{R}}X_{j,\nu}(\mathbf{R})$, where $\psi_{j,\mathbf{R}}$, is an electronic state corresponding to the jth BO level with energy $\epsilon_j(\mathbf{R})$, $\mathbf{R}$ is the nuclear space coordinate (we focus on a single nucleus, incoherent scattering), and $X_{j,\nu}(\mathbf{R})$ is the ν nuclear eigenfunction on the jth potential surface. Fermi's pseudopotential operator for a NN collision that results in momentum transfer $\mathbf{q}$ to the nucleus is $\hat{V}_{\mathbf{q}}=\hat{b}e^{i\mathbf{q}\cdot\mathbf{R}}$, where $\hat{b}$ is the scattering length operator acting on spin degrees of freedom.[8] The amplitude to excite electron-nuclear level $\psi_{n,\mathbf{R}}X_{n,\mu}(\mathbf{R})$ starting from $\psi_{j,\mathbf{R}}X_{j,\nu}(\mathbf{R})$ is proportional to

$$\int d\mathbf{R}X^*_{n,\mu}(\mathbf{R})\langle\psi_{n,\mathbf{R}}|e^{i\mathbf{q}\cdot\mathbf{R}}|\psi_{j,\mathbf{R}}\rangle X_{j,\nu}(\mathbf{R}). \tag{4}$$

The amplitude vanishes for $j\neq n$, since $\langle\psi_{n,\mathbf{R}}|\psi_{j,\mathbf{R}}\rangle=\delta_{n,j}$ for all $\mathbf{R}$.

However, it is indeed possible to excite electrons in a NN collision as Lovesey and co-workers[25] and Reiter and Platzman[26] suggest. Actually, the idea dates back to 1939, when Migdal investigated what happens when an atom in its ground state receives an impulse that increases its velocity by $\mathbf{v}$, in the limit that the impulse duration is very short compared with the electron period and with a/v, where a is the dimension of the atom. The problem is discussed as a worked example in Ref. 27. For a hydrogen atom, the probability the electron remains in its ground state is

$$\left[1+\frac{m^2a_0^2q^2}{(M_p+m)^2}\right]^{-4}, \tag{5}$$

where a_0 is Bohr's radius and $\mathbf{q}=(M_p+m)\mathbf{v}$ is the momentum transferred to the atom, and M_p and m are the proton and electron masses, respectively. Using a typical large value for the recoil energy from the recent experiments $\hbar^2q^2/(2M_p)=100$ eV, we find that the probability is 98.5%.

Clearly an excitation of a few percent of the electrons is not sufficient to explain the large shortfall observed in the experiments. The example is enlightening for another reason. It shows that, at least in the case of the atom, even though the nucleus has kinetic energy an order-of-magnitude larger than the separation of the electronic levels (for q values similar to the experimental), it still moves almost adiabatically carrying along its electrons. So, just the fact that the nuclear kinetic energy is much larger than the electronic gap is not sufficient to cause significant nonadiabatic electronic excitation.

In general, the nonadiabatic coupling between electronic levels j, n, depends on the matrix elements $\langle\psi_{n,\mathbf{R}}|\nabla_{\mathbf{R}}\psi_{j,\mathbf{R}}\rangle$ and $\langle\psi_{n,\mathbf{R}}|\nabla^2_{\mathbf{R}}\psi_{j,\mathbf{R}}\rangle$. The latter can be ignored as they play a role only when the electronic levels come close together. Obviously, to assess whether the nonadiabatic electronic excitation explains the anomaly, we need an estimate of the order of magnitude of the effect. Unfortunately, the nonadiabatic coupling matrix elements are not easy to calculate and the main goal of this work is to understand the underlying mechanism, why the BO separation may break down. This will allow us to estimate quantitatively the magnitude of the effect.

Conventionally, the BO approximation fails when two electronic levels cross, or come very close together, in a region where the nuclear wave function is nonzero. The typical scenario for the breakdown is that the nuclear wave function in that region accesses more than one electronic level and then the total wave function is not separable as an adiabatic product. Here, we are considering a different case where the electronic levels are not close. We will see, how-

ever, that after a NN collision of sufficiently high q, a similar mixing happens and the nuclear wave packet after collision accesses many electronic levels.

A. Mechanism for the breakdown of the Born-Oppenheimer scheme in a neutron-nuclear collision

It is timely to revisit time-dependent (TD) perturbation theory at this point. Initially, the space part of the nuclear wave function is in its vibrational ground state described by $X(\mathbf{R})$ with energy E. We include both nuclear and neutron spins in spin state $|s_i\rangle$ and the energy of the incoming neutron is E_0. We have $\hat{H}X(\mathbf{R})|s_i\rangle=(E+E_0)X(\mathbf{R})|s_i\rangle$, where $\hat{H}$ is the unperturbed Hamiltonian of the combined NN system. When Fermi's pseudopotential interaction $\hat{V}_\mathbf{q}$ is switched on for time t, the wave function in first order becomes $\exp[-i(E+E_0)t/\hbar]\, X(\mathbf{R})|s_i\rangle+\exp(-i\hat{H}t/\hbar)|\Psi_{\mathbf{q},\omega}(\mathbf{R},t)\rangle$, with

$$|\Psi_{\mathbf{q},\omega}(\mathbf{R},t)\rangle = \int_0^t dt' e^{i(\hat{H}t'/\hbar)}\hat{V}_\mathbf{q} e^{-i(\hat{H}t'/\hbar)}X(\mathbf{R})|s_i\rangle. \tag{6}$$

We find that $|\Psi_{\mathbf{q},\omega}(\mathbf{R},t)\rangle$ can be written as a product of a NN spin state $\Sigma_s|s\rangle\langle s|\hat{b}|s_i\rangle$ and a spatial function

$$\Psi_{\mathbf{q},\omega}(\mathbf{R},t) = \sum_{\mathbf{k}'} X_{\mathbf{k}'}(\mathbf{R}) \int d\mathbf{R}' X^*_{\mathbf{k}'}(\mathbf{R}') e^{i\mathbf{q}\cdot\mathbf{R}'} X(\mathbf{R}') \times \frac{\sin[(\hbar\omega+E-E_{k'})t/2\hbar]}{(\hbar\omega+E-E_{k'})/2\hbar}, \tag{7}$$

where we sum over a complete set of NN spin states $|s\rangle$ and nuclear eigenfunctions $X_{\mathbf{k}'}$ with energies $E_{k'}$, $\hbar\omega$ is the difference $\hbar\omega=E_0-E_1$, and E_1 is the energy of the outgoing neutron. When q is very large, the matrix element $\int d\mathbf{R}' X^*_{\mathbf{k}'}(\mathbf{R}')e^{i\mathbf{q}\cdot\mathbf{R}'}X(\mathbf{R}')$ is appreciable only when $X_{\mathbf{k}'}$ is a continuum state with momentum $\mathbf{k}'$ comparable in magnitude to $\mathbf{q}$. So, $\Psi_{\mathbf{q},\omega}(\mathbf{R},t)$ is a wave packet composed of plane waves with a distribution of momenta around $\mathbf{q}$ and moving with the recoil velocity. By Fermi's golden rule, the probability of transition from state $X(\mathbf{R})$ to the plane wave state $X_{\mathbf{k}'}(\mathbf{R})=\exp(i\mathbf{k}'\cdot\mathbf{R})/\sqrt{V}$ is proportional to

$$\left|\int d\mathbf{R}' X^*_{\mathbf{k}'}(\mathbf{R}')e^{i\mathbf{q}\cdot\mathbf{R}'}X(\mathbf{R}')\right|^2 \delta(\hbar\omega+E-E_{k'}). \tag{8}$$

Setting $\mathbf{k}'=\mathbf{q}+\mathbf{k}$, we find $\int d\mathbf{R}' X^*_{\mathbf{k}'}(\mathbf{R}')e^{i\mathbf{q}\cdot\mathbf{R}'}X(\mathbf{R}') = \sqrt{8\pi^3/V}\phi(\mathbf{k})$. From Eqs. (7) and (8) the norm $\int d\mathbf{R}|\Psi_{\mathbf{q},\omega}(\mathbf{R})|^2$ is proportional to $S(\mathbf{q},\omega)$.

Using the wave packet $\Psi_{\mathbf{q},\omega}$, we can calculate expectation values of nuclear operators. For the nth power of the nuclear Hamiltonian $\hat{h}$, we have

$$\langle\hat{h}^n\rangle_{\Psi_{\mathbf{q},\omega}} = \frac{\int d\mathbf{R}\Psi^*_{\mathbf{q},\omega}(\mathbf{R})\hat{h}^n\Psi_{\mathbf{q},\omega}(\mathbf{R})}{\int d\mathbf{R}'|\Psi_{\mathbf{q},\omega}(\mathbf{R}')|^2} = \frac{\sum_{\mathbf{k}'}(E_{k'})^n|\langle X_{\mathbf{k}'}|e^{i\mathbf{q}\cdot\mathbf{R}'}|X\rangle|^2\delta(\hbar\omega+E-E_{k'})}{S(\mathbf{q},\omega)}. \tag{9}$$

The integral on the right-hand side of

$$\langle\hat{h}^n\rangle_{\bar{\Psi}_\mathbf{q}} \doteq \hbar\int d\omega\langle\hat{h}^n\rangle_{\Psi_{\mathbf{q},\omega}}S(\mathbf{q},\omega) \tag{10}$$

is the average over $\hbar\omega$ of the expectation value $\langle\hat{h}^n\rangle_{\Psi_{\mathbf{q},\omega}}$. The double average can be interpreted rather loosely as the expectation value of $\hat{h}^n$ in terms of an average (over $\hbar\omega$) wave packet $\bar{\Psi}_\mathbf{q}$. We have denoted the double average by $\langle\hat{h}^n\rangle_{\bar{\Psi}_\mathbf{q}}$. With a little effort, we obtain from (9) the theorem

$$\langle\hat{h}^n\rangle_{\bar{\Psi}_\mathbf{q}} = \hbar\int d\omega(\hbar\omega+E)^n S(\mathbf{q},\omega). \tag{11}$$

A corollary of (11) is that the root-mean-square variance

$$\Delta E_{\bar{\Psi}_\mathbf{q}} \doteq \sqrt{\langle\hat{h}^2\rangle_{\bar{\Psi}_\mathbf{q}} - \langle\hat{h}\rangle^2_{\bar{\Psi}_\mathbf{q}}} \tag{12}$$

of the double distribution (i.e., of the average wave packet $\bar{\Psi}_\mathbf{q}$) is equal to the root-mean-square variance $\hbar/\tau_\mathbf{q}$ of the distribution $S(\mathbf{q},\omega)$ for fixed $\mathbf{q}$

$$\Delta E_{\bar{\Psi}_\mathbf{q}} = \frac{\hbar}{\tau_\mathbf{q}}. \tag{13}$$

From (3) we have that the energy spread of the average wave packet $\bar{\Psi}_\mathbf{q}$ is proportional to the square root of the recoil energy $\sqrt{\hbar^2q^2/(2M)}$ times the square root of the initial kinetic energy (isotropic potential) $\sqrt{\hbar^2\langle k^2\rangle_\phi/(2M)}$. We may write

$$\Delta E_{\bar{\Psi}_\mathbf{q}} = \sqrt{\tfrac{4}{3}E_qE_v}, \tag{14}$$

where E_q is the nuclear recoil energy and E_v the initial nuclear vibrational kinetic energy. Now, the mechanism for the breakdown of the BO approximation in a NN collision is obvious. When q is low, the average energy uncertainty of the recoil nucleus is small and the adiabatic separation of the nuclear and electronic motions is valid. When q increases, the spread of the recoil wave packet becomes large enough that the struck nucleus samples more than one electronic level. This signals the departure from the BO picture, where nuclei and electrons can be treated separately. The effect is stronger the higher the initial vibrational energy E_v of the nuclei. So, the nonadiabatic excitation of electrons will be much stronger in molecules and solids than what it is in atoms.

B. Model to estimate magnitude of electronic excitation

To model the nonadiabatic electronic excitation we say that only two electronic levels can be involved. We denote by $\alpha_{\mathbf{q}}$ and $\beta_{\mathbf{q}}$ the amplitudes that electrons, originally in their ground state, will remain in the ground state or will be excited by the NN collision. We have $|\alpha_{\mathbf{q}}|^2+|\beta_{\mathbf{q}}|^2=1$. Our results will be valid for small $\Delta E_{\Psi_{\mathbf{q}}}^{-}/E$, with $\overline{E}$ the mean-energy separation of the electronic levels. When $\Delta E_{\Psi_{\mathbf{q}}}^{-}$ becomes large, more than two electronic states will be accessed. We know from the previous discussion that the wave packet energy spread $\Delta E_{\Psi_{\mathbf{q}}}^{-}$ couples the electronic levels. To proceed, we model this coupling with that present in a 2×2 real matrix with diagonal elements separated by $\overline{E}$ and off-diagonal element $\Delta E_{\Psi_{\mathbf{q}}}^{-}$, obtaining the eigenvalue equation

$$\begin{pmatrix} 0 & \Delta E_{\Psi_{\mathbf{q}}}^{-} \\ \Delta E_{\Psi_{\mathbf{q}}}^{-} & \overline{E} \end{pmatrix} \begin{pmatrix} \alpha_{\mathbf{q}} \\ \beta_{\mathbf{q}} \end{pmatrix} = \lambda_{\mathbf{q}} \begin{pmatrix} \alpha_{\mathbf{q}} \\ \beta_{\mathbf{q}} \end{pmatrix}. \tag{15}$$

We expand the eigenvalues and eigenvectors in powers of $\Delta E_{\Psi_{\mathbf{q}}}^{-}/\overline{E}$ and ignore terms higher than second order

$$\lambda_{\mathbf{q}} = -\frac{\Delta E_{\Psi_{\mathbf{q}}}^{2-}}{\overline{E}}, \tag{16}$$

$$\lambda_{\mathbf{q}}' = \overline{E} + \frac{\Delta E_{\Psi_{\mathbf{q}}}^{2-}}{\overline{E}}, \tag{17}$$

$$|\alpha_{\mathbf{q}}|^2 = 1 - \frac{\Delta E_{\Psi_{\mathbf{q}}}^{2-}}{\overline{E^2}}, \tag{18}$$

$$|\beta_{\mathbf{q}}|^2 = \frac{\Delta E_{\Psi_{\mathbf{q}}}^{2-}}{\overline{E^2}}. \tag{19}$$

$|\alpha_{\mathbf{q}}|^2$ is the probability that electrons are not excited. For an isotropic potential $|\alpha_{\mathbf{q}}|^2=1-\hbar^4q^2\langle k^2\rangle_\phi/(3M^2\overline{E^2})$.

We can compare the prediction of our model with the analytic result for the hydrogen atom. From Eq. (5), the probability the electron remains in its ground state, for low q, is

$$1-4\frac{m^2a_0^2q^2}{(M_p+m)^2}. \tag{20}$$

For the hydrogen atom the energy levels are $E_n=-\hbar^2(M_p+m)/(2M_pma_0^2n^2)$. So, $\overline{E}=3\hbar^2(M_p+m)/(8M_pma_0^2)$ and $\langle k^2\rangle_\phi=1/a_0^2$. Therefore for our model, the probability that the electron is not excited is

$$1-2.37\frac{m^2a_0^2q^2}{(M_p+m)^2}, \tag{21}$$

the same as the exact result (20) within a numerical constant of order 2.

III. EXPLANATION OF APPARENT ANOMALY

This gives us confidence to proceed. After some algebraic manipulations, the response function for scattering of a neutron off a nucleus in the limit of high $\mathbf{q}$, allowing for nonadiabatic excitation of electrons becomes

$$S(\mathbf{q},\omega) = |\alpha_{\mathbf{q}}|^2 S_1(\mathbf{q},\omega) + |\beta_{\mathbf{q}}|^2 S_2(\mathbf{q},\omega), \tag{22}$$

where $S_{1,2}(\mathbf{q},\omega)$ are scattering functions (2) centered at $\hbar^2q^2/(2M)-\Delta E_{\Psi_{\mathbf{q}}}^{2-}/\overline{E}$ and $\hbar^2q^2/(2M)+\overline{E}+\Delta E_{\Psi_{\mathbf{q}}}^{2-}/\overline{E}$. For high q, the scattering function splits into two distributions, $S_1(\mathbf{q},\omega)$ (main) and $S_2(\mathbf{q},\omega)$ (secondary), separated by $\overline{E}+2\Delta E_{\mathbf{q}}^2/\overline{E}$. In the experiments, it is possible that neutrons scattered near the secondary peak have been missed, since one does not expect to find intensity at energies higher than the proton recoil peak. In a realistic system with many neighboring excited electronic levels available, the original distribution will actually split in the main peak and a series of weaker secondary peaks that will be hard or even impossible to observe. The apparent cross-sectional shortfall probably corresponds to the weight of the secondary peak $\Delta E_{\Psi_{\mathbf{q}}}^{2-}/\overline{E^2}$. Writing $\Delta E_{\Psi_{\mathbf{q}}}^{-}=\hbar/\tau_{\mathbf{q}}$ [Eq. (13)], we compare in Fig. 1 the plot of the weight of the main peak $|\alpha(\tau_{\mathbf{q}})|^2=1-\hbar^2/(\tau_{\mathbf{q}}{}^2\overline{E^2})$ against the plot of the relative proton to metal cross section for NbH and PdH. We used $\overline{E}=5$ eV. The line $|\alpha(\tau_{\mathbf{q}})|^2$ is meaningful (solid) for small $\hbar/(\tau_{\mathbf{q}}\overline{E})$. The density of states of both PdH and NbH show pronounced peaks on either side of the Fermi energy separated by about 5 eV and about 4 eV, respectively (Refs. 28 and 29).

The first-moment sum rule[8] is obeyed in second order, $E_q \doteq \hbar^2\int d\omega\omega S(\mathbf{q},\omega)=\hbar^2q^2/2M$, as expected. The main peak in (22) is shifted to a lower energy by $\Delta E_{\Psi_{\mathbf{q}}}^{2-}/\overline{E}=4/3E_qE_v/\overline{E}$ (isotropic potential). The shift is a consequence of the requirement of the first-moment sum rule that the average energy remains at the recoil energy, while at the same time some intensity appears at much higher energies. Cowley writes that since a significant shift of the main peak has not been observed experimentally, especially when the shortfall is large, the nonadiabatic excitation of electrons probably cannot account for the anomaly.[21] To investigate whether the predicted shift can be observed, we must estimate the difference in the scattering angle θ that corresponds to the peak shift. In terms of θ, the proton recoil energy is given by

$$E_q = \frac{\hbar^2q_1^2\tan^2\theta}{2M_p}, \tag{23}$$

where q_1 is the momentum of the scattered neutron.[4] Inverting (23) we may express the scattering angle in terms of the proton recoil energy

$$\theta = \arctan\left(\frac{\sqrt{2M_pE_q}}{\hbar q_1}\right). \tag{24}$$

A small change in the recoil energy δE_q amounts to a change in the scattering angle by

$$\delta\theta = \frac{\sin 2\theta}{4E_q}\delta E_q. \tag{25}$$

Setting δE_q equal to the shift, we obtain that the change in the scattering angle, due to the shift, is

$$\delta\theta_{\text{shift}} = \frac{E_v}{3E}\sin 2\theta. \tag{26}$$

The maximum change in the angle occurs at $\theta = 45°$, when the transfered energy is rather low ($\delta\theta_{\text{shift}}^{\max} \sim 0.6°$ for NbH and $\sim 0.4°$ for PdH). For example, in NbH and PdH, the shortfall becomes obvious for angles greater than 55°–60°.[4] At the same time, at $\theta = 45°$, the peak shift due to conventional final state effects is significant and comparable in magnitude to the new shift.[30] For large scattering angles, even though this new shift grows, the corresponding change in the angle is damped and the shift could not have been observed easily as the angle was determined within $\sim 0.2°$.[31] Obviously, to observe the shift, the error in determining the scattering angle should be much less than $\delta\theta_{\text{shift}}$. In the experiments, I believe these shifts, which were not anticipated, would have been confused with shifts due to conventional final state effects.

Looking at the mass dependence of $|\alpha_{\mathbf{q}}|^2$, one understands why for similar wave vector transfers the proton cross section appears reduced and the deuteron cross section unaffected. For deuterons, it would require about twice the momentum transfer needed for protons to see a similar cross-sectional reduction (our two-level model indicates that the ratio of the momentum transfers is $2^{3/4} \simeq 1.7$). Unpublished data on hydrated and deuterated yttrium, YH_3 and YD_3, agree with the prediction.

Our theory does not account for all experimental evidence in its present form. NCS experiments, in a class of systems, reveals that the drop of the proton cross section depends on the relative concentration of protons to deuterons.[1] Work is in progress to explain these experiments in terms of a more sophisticated theory of nonadiabatic electronic excitations.

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