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Molecular excitations: a new way to detect Dark Matter

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ABSTRACT

We believe that the Dark Matter (DM) search should be expanded into the domain of detectors sensitive to molecular excitations, and so that we should create detectors which are more sensitive to collisions with very light WIMPs. In this paper we investigate in detail diatomic molecules, such as fused silica material with large OH-molecule content, and water molecules. Presently, we do not have suitable low-cost IR detectors to observe single photons, however some OH-molecular excitations extend to visible and UV wavelengths and can be measured by bialkali photocathodes. There are many other chemical substances with diatomic molecules, or more complex oil molecules, which could be also investigated. This idea invites searches in experiments having large target volumes of such materials coupled to a large array of single-photon detectors with bialkali or infrared-sensitive photocathodes.

1. Introduction

A recent paper [1] discussed the possibility that the DAMA experiment [2] observes the effect of a light WIMP striking a hydrogen atom and creating a proton recoil, which then excites the NaI(Tl) crystal in which it is located. The target hydrogen atom is present as OH or H_2O contamination. The "classical" scintillation mechanism for atomic level excitation in NaI(Tl) is shown schematically in Fig. 1. The primary energy deposit has to exceed the band gap of NaI, which is 3.9 eV; thallium is added to lower the emission energy.

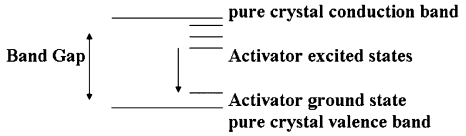

Fig. 1. Energy levels for an activated NaI(Tl) crystal, where Tl is the so-called activator. The Tl-levels lie somewhat below the conduction band so that the radiated photons are emitted with less energy than the band gap of the pure crystal.

The present paper considers another, even more sensitive, method to detect Dark Matter via molecular excitations (a preliminary version was presented in Ref. [3]). A very small energy-deposit, at a level of 2–3 eV, is needed to excite such vibrations; this is a factor of 2 lower in energy than the classical scintillation mechanism. Many diatomic molecules will vibrate when hit by a photon (or neutron or a WIMP) and some small fraction of such single photon excitations can be detected by a PMT working in the bialkali regime. However, most of the emitted energy is in the IR wavelength region, or is in the form of heat; the emission of visible photons is suppressed by at least 4–6 orders of magnitude compared to IR photons. Because the efficiency for Dark Matter to generate visible photons in water or ice is expected to be very small, a large detector volume is required, together with an extensive PMT coverage with single photon sensitivity. Examples of possible experiments to perform this measurement are the Ice Cube, BaBar DIRC and the Super-Kamiokande experiment.

Diatomic molecules are ideal for such studies, since they are simpler to understand, and have been studied extensively by chemists [4]. The energy levels of diatomic molecules can be calculated using the Schroedinger equation description of a harmonic oscillator, which has been described in many textbooks – e.g. see Refs. [5] and [6]. Fig. 2 and Table 1 provide examples of energy levels in a typical diatomic molecule, for a perfect harmonic oscillator, and for an anharmonic oscillator following the Morse potential [5]. The most significant difference between the two potentials is a transition selection rule. The harmonic oscillator allows only transitions obeying $\Delta\nu = \pm 1$. In contrast, the anharmonic oscillator allows the transitions $\Delta\nu = \pm 1, \pm 2, \pm 3$, etc. These transitions, ν_1, $2\nu_1$, $3\nu_1$, etc., are called overtones. We see that although the fundamental mode corresponds to an IR wavelength, the higher overtones correspond to visible or even UV wavelengths. This can provide a path to detection using bialkali photocathode-based PMTs; single-photon IR-sensitive detectors are more difficult to utilize at present for this purpose.

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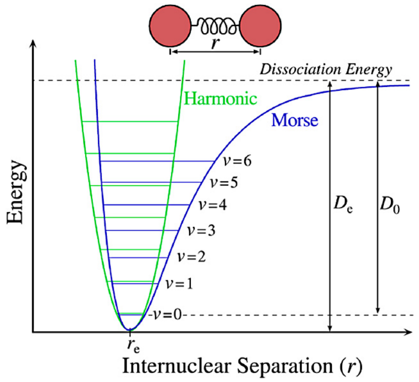

Fig. 2. Energy levels of diatomic molecules for a harmonic and an anharmonic oscillator, where the latter follows the more complex Morse potential; ν is the vibrational quantum number ($\nu = 0, 1, 2, \ldots$). The $\nu = 0$ level is the vibrational ground state. Unlike the energy levels of the harmonic oscillator potential, which are evenly spaced by $\hbar\omega$, the Morse potential level spacing decreases as the energy approaches the dissociation energy D_e [5].

Table 1
A simple calculation of the transition wavelength for several frequency overtones of the OH-radicals. The last two modes correspond to visible wavelengths. Higher modes can reach the UV regime [6].

OH-band identity	Transition	Calculated wavelength [nm]
ν_1	$0 \to 1$	2803
$2\nu_1$	$0 \to 2$	1436
$3\nu_1$	$0 \to 3$	980
$4\nu_1$	$0 \to 4$	755
$5\nu_1$	$0 \to 5$	619.5

We note that the OH-molecule has been studied extensively by many chemists using laser-induced fluorescence. An example of such a fluorescence measurement is the OH-molecule excitation by a 282 nm dye laser, followed by the observation of the 310 nm wavelength with a PMT with a notch filter [7]. This method was used to determine traces of OH-radicals in the atmosphere [8]. Fig. 3 shows schematically how WIMP scattering could excite energy levels in the OH-molecule, with a subsequent de-excitation via fluorescent photons at either ~282 nm or ~310 nm.

However, the picture outlined above is too simplistic, since the actual energy levels can be affected by the substance in which the OH-radical is located. In this paper we discuss the example of fused silica loaded with OH-molecules. Fused silica is a good example because it has been investigated previously in great detail. It is an ideal material in which to study the effects of the OH-molecular presence, because the basic material is very pure. In addition, fused silica can be prepared in the form of long fibers, which allows the accurate measurement of absorption resonances by using a monochromator. The next chapter will deal with this material in more detail.

Although fused silica is a well-understood material, pure water is even better understood. We have looked into its molecular vibration response also.

2. OH-molecular vibrations in fused silica

Ref. [9]] investigated IR absorption in wet and dry fused silica. Wet fused silica contains a large quantity of OH-molecules. In contrast, the dry fused silica has almost no OH-content and a minimum of other impurities, so that it is useful for fiber applications operating in the IR regime. The OH content is due to the presence of some moisture or hydrogen in the manufacturing process, which results in hydroxyl groups chemically bonded to the silica molecular network (SiOH). This hydroxyl (OH) affects the optical properties of silica due to the fundamental OH-absorption band with $\nu_3 = 2.72$ μm, the corresponding overtones, and the combination modes with the SiO_4 tetrahedron vibration. The OH content of the dry fused silica was 0.2 ppm (designated as F300), and the OH-content of the wet fused silica was about 700 ppm (designated as F100). Fig. 4 shows the absorption measurements for both types of fused silica in short-bulk samples. The spectrum of the wet silica is affected by the fundamental mode ν_3, the overtones $2\nu_3$, $3\nu_3$, and a few combination modes. Higher overtones, $n\nu_3$, were not observed because the sample was only 20 cm in length. However, the fundamental ν_3 frequency was observed in the wet sample. The dry sample does not exhibit major absorption peaks.

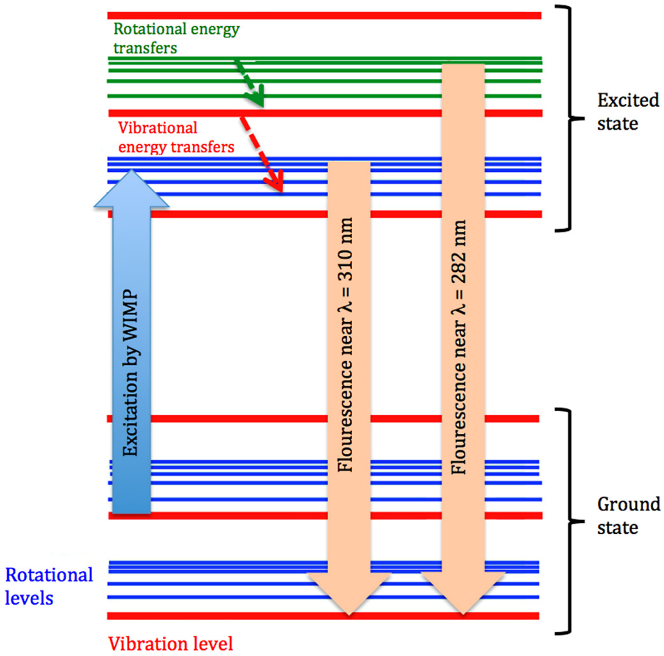

Fig. 3. A schematic picture of WIMP-scattering excitation of energy levels in the OH-molecule, with subsequent de-excitation via fluorescent photons at either ~282 nm or ~310 nm.

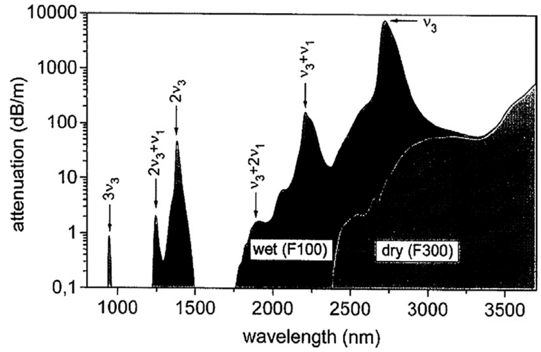

Fig. 4. Attenuation spectra of wet (F100) and dry (F300) fused silica short-bulk samples. Each sample is too short (20 cm) to be sensitive to higher harmonic modes [9].

Fig. 5 shows the absorption fiber spectra in the lower wavelength region using fibers 1 km in length. The wet silica spectrum is a good example of the principal pattern spectral positions and relative intensities of the OH-bands. Each of the overtones at 724 nm, 943 nm and 1383 nm is accompanied by two less-intense combination modes located on the short wavelength tail of the corresponding overtone absorption band. The basic attenuation is almost entirely governed by Rayleigh scattering. This is the reason why the experiment measures only the seventh overtone $7\nu_3$.