

Measuring the molecular Migdal effect with neutron scattering on diatomic gases

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The Migdal effect is a key inelastic signal channel which could be used to detect low-mass dark matter, but it has never been observed experimentally using Standard Model probes. Here we propose an experiment which could detect the Migdal effect in diatomic molecules through low-energy neutron scattering. The enhancement of the Migdal rate through non-adiabatic couplings, which are absent in isolated atoms, combined with the distinctive photon energies of electronic transitions in CO, suggest that a positive detection of the molecular Migdal effect may be possible with modest beam times at existing neutron facilities.

The Migdal effect, where nuclear scattering induces an electronic excitation in an atom, molecule, or solid, has been studied theoretically for nearly a century but has never been conclusively observed experimentally. The main challenge is the very small rate compared to elastic scattering, combined with the difficulty of distinguishing a primary Migdal event from a secondary electronic excitation or ionization following ordinary elastic nuclear scattering. The Migdal effect has been proposed to search for sub-GeV dark matter as a way to evade nuclear recoil thresholds via an electronic excitation signal (see Ref. [1] for an overview of low-threshold detection methods), but first this effect must be observed with Standard Model probes in order to calibrate it [2–6]

In this Letter, motivated by recent developments on the *molecular* Migdal effect relevant for dark matter detection [7], we propose a new technique for measuring the Migdal effect with low backgrounds. A low-energy (~ 100 eV) neutron beam is used to induce *bound* Migdal transitions through nuclear scattering in a molecular gas such as carbon monoxide (CO), with a probability of $\sim 10^{-5}$ per neutron scattering event, leading to the emission of UV and visible photons with a distinctive spectrum that can be efficiently detected. As we will show, such transitions are extremely rare if induced by secondary collisions following a primary elastic scattering event, and the transitions we focus on are well-separated from nearby molecular transitions such that the only irreducible source of background is absorption of ~ 10 eV photons to directly drive the transition. By using a beam such as the Spallation Neutron Source (SNS) at Oak Ridge National Laboratory with a definite time structure, time correlations can be exploited to further reduce backgrounds not associated with the source.

Schematic of proposed experiment. Our experimental design is schematically represented in Fig. 1. A low-energy, highly-collimated neutron beam traverses a ~ 1 m long cell of cross-sectional area ~ 1 cm² filled with carbon monoxide (CO) molecules in the gas phase. Following a Migdal scattering event, the molecule undergoes the transition $X^1\Sigma \rightarrow B^1\Sigma$ with an electronic energy gap of

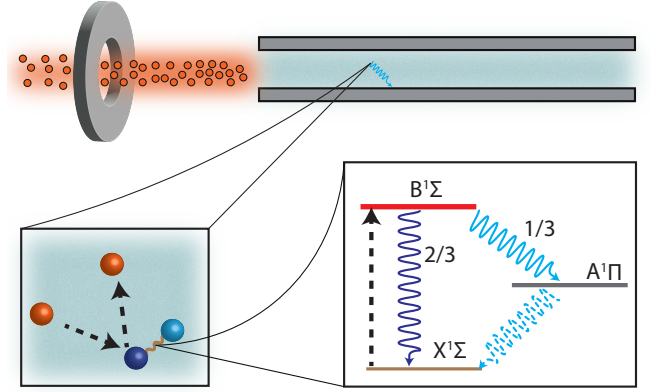


FIG. 1. Scheme of the experimental proposal. A collimated neutron beam collides with a gas of CO molecules. A neutron-molecule collision via the molecular Migdal effect induces the $X \rightarrow B$ transition in CO. This excitation has two decay pathways: one going back to the X state and another ending up in the A state. The Migdal signal is the $B \rightarrow A$ transition.

10.78 eV, whose decay leads to photon emission following two pathways. Pathway (1) (dark blue), the de-excitation back to the ground electronic state $B^1\Sigma \rightarrow X^1\Sigma$, has a branching ratio of $\approx 2/3$ and can induce the inverse process in nearby CO molecules, leading to a loss of signal from attenuation. On the other hand, pathway (2) (light blue), with a branching ratio of $\approx 1/3$, results in visible or near-UV photon emission peaking at ~ 400 nm from $B^1\Sigma \rightarrow A^1\Pi$ which streams freely, while the subsequent 158 nm photon from $A^1\Pi \rightarrow X^1\Sigma$ can excite the inverse transition in adjacent CO molecules and is attenuated. Therefore, our signal is the $B^1\Sigma \rightarrow A^1\Pi$ transition from (2), shown in solid light blue in Fig. 1. The signal photons can be detected with silicon photomultiplier (SiPM) detectors lining the walls of the gas cell, which have high efficiency at the signal wavelength.

The pressure p and temperature T of the gas cell should be chosen such that black-body radiation effects are irrelevant, collision-induced absorption is highly suppressed, and no collisional quenching of electronic transitions oc-

curs. For simplicity, we assume the gas cell is at room temperature ($T = 300$ K), but in a realistic implementation the temperature will be set by the requirements of the photodetector. The $B^1\Sigma$ state of CO has a lifetime $\tau_B = 22.3 \pm 0.5$ ns, which is typical of allowed molecular transitions. However, there is another zero-photon decay channel that can de-excite the molecule: CO-CO collisions, also known as self-quenching collisions. In the case of CO, its self-quenching cross section for the B state has been calculated to be $\sigma_{\text{self}} = 132 \text{ a}_0^2$ [8]. The typical collision time is $t_{\text{coll}} = \frac{1}{n(\sigma_{\text{self}})\langle v_{\text{CO}} \rangle}$, where $\langle v_{\text{CO}} \rangle$ denotes the average thermal velocity of CO molecules, n is the gas number density and $\langle \sigma_{\text{self}} \rangle$ is the thermally-averaged self-quenching cross section, which in this case we approximate as the constant σ_{self} . At $T = 300$ K, imposing that $t_{\text{coll}} > \tau_B$, we find that $n_{\text{CO}} < 3 \times 10^{16} \text{ cm}^{-3}$, which sets an upper bound on the pressure at $p \sim 1$ mbar.

Estimated rate. Calculating the expected rate of Migdal excitation is a straightforward modification of the formalism of Ref. [7], which computed dark matter-induced Migdal excitation in heteronuclear diatomic molecules, including to the same $B^1\Sigma$ state of CO. Throughout the rest of the analysis, we use particle physics units with $\hbar = c = 1$. The probability of Migdal excitation to an electronic state α with energy ϵ_α through nuclear scattering, via the non-adiabatic coupling channel, decomposes into electronic and nuclear matrix elements, $P_M^{(\alpha)}(\vec{q}) = P_e^{(\alpha)}(\vec{q}) \times P_N^{(\alpha)}(\vec{q})$, which depend on the momentum transfer $\vec{q}$. At 300 K, most of the molecules will be in the vibrational ground state; for simplicity, we will neglect rotational excitations which amounts to assuming that the initial and final rotational states of the molecule are the same, yielding a lower bound on the total rate. The electronic matrix element is

$$P_e^{(\alpha)} = \frac{q^2 \eta^2 |G_{\alpha 0}|^2}{M^2 (\epsilon_\alpha - \epsilon_0)^2}, \quad (1)$$

where $q = |\vec{q}|$, η is the cosine of the angle between $\vec{q}$ and the molecular axis, M is the total nuclear mass of the molecule, ϵ_0 is the ground-state energy, and $G_{\alpha 0}$ is the non-adiabatic coupling between α and the ground state, equal to 1.50 a_0^{-1} for the X-B transition in CO. The nuclear matrix element is [7, 9]

$$P_N^{(\alpha)} = \sum_{n=0}^{n_{\text{diss.}}} \left(\left| \left\langle \chi_n^{(\alpha)} \right| a_1 \frac{M_2}{\mu} e^{-i \frac{\mu}{M_1} q \rho \eta} - a_2 \frac{M_1}{\mu} e^{+i \frac{\mu}{M_2} q \rho \eta} \right| \chi_0 \right|^2 \right), \quad (2)$$

where χ_0 is the nuclear ground state wavefunction, $\chi_n^{(\alpha)}$ are the vibrational wavefunctions at harmonic oscillator level n associated to state α in the Born-Oppenheimer approximation, $n_{\text{diss.}}$ is the level at which the vibrational energy exceeds the dissociation energy of the

molecule, M_1 and M_2 are the masses of the two nuclei, $\mu = M_1 M_2 / M$ is the nuclear reduced mass, ρ is the inter-nuclear separation, and a_1 and a_2 are dimensionless coupling constants characterizing the interactions between the scattering probe and the nuclear targets. In the case of neutron scattering, it is more convenient to work in terms of the (dimensionful) neutron scattering lengths off free targets [10], $b_C = 6.64 \text{ fm} \times \frac{12}{13}$ and $b_O = 5.80 \text{ fm} \times \frac{16}{17}$, where the fractional factor accounts for the reduced mass between the neutron and the nucleus. Replacing a_1 and a_2 with scattering lengths b_1 and b_2 gives the nuclear matrix elements the dimension of a cross section, and so to avoid ambiguity we will write the neutron-induced Migdal cross section as

$$\sigma_M^{(\alpha)}(\vec{q}) = \frac{q^2 \eta^2 |G_{\alpha 0}|^2}{M^2 (\epsilon_\alpha - \epsilon_0)^2} \times \sum_{n=0}^{n_{\text{diss.}}} \left(\left| \left\langle \chi_n^{(\alpha)} \right| b_1 \frac{M_2}{\mu} e^{-i \frac{\mu}{M_1} q \rho \eta} - b_2 \frac{M_1}{\mu} e^{+i \frac{\mu}{M_2} q \rho \eta} \right| \chi_0 \right|^2 \right). \quad (3)$$

To obtain the total scattering rate, we integrate over the neutron spectrum and the possible momentum transfers. In Ref. [7], the molecules were taken to have a fixed orientation and the dark matter spectrum was parameterized by a velocity distribution. To make contact with this formalism, we can convert the neutron energy spectrum to a velocity distribution, which we pretend is isotropic in direction in order to model the random orientations of the target molecules. As a model for low-energy neutrons, we assume an E^{-1} spectrum between energies E_{min} and E_{max} [11, 12], leading to an effective neutron velocity distribution of

$$f_n(\vec{v}) = \frac{2}{\ln(E_{\text{max}}/E_{\text{min}})} \frac{1}{4\pi v^3} \Theta(v - v_{\text{min}}) \Theta(v_{\text{max}} - v), \quad (4)$$

where $v_{\text{min,max}} = \sqrt{2E_{\text{min,max}}/m_n}$. The first prefactor in Eq. (4) ensures that $\int d^3v f(\vec{v}) = 1$. In terms of this velocity distribution, the total rate per target molecule is given by Fermi's Golden Rule as

$$R = \frac{2\pi\rho_n}{m_n^3} \int d^3v f(\vec{v}) \int \frac{d^3q}{(2\pi)^3} \sigma_M^{(\alpha)}(\vec{q}) \delta(\Delta E - \omega_{\vec{q}}), \quad (5)$$

where ρ_n is the mass density of neutrons in the target volume, $\omega_{\vec{q}} = \vec{q} \cdot \vec{v} - \frac{q^2}{2m_n}$ accounts for the non-relativistic kinematics of the scattering, and ΔE is the total excitation energy, equal to $\epsilon_\alpha - \epsilon_0$ plus the vibrational excitation energy. Strictly speaking, there should be a different ΔE_n for each vibrational level, so the energy-conserving delta function gets pulled inside the sum which defines σ_M . The final modification to the dark matter formalism arises because the neutron flux $\Phi_n = \rho_n v / m_n$, rather than ρ_n , is the experimentally-provided quantity. The factor of v gets pulled inside the velocity integral, yielding our

final expression for the rate per target molecule,

$$R = \frac{\Phi_n}{m_n^2} \int d^3v \frac{f(\vec{v})}{v} \int \frac{d^3q}{4\pi^2} \sigma_M^{(\alpha)}(\vec{q}) \delta(\Delta E - \omega_{\vec{q}}). \quad (6)$$

To evaluate Eq. (6), we follow the prescription of Ref. [7] and fit the ground state χ_0 and the excited vibrational states $\chi_n^{(\alpha)}$ for $0 \leq n \leq 10$ to harmonic oscillator states at the same level n in order to exploit analytic formulas for the nuclear matrix elements in terms of Hermite polynomials. We choose $\chi_n^{(\alpha)}$ to be Morse potential wavefunctions, but as described in more detail in Ref. [7], the choice of nuclear wavefunction has a $\mathcal{O}(1)$ effect on the total rate and thus the harmonic oscillator approximation should suffice for an order-of-magnitude estimate. Using the energy eigenvalues of the Morse potential, there are in fact $n_{\text{diss.}} = 69$ vibrational levels available before exceeding the dissociation energy of 14 eV, so summing only up to $n = 10$ likely underestimates the rate slightly. Taking $E_{\text{min}} = 1$ eV, $E_{\text{max}} = 100$ eV, and $\Phi_n = 5 \times 10^8/\text{cm}^2/\text{s}$ (a typical neutron flux from sources such as the SPS [11]), and imagining a sample container with cross-sectional area $A = 1 \text{ cm}^2$ and length $L = 1 \text{ m}$, which contains $N_T = 2.3 \times 10^{18}$ molecular targets at the maximum density of $2.3 \times 10^{16}/\text{cm}^3$, we find a total rate

$$R_{\text{total}} \approx 2.6 \text{ events/min} \quad (7)$$

after accounting for the $\approx 1/3$ branching ratio of the signal pathway. If the neutron spectrum is chopped at 18 eV to reduce high-energy scattering events that could lead to ionization or dissociation (discussed further below), the Migdal rate is reduced by a factor of 10. The total neutron elastic scattering rate for this target density and volume is approximately $R_{\text{el.}} \approx \Phi_n(4\pi b_n^2)N_T = 5.2 \times 10^3 \text{ events/s}$, where $b_n \approx 6 \text{ fm}$ is an approximate average scattering length, so the Migdal rate is five or six orders of magnitude smaller. Nonetheless, the distinctive photon spectrum of the Migdal de-excitation will help to reduce backgrounds, as we will discuss below.

Signal photon spectrum. At $T = 300 \text{ K}$, most molecules are in the vibrational ground state $n_X = 0$. Using Eq. (6), we can calculate the relative probabilities of transitions from 0_X to each B vibrational state n_B , accounting for the expected neutron velocity distribution and integrating over allowed momentum transfers. The results are shown in the inset of Fig. 2 for two different choices of neutron energy cutoff. If the neutron spectrum extends to 100 eV (red), the final vibrational states are roughly equipartitioned, while if the neutron spectrum is chopped at 18 eV (blue), the transitions tend to end up in the ground vibrational state 0_B . The vibrational energies of the B states with respect to the 0_X ground-state energy range from 0.13 eV for 0_B to 2.5 eV for $n_B = 10$.

Next, a given n_B state will decay to the $A^1\Pi$ state following the usual dipole selection rules. The emission

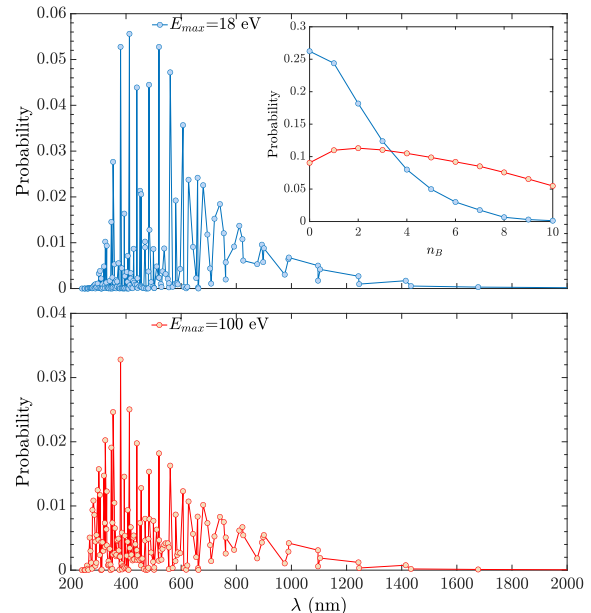


FIG. 2. The spectrum of signal photons resulting from the $B \rightarrow A$ transition after Migdal excitation of CO molecules. The top panel assumes $E_{\text{max}} = 18 \text{ eV}$, while the bottom panel assumes $E_{\text{max}} = 100 \text{ eV}$. The discrete peaks and troughs arise from vibrational splittings of the B and A levels. The inset shows the probability of $0_X \rightarrow n_B$ transitions which affect the overall shape of the spectrum.

intensity depends on the Franck-Condon factor, which allows us to calculate the spectral lineshape of the Migdal signal. The results, shown in the top panel of Fig. 2 for $E_{\text{max}} = 18 \text{ eV}$, show a distinctive photon spectrum centered at visible photon wavelengths that the SiPMs can easily detect, with the spectrum shifted slightly toward the near UV for the higher-energy neutrons with $E_{\text{max}} = 100 \text{ eV}$ (bottom panel). The open circles represent the wavelengths of narrow vibrational transitions.

Backgrounds. The dominant backgrounds will depend sensitively on the characteristics of the neutron beam, which we do not attempt to model here. Rather, we will argue that certain backgrounds are almost certainly negligible, while the presence of others imposes requirements on the associated photon spectrum of the beam.

First, photon absorption at $\sim 11 \text{ eV}$ can directly drive the $X^1\Sigma \rightarrow B^1\Sigma$ transition. Based on the oscillator strength for the 0-0 transition [13], in order for this rate to be below the signal rate, the photon flux at these energies would need to be $\lesssim 10^{-8} \Phi_n$. By doing a preliminary measurement with the gas cell emptied of target molecules, it may be possible to estimate the flux of these UV photons using the same SiPMs that are used to detect the signal photon, thus giving an in-situ estimate of the background rate. We note that the large energy of this transition makes thermal photons a negligible source of background, since at 300 K, there is a

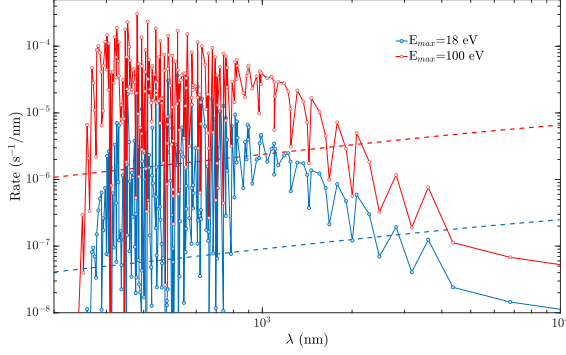


FIG. 3. Rate per unit wavelength of collision-induced emission, for $E_{\max} = 100$ eV (red dashed) and $E_{\max} = 18$ eV (blue dashed). The Migdal signal (open circles) in the 250–800 nm window gives a larger total rate in both cases.

Boltzmann suppression of $\sim e^{E_\gamma/T} = e^{-400}$. The first electronic state with the same spin as the ground state is the $A^1\Pi$ state, at 8.068 eV above the minimum of the ground electronic state [14, 15], with a transition wavelength of 158 nm. Therefore, there is no direct electronic transition from the ground state in the same wavelength range as the Migdal signal. Vibrational transitions may occur, but these are highly suppressed due to a negligible Franck-Condon factor and very small dipole moment. We expect that if the UV photon flux is sufficiently small to not drive the $X^1\Sigma \rightarrow B^1\Sigma$ transition at a rate above the neutron-induced Migdal rate, any other such transitions will occur at a lower rate.

Higher-energy X-ray photons, which are generically expected to accompany neutron beams, may also drive the

same transition through Compton scattering. As a rough estimate, the Compton cross section is $\mathcal{O}(\text{barn})$ [16], which is comparable to the elastic neutron cross section. Therefore, to avoid this source of backgrounds with a Migdal signal rate that is 10^{-5} of the elastic scattering rate, one would need to ensure that the X-ray photon flux is $\lesssim 10^{-5}\Phi_n$.

After an elastic neutron-CO collision, the CO molecule could subsequently collide with another CO molecule, leading to collision-induced emission in the same wavelength as our signal. The differential emission rate of photons per unit frequency ω is given by

$$A(\omega) = \frac{4\omega^3}{3} n_{\text{CO}} \int_a^\infty b db \langle v |\mathbf{d}(v, b, \omega)|^2 \rangle, \quad (8)$$

where v is the relative velocity of two CO molecules, b is the impact parameter, a is the diameter of a CO molecule, and $\mathbf{d}(v, b, \omega)$ is the Fourier transform of the transition dipole moment between the ground and the electronic state under consideration, and $\langle \cdot \rangle$ denotes an average over the relative velocity distribution. As a first estimate, we assume that the transition dipole moment is independent of the impact parameter, leading to the geometric cross section

$$A(\omega) = \frac{2a^2\omega^3}{3} n_{\text{CO}} \langle v |\mathbf{d}(v, \omega)|^2 \rangle. \quad (9)$$

Next, following the work of Karman et al. [17], it is possible to find an analytical expression for $|\mathbf{d}(v, \omega)|^2$, assuming that the excitation is due to short-ranged exchange interactions, yielding

$$|\mathbf{d}(v, \omega)|^2 = \left| \frac{4\mu d_0 e^{-\gamma a} \gamma \sqrt{\mu v} (\mu^2 v^2 + 2\mu\omega)^{1/4}}{(\gamma^2 + \mu^2 v^2)^2 + 2(\gamma^2 - \mu^2 v^2)(2\mu\omega + \mu^2 v^2) + (\mu^2 v^2 + 2\mu\omega)^2} \right|^2, \quad (10)$$

where μ is the reduced mass of the CO-CO system. In Eq. (10), the transition dipole moment is assumed to scale as $d = d_0 e^{-\gamma r}$, where d_0 is the transition dipole moment in the asymptotic region and γ is the length scale of the dipole surface, which we estimate as $\gamma = 3 \text{ a}_0^{-1}$ and $d_0 = 1$ Debye. Finally, we calculate the speed distribution of the scattered CO molecules $f_{\text{CO}}(v)$ using the kinematics of $2 \rightarrow 2$ hard-sphere scattering; this is formally identical to the standard calculation for dark matter-induced nuclear recoil [18]. The total rate per unit frequency, assuming every CO molecule undergoes a primary neutron scattering, is

$$A(\omega) = \frac{2a^2\omega^3}{3} n_{\text{CO}} \int f_{\text{CO}}(v) |\mathbf{d}(v, \omega)|^2 dv. \quad (11)$$

The emission spectra for two fiducial choices of maximum neutron beam energy are shown in Fig. 3, along with the signal spectra from Fig. 2 normalized to the total signal rate. Note that the background spectra are continuous while the signal spectra are discrete from the vibrational transitions shown in Fig. 2. Integrating the spectra over the range 250 – 800 nm, which contains the majority of the Migdal signal and represents a reasonable window for SiPM detection, yields background rates of $9.2 \times 10^{-4}/\text{s}$ for $E_{\max} = 100$ eV and $1.5 \times 10^{-5}/\text{s}$ for $E_{\max} = 18$ eV. Compared to the expected Migdal rates of 0.13/s for $E_{\max} = 100$ eV and 0.013/s for $E_{\max} = 18$ eV, the photon emission rate from secondary collisions is suppressed by more than two orders of magnitude in both cases, and thus is likely negligible in our setup.

Finally, we note that assuming the aforementioned backgrounds can be mitigated, the dark rate of the SiPMs will determine the required data-taking time for a given detection significance. For example, a dark rate of 1 Hz will yield $B = 1.44 \times 10^4$ background counts in 2 hours; we expect $S = 624$ signal events in the same interval, yielding an estimated sensitivity $S/\sqrt{B} = 5.2$ assuming that the dark counts are uncorrelated Poisson noise. Thus it is plausible that a statistically-significant detection can be achieved with $\mathcal{O}(\text{hours})$ of beam time.

Conclusions. In this Letter we have laid out a detection strategy for the molecular Migdal effect using low-energy neutron beams scattering off diatomic CO gas. The same approach is undoubtedly applicable to other diatomic gases, such as N_2 . However, further data on electronic quenching cross sections are required to make realistic predictions. Similarly, it could be possible to use highly polar molecules and, via a static electric field, exploit the distinctive directionality of the Migdal effect as studied in Ref. [7]. This setup could also further reduce backgrounds and avoid the reabsorption of photons coming from the $B \rightarrow X$ pathway, although the implementation is necessarily more complex than the present proposal. One could also consider using a buffer gas, such as He, to broaden the electronic transition [19] allowing for larger densities of molecules and thus a higher Migdal signal rate. We look forward to detailed follow-up studies on the feasibility of our proposed setup at neutron facilities such as the SNS.

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