Searching for dark matter with helium atom

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Abstract

With the help of the boost operator we can model the interaction between a weakly interacting particle (WIMP) of dark matter (DAMA) and an atomic nucleus. Via this “kick” we calculate the total electronic excitation cross section of the helium atom. The bound spectrum of He is calculated through a diagonalization process with a configuration interaction (CI) wavefunction built up from Slater orbitals. All together 19 singly- and doubly-excited atomic states were taken with total angular momenta of L=0,1 and 2. Our calculation may give a rudimentary estimation about the magnitude of the total excitation cross section which could be measured in later scintillator experiments. The upper limit of the excitation cross section is $9.7 \cdot 10^{-8}$ barn.

Key words: weakly interacting particles, dark matter, electronic excitation

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1 Introduction

Searching for DAMA with WIMP is an interesting question from both theoretical [1] and experimental sides. A considerable experimental work are in progress to measure DAMA-nucleus interaction in different scintillation set-ups such as liquid xenon [2], NaI [3] or different anisotropic crystals [4,5]. More technical details about the running experiments can be found under [6]. Theoretical considerations state that the WIMP can scatter from a nucleus either via a scalar (spin-independent) interaction or via an axial-vector (spin-dependent) interaction [7].

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In the following we use the binary encounter approach and apply the boost operator, to model the “kick” between the unknown WIMP-DAMA and the nucleus of the helium atom and calculate the total electronic excitation cross section. We use a CI wavefunction built up from Slater-like orbitals to describe the ground state and the low-lying bound spectrum of helium. Our CI wavefunction was successfully applied to describe different time-dependent problems such as heavy-ion helium collisions [8,9] or photoionization of helium in short XUV laser fields [10]. According to our knowledge, there are no theoretical calculations from this type forecasting measurable total excitation cross sections.

Atomic units are used throughout the paper unless otherwise mentioned.

2 Theory

At first we have to calculate the low-lying bound spectrum of the He. We obtain the eigenfunctions and the eigenvalues by diagonalizing the time-independent Schrödinger equation

\[
\hat{H}_{He} \Phi_j = E_j \Phi_j, \tag{1}
\]

where \( \hat{H}_{He} \) is the spin independent Hamiltonian of the unperturbed helium atom

\[
\hat{H}_{He} = \frac{\mathbf{p}_1^2}{2} + \frac{\mathbf{p}_2^2}{2} - \frac{2}{\mathbf{r}_1} - \frac{2}{\mathbf{r}_2} + \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}, \tag{2}
\]

and \( \Phi_j \) is the CI wavefunction built up by a finite linear combination of symmetrized products of Slater orbitals

\[
\phi(\mathbf{r}_1) = c(n, \kappa) r_n^{-1} e^{-\kappa} Y_{l,m}(\theta, \varphi), \tag{3}
\]

where \( c(n, \kappa) \) is the normalization constant. We use Slater functions with angular momentum \( l = 0, 1, 2 \) and couple them to \( L = 0, 1 \) and 2 total angular momentum two-electron states. In our basis we apply 9 different s orbitals, 6 different p orbitals and 4 different d orbitals, respectively. Table I presents our bound He spectrum compared to other, much larger \textit{ab initio} calculations [11,12,13]. We implement the complex scaling [14] method to identify the double-excited states in the low-lying single continuum. It is well known that the 1s1s ground state is highly angular correlated, and further \( pp \) and \( dd \) terms are needed to have an accurate agreement with experimental data which is \( -2.904 \) a.u. [10]. We checked the role of these terms and found that the affect in the final total cross sections is negligible.

We may approximate the interaction between the unknown DAMA particle and the nucleus of the helium with the boost operator. If we suddenly “kick” the He nucleus with a \( \mathbf{k} \) boost in the direction of \( \mathbf{r} \) that is equivalent to a
collective \(-k/2\) “kick” of the two atomic electrons according to the center-of-
mass. For a better understanding the geometry of the interaction is presented
in Figure 1.

The total excitation amplitude can be calculated in the following way:

\[
a_{\text{exc}} = \sum_f \langle \Phi(r_1, r_2) | e^{-ir_1k/2-i r_2k/2} | \Phi(r_1, r_2) \rangle_{1s1s},
\]

(4)

where \(1s1s\) is the ground state of He and the summation \(f\) runs over the
singly- and doubly-excited final states. For elastic collision only the ground
state to ground state transition is considered. The energy of the unknown
DAMA is \(E = k^2/2\). The DAMA-electron interaction is evaluated thought the
transition matrix elements of the boost operator between two Slater orbitals
\(\langle \phi_1(r) e^{-irk/2} | \phi_2(r) \rangle\). To separate the radial and the angular part of the matrix
element we expand the plane wave through spherical Bessel functions in the
well-known way [15]:

\[
e^{ir\cdot k} = e^{k\cdot r \cos(\theta)} = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} j_{l}(kr) Y_{l,m}(\theta_k, \varphi_k) Y_{l,m}(\theta_r, \varphi_r).
\]

(5)

After some algebra the angular part of the matrix element gives us the Clebsch-
Gordan coefficient

\[
\int_{\Omega} Y_{l_1,m_1}^*(\theta, \varphi) Y_{l,m}(\theta, \varphi) Y_{l_2,m_2}(\theta, \varphi) d\Omega = \sqrt{(2l_2 + 1)(2l + 1)} \times
\]

\[
\begin{align*}
&\sqrt{(2l_2 + 1)} \times
\end{align*}
\]

\[
(l_2, l, l_1|m_2, m, m_1) \cdot (l_2, l, l_1|0, 0, 0).
\]

(6)

According to the definition of the spherical Bessel functions [17]a \(j_l(kr) = \sqrt{\frac{2}{\pi kr}} J_{l+1/2}(kr)\) the radial part of the matrix element has the analytic solution
of [16]:

\[
\int_0^{\infty} J_{\nu}(kr) e^{-\alpha r} r^{\mu-1} dr = \frac{\left(\frac{k}{2}\right)^\nu \Gamma(\nu + \mu)}{\Gamma(\nu + 1) \sqrt{(k^2 + \alpha^2)^{\nu+\mu}}} \times
\]

\[
\left(2F_1\left(\frac{\nu + \mu}{2}, 1 - \mu + \nu \quad ; \nu + 1; \frac{k^2}{k^2 + \alpha^2}\right)\right),
\]

(7)

where \(\Gamma\) is the gamma function and \(2F_1\) is the hypergeometric function with the
following real arguments \(\mu - 1 = n_1 + n_2 - 1/2, \nu = l + 1/2\) and \(\alpha = \kappa_1 + \kappa_2\). We
tried to simplify the final formula but unfortunately, we could not succeed,
and have to calculate the hypergeometric function numerically with a well-behaving complex contour integral \[17\]\text{b}. It is worth to mention that with additional constraints among the parameters \([\alpha, k, \nu, \mu]\) this radial integral can be simplified, but not in our general case.

The total excitation cross section can be evaluated with the following formula

\[
\sigma_{exc} = r_\alpha^2 \pi P_{exc},
\]

where \(r_\alpha = 1.76 \cdot 10^{-15} m\) is the radius of the He nucleus and \(P_{exc} = |a_{exc}|^2\) is the total excitation probability. For elastic collision only the ground state to ground state transition is considered.

3 Results and discussion

Figure 2 presents our elastic and excitation total cross sections in function of the impulse of the DAMA. The cross sections are given in barns and the wave number of the unknown particle is given in atomic units. If the velocity of the DAMA is known then the mass can be calculated from \(m = k/v\).

The maximum of the excitation cross section is \(9.7 \times 10^{-8}\) barn at \(k=3\) a.u. DAMA impulse. At low wave numbers (\(k\)) the boost operator can be well approximated with its Taylor series which is similar to the dipole interaction, and used in photoionization calculations. At low \(k\) values the elastic cross section is many magnitude higher than the excitation one, which meets our physical intuition. At larger wave numbers, however, the dipole approximation breaks down and the general matrix element have to be calculated where the non-dipole contributions play a significant role. Above \(k = 30\) a.u. the elastic and excitation cross sections run together, but the excitation cross sections are a factor of 2-4 higher than the elastic ones. At wave numbers larger than 10, due to the quick oscillations of the boost operator, the cross sections have a strong decay which can be excellently fitted with the following power law:

\[
\sigma_{exc} = 2.3566 \times 10^5 \cdot k^{-13.782},
\]

where the standard error of the exponent is 0.074 and the standard error of the scaling constant is 0.48, respectively.

At \(k > 10000\) wave numbers the cross sections stop decaying and show spurious oscillations, which are numerical art-effects due to the limited accuracy of the calculations. These cross sections are not presented in Fig. 2.

We can not enhance the total angular momenta of the two electron wavefunction in our calculation, and the number of the available bound states are also
limited. The role of the highly-excited Rydberg states are out of our scope too. In this sense we can not rigorously prove the convergence of our calculation, but our experience shows that for excitation the significant contributions always came from the lowest excited states. We interpret our results as a rude approximation for the dark matter He interaction which may stimulate further investigations.

4 Summary and Outlook

With the help of the boost operator we gave a “simple-man’s model” for the DAMA-helium nucleus interaction and calculated total electronic excitation and elastic collision cross sections which can be measured in future scintillator experiments. Our calculation could be generalized for atoms with electrons more than two, (even for Xe) if the wavefunction of the ground state and a significant large number of excited states are present with sufficient accuracy. We think that this problem could be solved with the General Relativistic Atomic Structure (GRASP) code [18], which is out of our capability. The aim of this paper was twofold. First, we presented our model for the DAMA-He interaction calculating cross sections. Secondly, we advised our model to many-electron-atom theorists to calculate DAMA-Xe interaction.

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Fig. 1. The geometry of the DAMA-He interaction.

Table 1
The energy levels of bound, singly- and doubly-excited states used in our calculations, compared with a) basis set calculations from [11] b) CI calculation results [12] and c) complex-coordinate rotation calculations from [13].

| states | our results | other theory | states | our results | other theory | states | our results | other theory |
|--------|-------------|--------------|--------|-------------|--------------|--------|-------------|--------------|
| 1s1s   | −2.8821     | −2.9037<sup>a</sup> | 1s2p   | −2.1233     | −2.1238<sup>b</sup> | 1s3d   | −2.0556     | −2.0556<sup>b</sup> |
| 1s2s   | −2.1441     | −2.1460<sup>a</sup> | 1s3p   | −2.0550     | −2.0551<sup>b</sup> | 1s4d   | −2.0312     | −2.0313<sup>b</sup> |
| 1s3s   | −2.0607     | −2.0612<sup>a</sup> | 1s4p   | −2.0259     | −2.0310<sup>b</sup> | 2s3d   | −0.5597     | −0.5692<sup>c</sup> |
| 1s4s   | −2.0333     | −2.0335<sup>a</sup> | 2s2p   | −0.6572     | −0.6931<sup>c</sup> | 2s4d   | −0.5305     | −0.5564<sup>c</sup> |
| 2s2s   | −0.7297     | −0.7779<sup>a</sup> | 2s3p   | −0.5821     | −0.5971<sup>c</sup> |
| 2s3s   | −0.5711     | −0.5899<sup>a</sup> | 2s4p   | −0.5401     | −0.5640<sup>c</sup> |
| 2s4s   | −0.5372     | −0.5449<sup>a</sup> | 2s5p   | −0.5225     | −0.5470<sup>c</sup> |
| 2s5s   | −0.5133     | −0.5267<sup>a</sup> | 3s3p   | −0.2998     | −0.3356<sup>c</sup> |
Fig. 2. Elastic (dashed line) and excitation (solid line) total cross sections for DAMA-He collision.