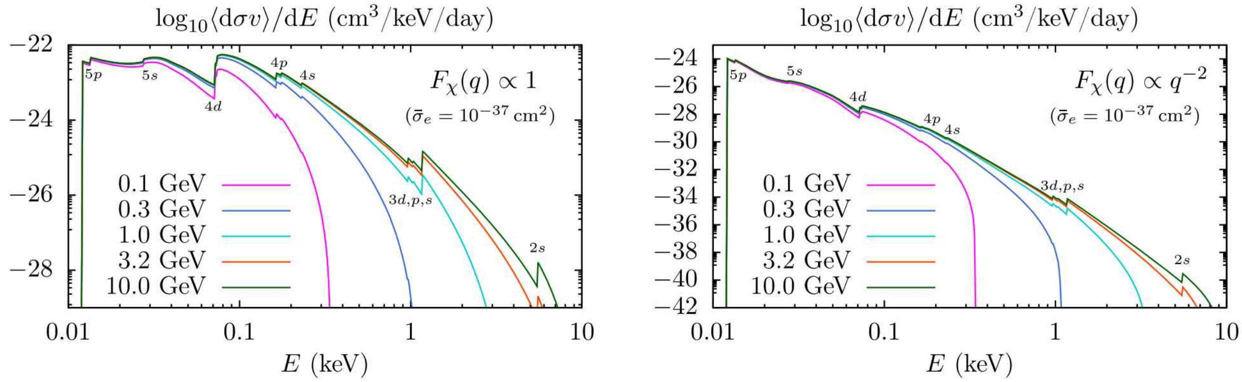

FIG. 2. Velocity-averaged differential cross section for a single Xe atom, with $\bar{\sigma}_e = 10^{-37}$ cm^2. The left panel is for a contact (heavy mediator) interaction, and the right is for a long-range (Coulomb-like) interaction. The kinks in the plots are due to the opening up of deeper electron shells. There is no signal above $E_{\rm max} = m_\chi v_{\rm max}^2/2$, where $v_{\rm max}$ is the maximum DM velocity.

the cross section. This is because such functions have incorrect scaling at distances close to the nucleus, which is the only part of the electron wave function that can contribute enough momentum transfer.

Another common approach is to approximate the outgoing ionization electron wave function as a plane-wave state. Such functions also have the incorrect scaling at small distances and underestimate the cross section by orders of magnitude for large q. (This is mostly due to the missing Sommerfeld enhancement as discussed in Ref. [47].) More details regarding this point are given in Appendix.

Therefore, to perform accurate calculations, one must employ a technique known to accurately reproduce the electron orbitals, namely, the relativistic Hartree-Fock method, including finite-nuclear size, and using continuum energy eigenstates as the outgoing electron orbitals. Detailed calculations and discussion were presented in Ref. [17]. Formulas are given in Appendix.

Given the extreme dependence on the atomic physics seen in Fig. 1, it is important to estimate the uncertainty in the calculations. To gauge this, we also calculate the cross section using other (simpler) methods. Namely, we exclude the effect of the exchange potential from the Hartree-Fock method and also solve the Dirac equations using only a local parametric potential (chosen to reproduce the ionization energies) instead of the Hartree-Fock equations. The effect this has on the calculations is very small, with the main difference coming from small changes in the calculated values for the ionization energies. This is as expected, since the cross section is due mainly to the value of the wave functions on small distances, close to the nucleus, where many-body electron effects are less important (but the correct scaling is crucial). All of these methods (unlike the effective Z method, or plane-wave assumption) give the correct small-r scaling of the bound and continuum electron orbitals.

The finite-nuclear size correction is important for large values of q but is small compared to the relativistic corrections and ultimately is not a leading source of error. In any case, we include this in an *ab initio* manner, by directly solving the electron Dirac equation in the field created by the nuclear charge density, which we take to be given by a Fermi distribution, $\rho(r) = \rho_0[1+\exp(r-c/a)]^{-1}$. Here, $t \equiv 4a\ln 3 \simeq 2.3$ fm and $c \simeq 1.1A^{1/3}$ fm are the nuclear skin-thickness and half-density radius, respectively, e.g., Ref. [48], and ρ_0 is the normalization factor. We note that the uncertainties stemming from the atomic physics errors are small compared to those coming from the assumed dark matter velocity distribution and detector performance, as discussed in the following sections.

Plots of the velocity averaged differential cross sections for several WIMP masses and mediator types are presented in Fig. 2. We find very good agreement with similar recent calculations for Xe atoms in Ref. [49]. We present these plots for the xenon atom, since it is the most common target material. For DAMA/LIBRA experiment, the cross section is dominated by scattering off iodine ($Z = 53$), which has an electron structure very similar to that of xenon ($Z = 54$).

C. Annual modulation

We assume the DM velocity distribution is described by the standard halo model, with a cutoff (in the galactic rest frame) of $v_{\rm esc} = 550(55)$ km/s, and a circular velocity of $v_0 = 220(20)$ km/s; see, e.g., Ref. [6,50]. The numbers in the parentheses above represent estimates for the uncertainties in the values. This is important, due to the strong velocity dependence of the cross section (see also, e.g., Ref. [46]). We use these uncertainties to estimate the resulting uncertainty in the calculated event rates.

For the calculations, the velocity distribution is boosted into the Earth frame, which has a speed of

$$v_E(t) \approx v_L + v_{\rm orb}\cos\beta\cos(2\pi\cdot{\rm yr}^{-1}t+\phi). \qquad (9)$$