Estimating the Magnetic Flux Generated By a Nuclear-Spin-1/2 Polarized Sample

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1 Introduction

One of the near-term goals of the Noble Gas Ice Project is to demonstrate the viability of matrix-isolated diamagnetic atoms with nonzero nuclear spins as a “next-generation” tool for nuclear EDM searches, see for example Tab. (1). The major potential benefit of this approach would be the increased statistical sensitivity to the EDM signal due to the orders of magnitude higher number of atoms in the sample relative to the sample size of traditionally optically-trapped atomic species. Once polarized, the nuclear spins are expected to retain their nonthermal polarization for a very long time, which is ideal for an EDM search. Towards this end, we have chosen to demonstrate the proof-of-principle of this approach with Ytterbium (Yb) atoms embedded in a solid-Neon (s-Ne) matrix.

Our goal is to optically pump Yb atoms while embedded in the s-Ne matrix and detect the resulting magnetization due to the nuclear spin polarization of Yb-171 in natural abundance Yb. Any detection technique that takes advantage of the coupling between this magnetization and a “pickup” coil requires knowledge of the magnetic flux due to the polarized Yb atoms. In the following sections, we list the equations necessary to perform this calculation and then estimate the size of the flux for one particular experimental configuration.

The magnitude of the voltage that one will ultimately use as a gauge of the nuclear polarization depends on the scheme that is used to transform the magnetic flux into an observable (e.g. SQUID-based detection, traditional NMR spectrometer, etc.). At present, these considerations are beyond the scope of this document. Furthermore, the degree of nuclear polarization that can be obtained via optical pumping will be discussed in a separate, upcoming note.

isotope	Z	state	half-life	abd.	g (μ_N)	ν (Hz)
neutron	0	free	885.7 s		-3.82608546	2916.5
proton	1	H_2	stable	0.999885	+5.585694712	4257.7
triton	1	T_2	12.33 y		+5.957924896	4541.5
He-3	2	$^1S_0$	stable	1.34 ppm	-4.254995436	3243.4
Sr-81	38	$^1S_0$	22.3 m		+1.088	829.3
Cd-111	48	$^1S_0$	stable	0.1280	-1.1897722	906.9
Cd-113	48	$^1S_0$	9.3E15 y	0.1222	-1.2446018	948.7
Cd-115	48	$^1S_0$	53.46 h		-1.2968518	988.5
Xe-127	54	$^1S_0$	36.4 d		-1.0078	768.2
Xe-129	54	$^1S_0$	stable	0.264006	-1.5559526	1186.0
Ba-125	56	$^1S_0$	3.5 m		+0.354	269.8
Ba-127	56	$^1S_0$	12.7 m		+0.178	135.7
Ba-129	56	$^1S_0$	2.23 h		-0.796	606.8
Ba-131	56	$^1S_0$	11.50 d		-1.416226	1079.5
Ba-133	56	$^1S_0$	10.52 y		-1.543348	1176.4
Yb-171	70	$^1S_0$	stable	0.1428	+0.98734	752.6
Hg-195	80	$^1S_0$	9.9 h		+1.0829498	825.5
Hg-197	80	$^1S_0$	64.14 h		+1.0547488	804.0
Hg-199	80	$^1S_0$	stable	0.1687	+1.011771	771.2
Hg-205	80	$^1S_0$	5.2 m		+1.202	916.2
Rn-211	86	$^1S_0$	14.6 h		+1.202	916.2
Ra-213	88	$^1S_0$	2.74 m		+1.2266	935.0
Ra-225	88	$^1S_0$	14.9 d		-1.4676	1118.7

Table 1: Table of Spin-1/2 Isotopes. These species all have $S = J = 0$ for the electronic ground state and a half-life of at least 100 seconds. The g-factor is listed in units of the nuclear magneton μ_N. The NMR frequency ν is listed for a field of 1 Gauss. Data from [1, 2, 3]

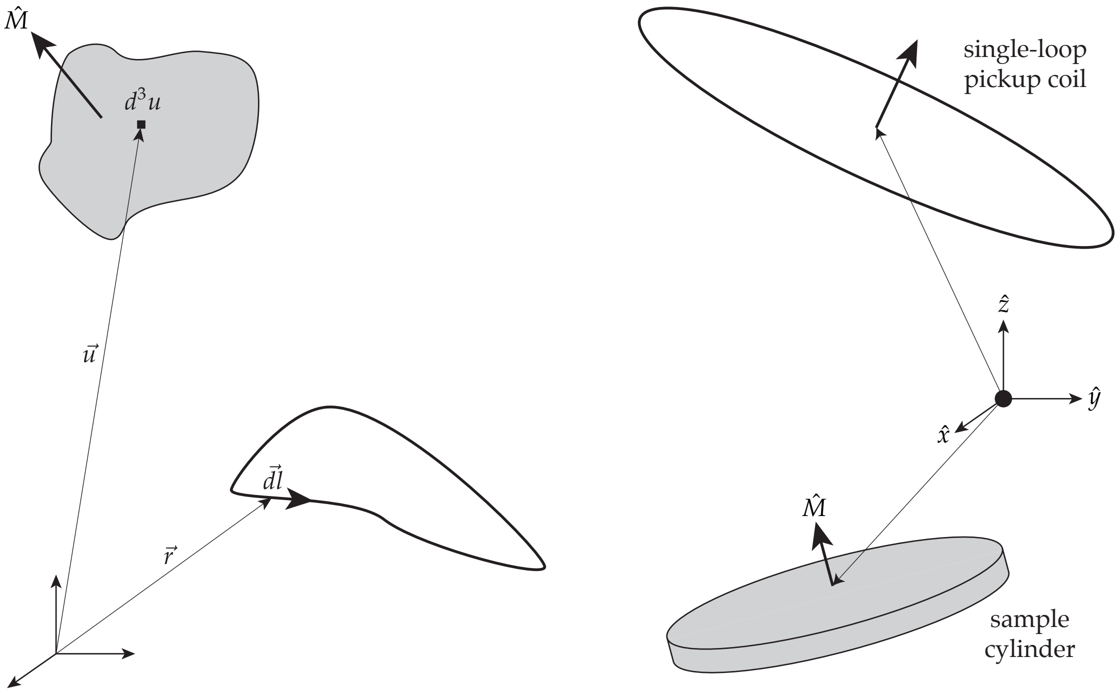

Figure 1: Geometry for Flux Calculation. *Left:* Arbitrary Sample & Coil Shapes. *Right:* Cylindrical Sample and Single-Loop Pickup Coil. This latter configuration is a model for the Noble Gas Ice Project.

2 Magnetic Vector Potential

Nuclear polarization can be detected by measuring the effect of the magnetic field $\vec{B}_n$ produced by the spin-polarized nuclei in a sample. This magnetic field depends on the geometry of the sample and the location $\vec{r}$ of the measurement by [4]:

$$\vec{B}_n(\vec{r},t) = \vec{\nabla} \times \vec{A}_n(\vec{r},t) \qquad \vec{A}_n(\vec{r},t) = \frac{\mu_0}{4\pi} \int \frac{\vec{M}(\vec{u},t) \times (\vec{r}-\vec{u})}{|\vec{r}-\vec{u}|^3} d^3u \tag{1}$$

where $\vec{A}_n(\vec{r},t)$ is the magnetic vector potential of the polarized sample, t is time, μ_0 is magnetic constant, $\vec{M}(\vec{u},t)$ is the magnetization of the polarized sample at a location $\vec{u}$, and the integral is performed over the volume of the sample, see left half of Fig. (1). The magnetization is defined as the average magnetic moment per unit volume:

$$\vec{M}(\vec{u},t) = \langle \vec{\mu}(\vec{u},t) \rangle \, \rho(\vec{u},t) \tag{2}$$

where ρ is local nuclear spin number density and $\langle\vec{\mu}\rangle$ is the combined statistical & quantum mechanical expectation value of the nuclear magnetic dipole moment:

$$\langle\vec{\mu}(\vec{u},t)\rangle = g\mu_N \left\langle \vec{I}(\vec{u},t) \right\rangle = g\mu_N I \vec{P}(\vec{u},t) \tag{3}$$

where g is the g-factor in units of the nuclear magneton μ_N, $\vec{I}$ is the (unitless) nuclear spin vector operator, I is the nuclear spin, and $\vec{P}$ is the polarization vector given by:

$$\vec{P} = \hat{x}P_x + \hat{y}P_y + \hat{z}P_z \equiv \frac{\langle\vec{I}\rangle}{I} \tag{4}$$

3 Magnetic Flux

By representing the field as the magnetic vector potential and applying Stokes's Theorem, the magnetic flux integral over the area of the coils can be reduced to an integral around the path of the coils:

$$\Phi = \int \vec{B}_n(\vec{r},t)\cdot d\vec{a} = \int \left(\nabla \times \vec{A}_n(\vec{r},t)\right)\cdot d\vec{a} = \oint \vec{A}_n(\vec{r},t)\cdot d\vec{l} \tag{5}$$

If we assume that the polarization and density of spins are both uniformly distributed within the sample (i.e. there are no polarization or density gradients), then the magnetic flux can be written as:

$$\Phi(t) = \sum_k \Phi_k P_k(t) = B_{\text{scale}} \sum_k a_k P_k(t) \tag{6}$$

where k labels one of the three orthonormal unit vectors, P_k is the (unitless) possibly time-dependent polarization component in the k-direction, B_{scale} is the "scale" magnetic field of the nuclear spins, and a_k is the effective "area" enclosed by the pickup coils relative to the k-direction. The scale magnetic field is given by:

$$B_{\text{scale}} \equiv \frac{\mu_0\mu_N g I\rho}{4\pi} = 67.85\text{ nG}\left[\frac{g}{1}\right]\left[\frac{I}{1/2}\right]\left[\frac{\rho}{10^{-3}\text{ amg}}\right] \tag{7}$$

where μ_0 is the magnetic constant, μ_N is the nuclear magneton, g is the g-factor of the nucleus, I is the nuclear spin, ρ is the number density of the nuclear spins in the sample, 1 amg ($= 2.6868 \times 10^{19}/\text{cm}^3$) is the number density of an ideal gas at 1 atm and 0 °C, and we've used the following useful relation:

$$\frac{\mu_0 \mu_N}{4\pi} = \frac{135.7\ \mu\text{G}}{\text{amg}} = \frac{1.357\ \text{nV}}{\text{amg} \cdot \text{cm}^2 \cdot \text{kHz}} \tag{8}$$

The effective area of the coils is given by the following integral:

$$a_k \equiv \int \oint \left[\hat{x}_k \times \frac{\vec{r} - \vec{u}}{|\vec{r} - \vec{u}|^3} \right] \cdot \vec{dl}\ \ d^3u \propto \frac{\cos(\theta_k) l_c V_n}{d^2} \tag{9}$$

where $\hat{x}_k$ is the unit vector in the k-direction, $\vec{u}$ is the displacement vector from the origin to the infinitesimal volume element d^3u inside the sample, $\vec{r}$ is the displacement vector from the origin to the infinitesimal line element $\vec{dl}$ of the pickup coil, θ_k is the angle between the unit vector along the k-direction and the normal vector of the coil, l_c is the effective length of the coil, V_n is the volume of the sample, and d is the characteristic distance between the coil and the sample.

4 Numerical Calculation for the Noble Gas Ice Project

In this section, we calculate the effective coil area, Eqn. (9), for a thin disk sample near a single-loop pickup coil as depicted in the right half of Fig. (1). These integrals are calculated numerically using Simpson's rule. We orient the axis of the sample, coils, and magnetization along the along the z-direction. These and other parameters used in the calculation are listed in Tab. (2). Furthermore, we've taken the number density of s-Ne to be 1604 amg [5] and the natural abundance & g-factor of Yb-171 listed in Tab. (1).

parameter	value	units
number of slices along the disk axis	$2 \times 1 + 1$	-
number of radial slices, azimuthal sectors	$16, 16^2$	-
disk thickness	0.003	cm
disk radius	0.50	cm
disk center	$(0.0, 0.0, 0.0)$	cm
magnetization unit vector, $\hat{M}$	$(0.0, 0.0, +1.0)$	-
number of coil loop line elements	101	-
loop radius	0.50	cm
loop center	$(0.0, 0.0, +0.2)$	cm
loop area unit vector	$(0.0, 0.0, +1.0)$	-

Table 2: Baseline Parameters Used for Flux Calculation.

4.1 Absolute Flux

For the case of longitudinal polarization, we orient the bias B-field along the z-direction and using the baseline parameters, we find:

$$\Phi = (0.0151\Phi_0)\left[\frac{[\mathrm{Yb}]/[\mathrm{Ne}]}{10^{-5}}\right]\left[\frac{[^{171}\mathrm{Yb}]/[\mathrm{Yb}]}{0.1428}\right]\left[\frac{a_z}{0.0203\ \mathrm{cm}^2}\right]\left[\frac{P_z}{100\%}\right] \tag{10}$$

where $\Phi_0 = h/(2e) = 206.8\ \mathrm{nG}\cdot\mathrm{cm}^2$ is the unit of flux quantum.

4.2 Induced Voltage

For the case of transverse polarization, we orient the bias B-field along the x-direction. This results in the precession of the nuclear spins about the x-axis which induces a voltage $\mathcal{V}$ in a set of pickup coils given by Faraday's Law [6]:

$$\mathcal{V} = -\frac{d\Phi}{dt} = -\omega B_{\mathrm{scale}} a_z P\cos(\omega t) = -V_{\mathrm{scale}}\cos(\omega t) \tag{11}$$

$$V_{\mathrm{scale}} = (31.2\ \mathrm{fV})\left[\frac{\omega}{1\ \mathrm{kHz}}\right]\left[\frac{[\mathrm{Yb}]/[\mathrm{Ne}]}{10^{-5}}\right]\left[\frac{[^{171}\mathrm{Yb}]/[\mathrm{Yb}]}{0.1428}\right]\left[\frac{a_z}{0.0203\ \mathrm{cm}^2}\right]\left[\frac{P_z}{100\%}\right] \tag{12}$$

4.3 Scaling Properties

Fig. (2) depicts the dependance on the effective area on the coil to substrate radius ratio when the two are separated by 2 mm. The maximum area occurs at a coil radius that is about 15% larger than the substrate radius. For a coil to substrate radius ratio of unity, the effective area is only about 10% smaller than the maximum value. When the coil is much smaller than the substrate, the effective area scales almost linearly with the physical area.

Fig. (3) depicts the dependence on the effective area on the separation between the coil and substrate and the substrate radius, assuming a unity coil to substrate radius ratio. As can be readily seen, the effective area drops off very fast as the coil and substrate are separated. This would seem to indicate that a gradient coil pair constructed from two separated coils would provide a larger net signal from the substrate than two coplanar coils with different radii.

Next, we see that, with a fixed sample density, increasing the substrate radius R results in only a linear scaling of the effective area. This can be understood from the scaling relationship in Eqn. (9): the length of the coil scales as R, the volume of the sample scales as R^2, and the characteristic separation scales as R. Putting this altogether gives a scalling of R, which is what the calculation shows as well. Finally, we'll note that the effective area scales linearly with the thickness of the sample since this linearly increases, for a fixed density, the total number of polarized nuclei.

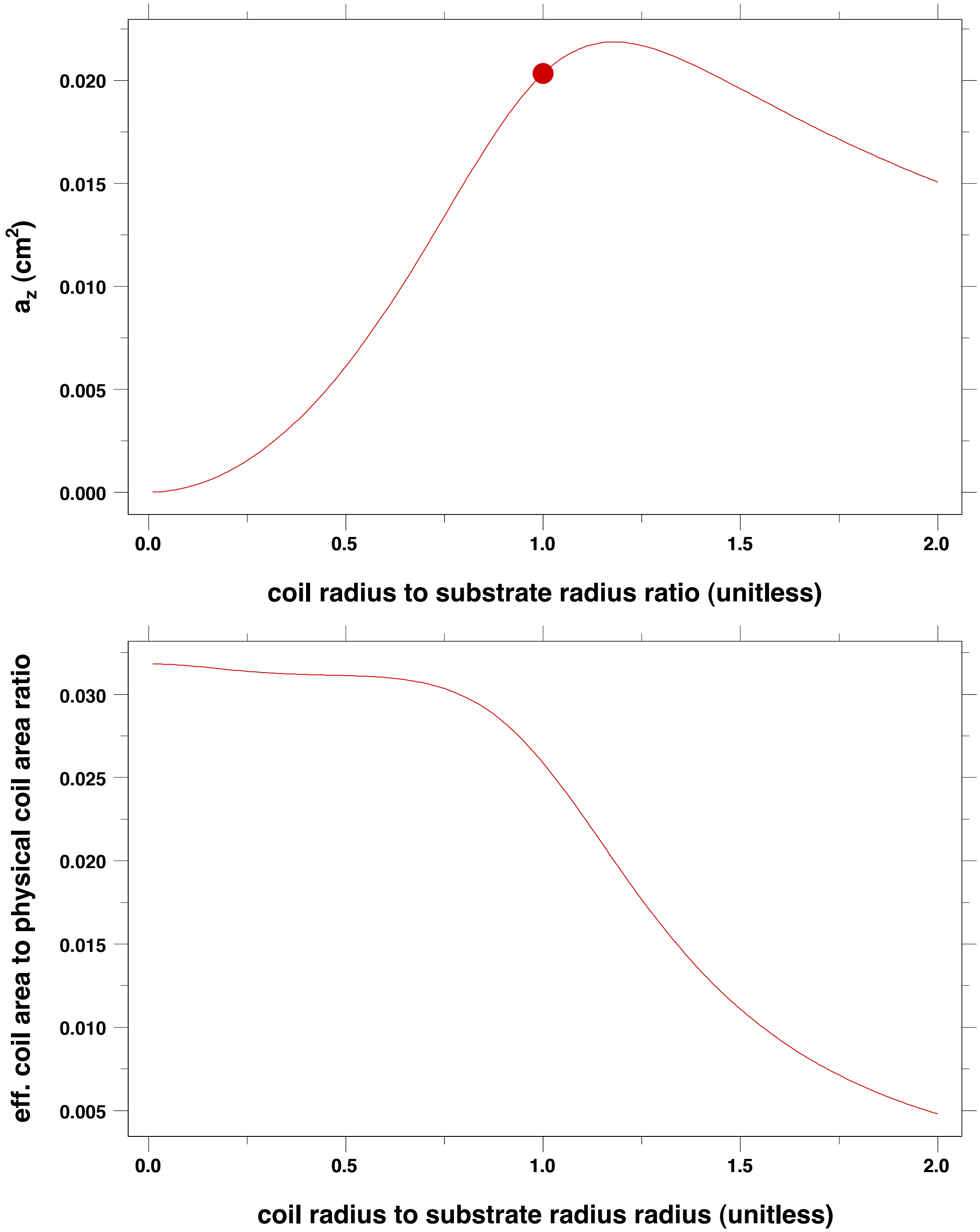

Figure 2: Effective Area as a Function of Coil to Substrate Radius Ratio. Results are plotted assuming a 2 mm separation between the coil and substrate. The red dot indicates the result obtained for the baseline parameters.

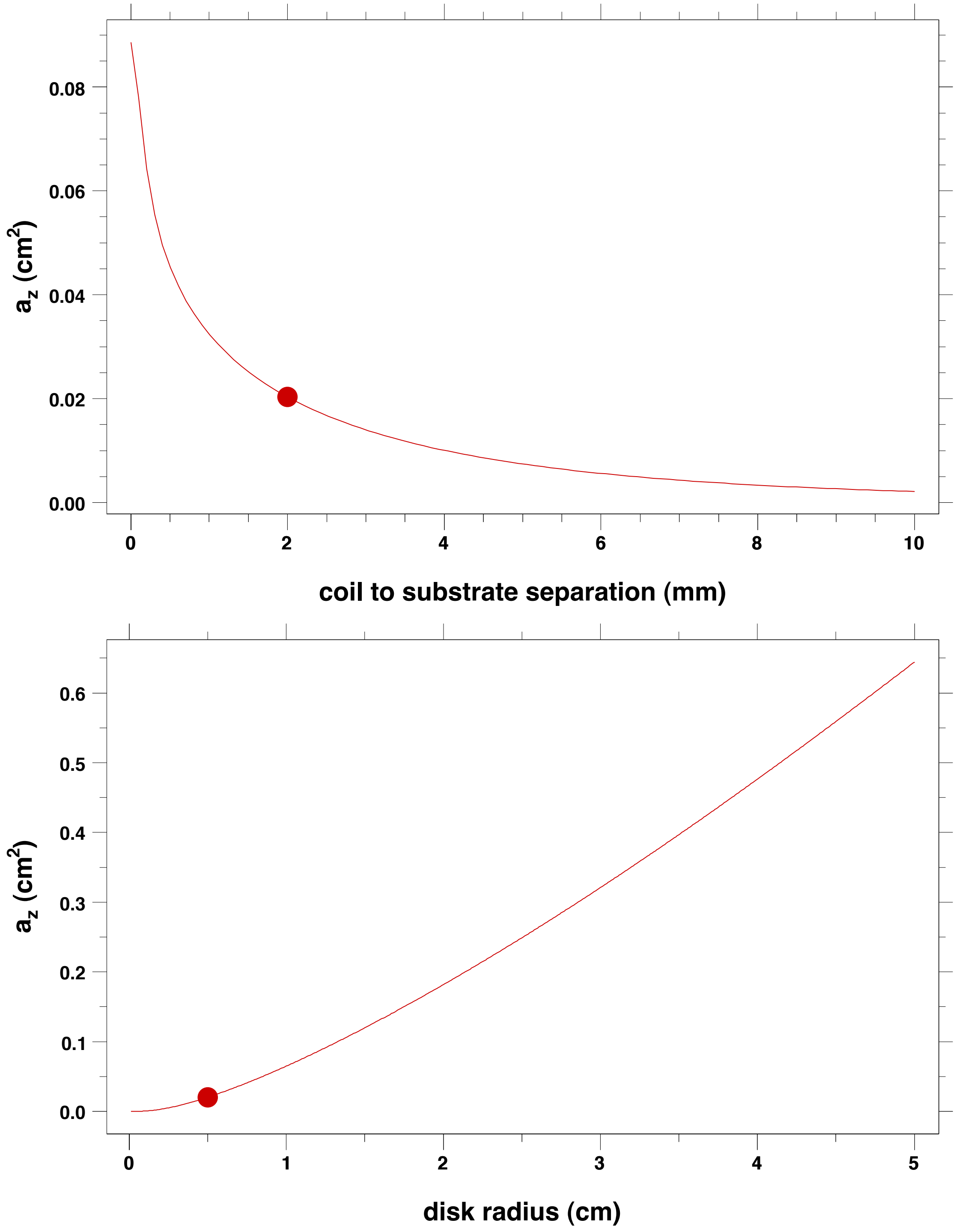

Figure 3: Effective Area as a Function of Separation and Substrate Radius. Results are plotted assuming a coil to substrate radius of unity. The red dot indicates the result obtained for the baseline parameters.

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