Gravitational effects in g-factor measurements and high-precision spectroscopy: Limits of Einstein's equivalence principle

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We study the interplay of general relativity, the equivalence principle, and high-precision experiments involving atomic transitions and g factor measurements. In particular, we derive a generalized Dirac Hamiltonian, which describes both the gravitational coupling for weak fields, as well as the electromagnetic coupling, e.g., to a central Coulomb field. An approximate form of this Hamiltonian is used to derive the leading gravitational corrections to transition frequencies and g factors. The position-dependence of atomic transitions is shown to be compatible with the equivalence principle, up to a very good approximation. The compatibility of g factor measurements requires a deeper, subtle analysis, in order to eventually restore the compliance of g factor measurements with the equivalence principle. Finally, we analyze small, but important limitations of Einstein's equivalence principle due to quantum effects, within high-precision experiments. We also study the relation of these effects to a conceivable gravitationally induced collapse of a quantum mechanical wave function (Penrose conjecture), and space-time noncommutativity, and find that the competing effects should not preclude the measurability of the higher-order gravitational corrections. Surprisingly large higher-order gravitational effects are obtained for transitions in diatomic molecules.

CONTENTS

I. INTRODUCTION

According to Einstein's theory of gravitation, space-time is locally flat, and the Einstein form of the equivalence principle states that the outcome of any non-gravitational experiment should be independent of where and when in the Universe it is performed. Among the most accurately measured quantities in physics, we find transition frequencies in simple atomic systems and g factor experiments, both for free and bound leptons (electrons and muons). Leptons are described, in curved space-time, by the gravitationally and electromagnetically coupled Dirac equation. Here, we derive a generalized Dirac Hamiltonian which describes both mentioned couplings for light fermions, in electromagnetic and (weak) gravitational fields, and establish its properties under a particle-antiparticle transformation. We also find its nonrelativistic form by a Foldy–Wouthuysen transformation.

As convincingly demonstrated by the Shapiro delay, measured to excellent accuracy by the Cassini spacecraft in superior conjunction [1], we must assign a coordinate dependence to the vacuum permittivity and vacuum permeability, in global coordinates. Based on these assumptions, we investigate the position-dependence of atomic transitions and find (in agreement with Ref. [2]) that the position-dependence of their frequencies is largely compatible with the equivalence principle.

For free and bound g factor experiments, gravitational frequency shifts of spin-flip transitions have been the subject of rather intense discussions [3–8]. Our paper addresses part of these questions but otherwise has a much broader scope. Furthermore, it has long been conjectured that subtle limitations to the Einstein equivalence

principle should occur within a full quantum theory. We find such limitations, both due to the Fokker precession as well as due to the noncommutativity of the electron's momentum operator with the global space-time coordinates.

It is our goal to present a comprehensive and relatively easily digestible account of related matters, despite the length of the current article. For clarification, we should point out that throughout this paper, we consider gravitational effects for an atom at rest with respect to a center of gravity, in contrast to Refs. [9–11], where the authors refer to an atom in a freely falling reference frame. Note that in Ref. [12], the results of Refs. [9–11] are generalized to accelerated and rotating reference frames; such frames are not of interest for the current study. Furthermore, we assume, throughout the paper, that local Lorentz invariance is conserved. Conceivable correction terms beyond this approximation are considered in Ref. [13]. In detail, the paper is organized as follows. In Sec. II, we consider the gravitationally and electromagnetically coupled Dirac equation, and the scaling of atomic transition frequencies, and bound-state g factors, induced by the gravitational coupling. The interrelation of quantum mechanics and Einstein's equivalence principle is being studied in Sec. III. Roughly speaking, the question is whether a non-deterministic theory (namely, quantum mechanics) can in principle be fully compatible with a fully deterministic theory (namely, general relativity), given the fact that position and momentum operators in quantum mechanics behave differently from their classical counterparts. We shall find tiny, but important corrections to the so-called $\sqrt{T}$ scaling which otherwise ensures the compatibility of the gravitationally corrected frequencies with the equivalence principle. The measurability of the higher-order gravitational corrections is discussed in Sec. IV. Conclusions are reserved for Sec. V.

II. GRAVITY AND SCALING

A. Coupled Dirac Hamiltonian

We use units with $\hbar = c = \epsilon_0 = 1$. The relativistic (gravitationally coupled) Dirac–Schwarzschild Hamiltonian is [14]

$$H_{\text{DS}} = \frac{1}{2} \left\{ \vec{\alpha} \cdot \vec{p}, \left(1 - \frac{r_s}{r}\right) \right\} + \beta m \left(1 - \frac{r_s}{2r}\right), \quad (1)$$

where $\vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix}$ and $\beta = \begin{pmatrix} \mathbb{1}_{2\times 2} & 0 \\ 0 & \mathbb{1}_{2\times 2} \end{pmatrix}$ are Dirac matrices, and m denotes the fermion (electron) mass. The (2×2) Pauli spin matrices are denoted as $\vec{\sigma}$. Hermiticity properties of this Hamiltonian are discussed in App. A 1, while a comparison of this result to other literature reference is the subject of App. A 2.

The Foldy–Wouthuysen (FW) transformed Dirac–Schwarzschild Hamiltonian has been found in Ref. [14],

$$H_{\text{FW}} = \beta \left(m + \frac{\vec{p}^2}{2m} - \frac{\vec{p}^4}{8m^3} - \beta \frac{m r_s}{2 r} - \frac{3 r_s}{8m} \left\{ \vec{p}^2, \frac{1}{r} \right\} \right. $$
$$\left. + \frac{3\pi r_s}{4m} \delta^{(3)}(\vec{r}) + \frac{3 r_s}{8m} \frac{\vec{\Sigma} \cdot \vec{L}}{r^3} \right), \quad (2\text{a})$$

which can be reformulated as

$$H_{\text{FW}} = \beta \left(m + \frac{\vec{p}^2}{2m} \right)$$
$$- \beta \left(\frac{\vec{p}^4}{8m^3} - \frac{m r_s}{2 r} - \frac{3}{16m} \left\{ \vec{\Sigma} \cdot \vec{p}, \left\{ \vec{\Sigma} \cdot \vec{p}, \frac{r_s}{r} \right\} \right\} \right), \quad (2\text{b})$$

where r_s is the Schwarzschild radius, and r is the radial variable in Eddington coordinates [15]. The latter form is obtained from the first by applying the operator identity $\{A, \{A, B\}\} = 2\{A^2, B\} - [A, [A, B]]$, for $A = \vec{\Sigma} \cdot \vec{p}$ and $B = 1/r$, where the (4×4) spin matrices are $\vec{\Sigma} = \begin{pmatrix} \vec{\sigma} & 0 \\ 0 & \vec{\sigma} \end{pmatrix}$. The generalization of the Dirac–Schwarzschild Hamiltonian (1) to the case of an additional external electromagnetic fields [denoted here as the Dirac–Schwarzschild–Coulomb (DSC) Hamiltonian] involves the replacement of the kinetic momentum operators $\vec{p}$ by the canonical momentum operators $\vec{\pi} = \vec{p} - e \vec{A}$, and the addition of the scalar potential term $e A^0$. Here, $e = -|e|$ is the physical electron charge. It reads as follows,

$$H_{\text{DSC}} = \frac{1}{2} \left\{ \left(1 - \frac{r_s}{r}\right), \vec{\alpha} \cdot \vec{\pi} \right\} + e A^0 \mathbb{1}_{4\times 4} + \beta m \left(1 - \frac{r_s}{2r}\right). \quad (3)$$

After a Foldy–Wouthuysen transformation, one obtains the Hamiltonian H_{EM} which describes the coupling to external electromagnetic fields,

$$H_{\text{EM}} = \beta \left(m + \frac{(\vec{\Sigma} \cdot \vec{\pi})^2}{2m} - \frac{(\vec{\Sigma} \cdot \vec{\pi})^4}{8m^3} \right) + e A^0 \mathbb{1}_{2\times 2}$$
$$- \beta \left(\frac{m r_s}{2 r} + \frac{3}{16m} \left\{ \vec{\Sigma} \cdot \vec{\pi}, \left\{ \vec{\Sigma} \cdot \vec{\pi}, \frac{r_s}{r} \right\} \right\} \right)$$
$$+ \left\{ 1 + \frac{r_s}{r}, \frac{e}{16m^2} \left(\vec{\nabla} \cdot \vec{E} + \vec{\Sigma} \cdot (\vec{E} \times \vec{\pi} - \vec{\pi} \times \vec{E}) \right) \right\}. \quad (4)$$

This Hamiltonian is a (4×4)-matrix, diagonal in the space of (2×2)-submatrices. The (2×2)-particle Hamiltonian H_{EM}^+ is obtained by replacing $\beta \to 1$:

$$H_{\text{EM}}^+ = m + \frac{(\vec{\sigma} \cdot \vec{\pi})^2}{2m} - \frac{(\vec{\sigma} \cdot \vec{\pi})^4}{8m^3} + e A^0$$
$$- \frac{m r_s}{2 r} - \frac{3}{16m} \left\{ \vec{\sigma} \cdot \vec{\pi}, \left\{ \vec{\sigma} \cdot \vec{\pi}, \frac{r_s}{r} \right\} \right\}$$
$$+ \left\{ 1 + \frac{r_s}{r}, \frac{e}{16m^2} \left(\vec{\nabla} \cdot \vec{E} + \vec{\sigma} \cdot (\vec{E} \times \vec{\pi} - \vec{\pi} \times \vec{E}) \right) \right\}. \quad (5)$$

The antiparticle Hamiltonian H_{EM}^- is obtained from H_{EM} by replacing $\beta \to -1$, taking into account an overall factor -1 due to the reinterpretation principle, replacing $\vec{\Sigma} \to -\vec{\sigma}$, and $\vec{p} \to -\vec{p}$, again due to reinterpretation for antiparticles. One can convince oneself that the antiparticle Hamiltonian H_{EM}^- can be obtained from the particle Hamiltonian H_{EM}^+ by the replacement $e \to -e$ (charge conjugation, hence $\vec{\pi} \to \vec{\pi}' = \vec{p} + e\vec{A}$)), while all the gravitational terms are invariant under the particle-antiparticle transformations [14], establishing the equivalence principle for anti-particles.

We now continue to work with the particle Hamiltonian (5), which can be simplified based on the identity $(\vec{\sigma} \cdot \vec{\pi})^2 = \vec{\pi}^2 - e\,\vec{\sigma} \cdot \vec{B}$, which implies that

$$
\begin{aligned}
H_{\mathrm{EM}}^+ = {} & m + \frac{\vec{\pi}^2}{2m} - \frac{\vec{\pi}^4}{8m^3} - \frac{e}{2m}\,\vec{\sigma} \cdot \vec{B} \\
& + e\,A^0 + \frac{e}{8m^3}\{\vec{\sigma} \cdot \vec{B}, \vec{\pi}^2\} - \frac{m\,r_s}{2\,r} + \frac{3\pi r_s}{4m}\delta^{(3)}(\vec{r}) \\
& - \frac{3}{8m}\left\{\vec{\pi}^2 - e\,\vec{\sigma} \cdot \vec{B}, \frac{r_s}{r}\right\} + \frac{3r_s}{8mr^3}\vec{\sigma} \cdot \vec{r} \times \vec{\pi} \\
& + \left\{1 + \frac{r_s}{r}, \frac{e}{16m^2}\left(\vec{\nabla} \cdot \vec{E} + \vec{\sigma} \cdot \vec{E} \times \vec{\pi} - \vec{\sigma} \cdot \vec{\pi} \times \vec{E}\right)\right\}.
\end{aligned}
\tag{6}
$$

We should note that related calculations have recently been considered in other contexts [16–18], with an important clarifying remark given in the text following Eq. (7.33) of Ref. [18] (see also Ref. [19]).

We now discuss a general metric for weak gravitational fields and gravitational red shifts. For inspiration, we start with the Schwarzschild metric [20] in isotropic form (Sec. 43 of Chap. 3 of Ref. [15]),

$$
\mathrm{d}s^2 = \left(\frac{1 - r_s/(4r)}{1 + r_s/(4r)}\right)^2 \mathrm{d}t^2 - \left(1 + \frac{r_s}{4r}\right)^4 \mathrm{d}\vec{r}^2.
$$

This metric can be expanded to first order in the potential $\Phi(\vec{r}) = -GM/r$, where M is the mass of the central gravitational object, and generalized to arbitrary (weak) gravitational potentials Φ,

$$
\begin{aligned}
\mathrm{d}s^2 &= \left(1 - \frac{r_s}{r}\right)\mathrm{d}t^2 - \left(1 + \frac{r_s}{r}\right)\mathrm{d}\vec{r}^2 \\
&= (1 + 2\Phi)\,\mathrm{d}t^2 - (1 - 2\Phi)\,\mathrm{d}\vec{r}^2 \\
&= T\,\mathrm{d}t^2 - H\,\mathrm{d}\vec{r}^2 = \overline{g}_{\mu\nu}\,\mathrm{d}x^\mu\,\mathrm{d}x^\nu.
\end{aligned}
\tag{7}
$$

Here, $\overline{g}_{\mu\nu} = \mathrm{diag}(T, -H, -H, -H)$ is the curved-space metric, while we reserve the symbol $\widetilde{g}_{\mu\nu}$ for the metric of free space [14]. In the following, we use the symbols T and H for the case of a general gravitational potential Φ.

In a metric of the form (7) (see Refs. [21–23]) one has for light, which travels on a zero geodesic with $\mathrm{d}s^2 = 0$,

$$
\left|\frac{\mathrm{d}\vec{r}}{\mathrm{d}t}\right|^2 = \frac{1 + 2\Phi}{1 - 2\Phi} = \frac{T}{H} \approx 1 + 4\Phi.
\tag{8}
$$

We thus generalize (8) to general gravitational fields. The Shapiro time delay [24–28] is consistent with an effective

speed of light, of the form $c_{\mathrm{eff}} = 1 + 2\Phi = \sqrt{T/H}$, to first order in the gravitational potential. This implies that in electrodynamics, we must assign a slight gravitational dependence to the vacuum permittivity ϵ and vacuum permeability μ, so that

$$
c_{\mathrm{eff}}^2 = \frac{1}{\epsilon\,\mu} = \frac{T}{H}, \qquad \epsilon = \mu = \sqrt{\frac{H}{T}},
\tag{9}
$$

consistent with Eq. (4) of Ref. [2].

B. Gravity and atomic transitions

The generalization of the Hamiltonian (3) to a general gravitational potential Φ can be found by realizing that the derivation, outlined in Ref. [14], goes through for a general metric of the form given in Eq. (7). The Hamiltonian reads as

$$
H_{\mathrm{DSC}} = \frac{1}{2}\{1 + 2\Phi, \vec{\alpha} \cdot \vec{\pi}\} + e\,A^0 + \beta m\,(1 + \Phi)
\tag{10}
$$

$$
= \frac{1}{2}\left\{\sqrt{\frac{T}{H}}, \vec{\alpha} \cdot \vec{\pi}\right\} + e\,A^0 + \beta m\sqrt{T}.
\tag{11}
$$

If we ignore commutators of the gravitational fields and the momentum operators, then we may approximate

$$
H_{\mathrm{DSC}} \approx \sqrt{\frac{T}{H}}\,\vec{\alpha} \cdot \vec{\pi} + \sqrt{T}\,\beta\,m + e\,A^0.
\tag{12}
$$

We here confirm the result given in Eq. (14) of Ref. [2], and show that anticommutators are needed in order to turn the Hamiltonian into a manifestly Hermitian entity. The approximation (12) is valid if we assume that T and H remain constant to very good approximation, over the distance scales relevant to the described quantum mechanical phenomena.

We consider the Hamiltonian (12) for the case $\vec{A} = \vec{0}$, and $e\,A^0 = -Ze^2/(4\pi\epsilon|\vec{\rho}|)$, where $|\vec{\rho}|$ is the distance to the atomic nucleus. In this case, the Hamiltonian becomes

$$
H_{\mathrm{DSC}} = \sqrt{\frac{T}{H}}\,\vec{\alpha} \cdot \vec{p} + \sqrt{T}\,\beta\,m - \frac{Ze^2}{4\pi\epsilon|\vec{\rho}|},
\tag{13}
$$

where the subscripts refer to Dirac, Schwarzschild and Coulomb (DSC). The energy eigenvalue equation is

$$
H_{\mathrm{DSC}}\,\psi = E\,\psi.
\tag{14}
$$

With Ref. [2], we now perform the following scaling,

$$
m = \bar{m}\,\frac{1}{\sqrt{H}}, \qquad e^2 = \bar{e}^2\sqrt{\frac{T}{H}}\,\epsilon, \qquad E = \bar{E}\sqrt{\frac{T}{H}},
\tag{15}
$$

which turns the eigenvalue problem (13) into

$$
\left(\vec{\alpha} \cdot \vec{p} + \beta\,\bar{m} - \frac{Z\bar{e}^2}{4\pi|\vec{\rho}|}\right)\psi = \bar{E}\,\psi.
\tag{16}
$$

The energy can be given in terms of the scaled function $f(n, J, Z\bar{\alpha})$ which has been introduced by Sapirstein and Yennie in Ref. [29],

$$\bar{E} = \bar{m}\, f(n, J, Z\bar{\alpha})\,, \tag{17a}$$

$$f(n, J, Z\bar{\alpha}) = \left(1 + \frac{(Z\bar{\alpha})^2}{[n_r + \sqrt{(J+1/2)^2 - (Z\bar{\alpha})^2}]^2}\right)^{-\frac{1}{2}}, \tag{17b}$$

where $n_r = n - J - 1/2$ is the "reduced" principal quantum number. The electron's orbital angular momentum quantum number is ℓ, while its total angular momentum is J. Finally, the gravitationally "modified" (as it turns out, invariant) fine-structure constant is

$$\bar{\alpha} = \frac{\bar{e}^2}{4\pi} = \sqrt{\frac{H}{T}}\,\frac{e^2}{4\pi\epsilon} = \sqrt{\frac{H}{T}}\,\frac{e^2}{4\pi}\sqrt{\frac{T}{H}} = \frac{e^2}{4\pi} = \alpha\,. \tag{17c}$$

The position-independence of the fine-structure constant has been verified experimentally, in a dedicated experiment described in Ref. [30]. We should notice that experimental possibilities to search for a temporal as well as spatial variation of the fine-structure constant have since dramatically improved in accuracy [31–34]. The scaling of the bound-state energy is found as

$$E = \sqrt{\frac{T}{H}}\,\bar{E} = \sqrt{\frac{T}{H}}\,\bar{m}\, f(n, J, Z\alpha) = \sqrt{T}\, m\, f(n, J, Z\alpha)\,, \tag{18}$$

valid for both main-structure (change in the principal quantum number) as well as fine-structure transitions.

C. Gravity and g factor

We start from Eq. (12), but this time we include the static vector potential $\vec{A} = \frac{1}{2}(\vec{B} \times \vec{r})$, which describes a constant $\vec{B}$ field. Hence, H_{DSC} attains the form

$$H_{\mathrm{DSC}} = \sqrt{\frac{T}{H}}\,\vec{\alpha} \cdot (\vec{p} - e\,\vec{A}) + \sqrt{T}\,\beta\, m + e\, A^0\,. \tag{19}$$

Taking into account that $\vec{A} = \frac{1}{2}(\vec{B} \times \vec{r})$, one can write the Hamiltonian H_M which describes the magnetic coupling of the electron to the external field as

$$H_M = -\sqrt{\frac{T}{H}}\, e\, \vec{\alpha} \cdot \vec{A} = -\sqrt{\frac{T}{H}}\,\frac{e}{2}\, \vec{\alpha} \cdot (\vec{B} \times \vec{r})\,. \tag{20}$$

Canonically, one assumes that $\vec{B}$ is directed along the z axis [35]. The Landé g factor (written as g_J) and the expectation value for a hydrogenic state in a homogeneous $\vec{B}$ field can be expressed as

$$\langle H_M \rangle = -g_J\,\frac{e}{2m}\, |\vec{B}|\, \mu_J\,, \tag{21}$$

where μ_J is the projection of the electron's total angular momentum (angular+spin) onto the axis of the $\vec{B}$

field. The expectation value in Eq. (21) is to be taken in an eigenstate of the unperturbed problem, i.e., in a (gravitationally modified) Dirac–Coulomb eigenstate of the Hamiltonian (13).

Let us therefore consider the Hamiltonian (19) under the same scaling as the one used in Eq. (15). The eigenvalue problem transforms into

$$\left(\vec{\alpha} \cdot (\vec{p} - \bar{e}\,\vec{A}) + \beta\,\bar{m} - \frac{Z\bar{e}^2}{4\pi|\vec{x}|}\right)\psi = \bar{E}\,\psi\,. \tag{22}$$

For the magnetic-field coupling Hamiltonian, written in terms of the scaled variables,

$$\bar{H}_M = -\frac{\bar{e}}{2}\,\vec{\alpha} \cdot (\vec{B} \times \vec{r})\,, \tag{23}$$

we therefore have the following relation, which holds in view of the analogy with the unperturbed Dirac problem (see Ref. [35]):

$$\langle \bar{H}_M \rangle = -\bar{g}_J\,\frac{\bar{e}}{2\bar{m}}\, |\vec{B}|\, \mu_J\,, \tag{24}$$

$$\bar{g}_J = \frac{\varkappa}{J(J+1)}\left(\varkappa\,\frac{\bar{E}}{\bar{m}} - \frac{1}{2}\right)$$

$$= \frac{\varkappa}{J(J+1)}\left(\varkappa\, f(n, J, Z\alpha) - \frac{1}{2}\right)\,. \tag{25}$$

Here, $\varkappa$ is the Dirac angular quantum number, which is given as $\varkappa = (-1)^{J+\ell+1/2}\left(J + \frac{1}{2}\right)$. A comparison of the Hamiltonian H_M given in Eq. (20) to the Hamiltonian $\bar{H}_M$ given in Eq. (23) reveals that $\langle H_M \rangle = -(T/H)^{1/2}\langle \bar{H}_M \rangle$ so that, in view of Eq. (21),

$$g_J = \frac{\sqrt{T}}{H}\,\bar{g}_J = \frac{\sqrt{T}}{H}\,\frac{\varkappa}{J(J+1)}\left(\varkappa\, f(n, J, Z\alpha) - \frac{1}{2}\right)\,. \tag{26}$$

For the ground state, one has with $\varkappa = -1$ and $J = 1/2$,

$$g_J = \frac{\sqrt{T}}{H}\,\frac{4}{3}\left(\sqrt{1 - (Z\alpha)^2} + \frac{1}{2}\right)\,. \tag{27}$$

The free-electron g factor is obtained from this expression, in the limit $Z\alpha \to 0$, and is equal to $g_S = 2\sqrt{T}/H$. This result is compatible with Eq. (6), under an isolation of the terms proportional to $\vec{\sigma} \cdot \vec{B}$ in the latter formula.

At this stage, we have clarified the gravitational corrections to the *non-anomalous* part of the electron's magnetic moment. For the anomalous part, we need to consider the generalized Dirac equation, which necessitates the introduction of form factors. We recall that in flat space, the electromagnetically coupled Dirac equation reads as $[\widetilde{\gamma}^\mu(p_\mu - e\,A_\mu) - m]\,\psi = 0$, where the $\widetilde{\gamma}^\mu$ are Dirac γ matrices which fulfill the anti-commutator relations $\{\widetilde{\gamma}^\mu, \widetilde{\gamma}^\nu\} = 2\widetilde{g}^{\mu\nu} = \mathrm{diag}(1, -1, -1, -1)$. In order to describe the anomalous magnetic moment, one replaces the Dirac γ matrices by a form-factor expression (see Chap. 7 of Ref. [36]),

$$\widetilde{\gamma}^\mu \to \widetilde{\gamma}^\mu\, F_1(q^2) + \frac{\mathrm{i}\widetilde{\sigma}^{\mu\nu}\, q_\nu}{2m}\, F_2(q^2)\,, \tag{28}$$

where the spin matrices are given as $\widetilde{\sigma}^{\mu\nu} = \frac{i}{2}[\widetilde{\gamma}^\mu, \widetilde{\gamma}^\nu]$. The replacement leads to the modified Dirac (MD) Hamiltonian [37],

$$H_{\mathrm{MD}} = \vec{\alpha} \cdot \left[\vec{p} - e\, F_1(\vec{\nabla}^2)\, \vec{A}\right] + \beta\, m + \mathrm{e}\, F_1(\vec{\nabla}^2)\, A^0$$
$$+ F_2(\vec{\nabla}^2) \frac{e}{2\,m} \left(\mathrm{i}\,\vec{\gamma}\cdot\vec{E} - \beta\,\vec{\sigma}\cdot\vec{B}\right). \qquad (29)$$

In the following, we shall approximate

$$F_1(q^2) \approx F_1(0) = 1\,, \qquad F_2(q^2) \approx F_2(0) = \kappa \approx \frac{\alpha}{2\pi}\,, \qquad (30)$$

and set the external electric field equal to zero, $\vec{E} = \vec{0}$. [We remember that, if we set $\vec{E}$ equal to the Coulomb electric field, the corresponding term in Eq. (29) describes the anomalous magnetic-moment correction to the Lamb shift.] Here, κ describes the anomalous magnetic moment correction to the electron's spin g factor, and is approximated by the Schwinger term $\alpha/(2\pi)$.

With the approximations outlined in Eq. (30), the Hamiltonian (29) becomes

$$H_{\mathrm{MD}} = \vec{\alpha}\cdot\left(\vec{p} - e\,\vec{A}\right) + \beta\,m + e\,A^0 - \kappa\,\frac{e}{2\,m}\,\beta\,\vec{\sigma}\cdot\vec{B}\,. \quad (31)$$

We carry out a replacement analogous to Eq. (28) in curved space,

$$\overline{\gamma}^\mu \to \overline{\gamma}^\mu\, F_1(q^2) + \frac{\mathrm{i}\overline{\sigma}^{\mu\nu}\, q_\nu}{2m}\, F_2(q^2)\,, \qquad \{\overline{\gamma}^\mu, \overline{\gamma}^\nu\} = 2\overline{g}^{\mu\nu}\,, \qquad (32)$$

where $\overline{g}^{\mu\nu} = \mathrm{diag}(1/T, -1/H, -1/H, -1/H)$ is the inverse of the metric $\overline{g}_{\mu\nu}$ given in Eq. (7). The curved-space Dirac spin matrices $\overline{\sigma}^{\mu\nu} = \frac{1}{2}[\overline{\gamma}^\mu, \overline{\gamma}^\nu]$ fulfill $\overline{\sigma}^{\mu\nu} = \widetilde{\sigma}^{\mu\nu}/H$, and the gravitational modification of Eq. (31) reads as

$$H = \sqrt{\frac{T}{H}}\,\vec{\alpha}\cdot(\vec{p} - e\,\vec{A}) + \sqrt{T}\,\beta\,m + e\,A^0 - \frac{\sqrt{T}}{H}\,\kappa\,\frac{e}{2\,m}\,\beta\,\vec{\sigma}\cdot\vec{B}\,. \quad (33)$$

The gravitationally modified electron g_J factor (for the $1S$ state) thus is, in view of Eq. (27) and Eq. (33),

$$g_J = \frac{\sqrt{T}}{H}\,\frac{4}{3}\left(\sqrt{1 - (Z\alpha)^2} + \frac{1}{2} + \frac{3}{2}\,\kappa\right), \qquad (34)$$

where the free-electron term is obtained in the limit $Z\alpha \to 0$. The scaling with $\sqrt{T}/H$ is thus established as a universal scaling of the free-electron and bound-electron g factors, including the anomalous-magnetic-moment correction.

D. Equivalence principle and g factor

According to Eq. (18), atomic transition frequencies receive a gravitational correction proportional to $\sqrt{T}$, while according to Eq. (34), the $1S$ electron g factor receives a correction proportional to $\sqrt{T}/H$. The prefactor $\sqrt{T}$

in Eq. (18) describes the transition from coordinate time to laboratory time, This is evident from the metric (7), $\mathrm{d}s^2 = T\,\mathrm{d}t^2 - H\,\mathrm{d}\vec{r}^2 = \mathrm{d}\tau^2$, where $\mathrm{d}\tau^2$ measures the (square of the) time interval in the local Lorentz frame. We can convert the time derivative operator from coordinate time to the time elapsed in the local Lorentz frame,

$$\sqrt{T}\,\mathrm{d}t = \mathrm{d}\tau\,, \qquad \mathrm{i}\frac{\partial}{\partial\tau} = \frac{\mathrm{i}}{\sqrt{T}}\,\frac{\partial}{\partial t}\,. \qquad (35)$$

The energy (18) is formulated with respect to the coordinate time, and so, the energy in the laboratory can be obtained by dividing the energy E given in Eq. (18) by a factor $1/\sqrt{T}$, and one obtains the laboratory atomic energy levels as being given by the expression $m\,f(n, J, Z\alpha)$.

Let us put this statement into the context of the weak and strong forms of the equivalence principle. The "weak equivalence principle" (WEP) asserts the proportionality of "mass" ("inertial mass") and "weight" (which enters the gravitational force law). The Einstein equivalence principle (EEP) states that *(i)* WEP is valid, *(ii)* the outcome of any local non-gravitational experiment is independent of the velocity of the freely-falling reference frame in which it is performed (local Lorentz invariance, LLI), and *(iii)* the outcome of any local non-gravitational experiment is independent of where and when in the universe it is performed (local position invariance, LPI).

The scaling with $\sqrt{T}/H$ of the electron's g factor, in coordinate time, taken at face value, would imply a scaling with $1/H$ in the local Lorentz frame of each laboratory, after dividing out the factor $\sqrt{T}$. This would make the outcome of a non-gravitational experiment (the measurement of the electron's g factor) dependent on the position, limit the validity principle of local position invariance, and, hence, the EEP.

In order to resolve the problem, we note that we have assumed, in our derivation, that the $\vec{A}$ field is given in terms of the components of the covariant basis,

$$\vec{A} = A^i\,\vec{e}_i\,, \qquad \vec{e}_i\cdot\vec{e}_j = H\,\delta_{ij}\,. \qquad (36)$$

Latin indices indicate spatial components ($i, j, k, \ldots = 1, 2, 3$). However, the "Cartesian" unit vectors (index c) which span the local Lorentz frame are

$$\hat{e}_i = \frac{1}{\sqrt{H}}\,\vec{e}_i\,, \qquad \hat{e}_i\cdot\hat{e}_j = \delta_{ij}\,. \qquad (37)$$

Let x^i denote the components of the position vector $\vec{r}$ in the basis spanned by the $\vec{e}_i$, while the components x_c^j are relevant to the basis spanned by the $\hat{e}_i$. Then,

$$x_c^j = \sqrt{H}\,x^j\,, \qquad A_c^i = \sqrt{H}\,A^j\,. \qquad (38)$$

We denote by ϵ^{ijk} the totally antisymmetric Levi-Cività tensor (under the normalization $\epsilon^{123} = 1$). Then, we have

$$\vec{A} = \frac{1}{2}\,\vec{B}_c \times \vec{r}_c = \frac{1}{2}\,\hat{e}_i\,\epsilon^{ijk}\,B^j\,x_c^k\,, \qquad (39)$$

which is the appropriate vector potential for a magnetic field with "Cartesian" components B_c^i, measured in the local Lorentz frame. The curl of $\vec{A}$ enters into Eq. (27); it is calculated with momentum operators $\vec{p} = -i\vec{\nabla}$ where $\nabla^k = -i\partial/\partial x^k$, and hence,

$$B^i = \epsilon^{ijk} \frac{\partial}{\partial x^j} A^k = \frac{1}{2}\,\epsilon^{ijk} \frac{\partial}{\partial x^j} \epsilon^{k\ell m} B_c^\ell \sqrt{H}\, x^m = \sqrt{H}\, B_c^i\,. \tag{40}$$

For the vector $\vec{B}$, this means that

$$\vec{B} = B^i\,\vec{e}_i = (\sqrt{H}\, B_c^i)\,(\sqrt{H}\hat{e}_i) = H\, B_c^i\,\hat{e}_i\,. \tag{41}$$

Thus, the ith component of $\vec{B}$, written in our basis, is equal to H times the B field measured by a local observer, in their own Lorentz frame. This implies that, when normalized to the local B field, spin-flip frequencies transform with a factor $\sqrt{T}$, not $\sqrt{T}/H$, respecting the equivalence principle. We note that the same factor H is obtained in Ref. [2] for the transformation of the hyperfine-structure generating B field of a nucleus, from global coordinates to the local Lorentz frame; however, the derivation proceeds in a completely different way [see Eqs. (32)—(34) of Ref. [2]]. One notes that the restoration of the $\sqrt{T}$ scaling actually is absolutely crucial for the validity of the current adjustment of the fundamental constants [38].

III. QUANTUM MECHANICS AND EQUIVALENCE PRINCIPLE

A. Leading order and $\sqrt{T}$ scaling

We recall, from Sec. II A, that relatively weak gravitational fields give rise to a metric

$$\mathrm{d}s^2 = T\,\mathrm{d}t^2 - H\,\mathrm{d}\vec{r}^2\,, \tag{42}$$
$$T = 1 + 2\,\Phi\,, \qquad H = 1 - 2\,\Phi\,, \tag{43}$$

where Φ is the gravitational potential. Hence, if, in global coordinates, an energy goes as

$$E = \sqrt{T}\, E_c\,, \tag{44}$$

where E_c is the energy measured in a local, Cartesian Lorentz frame, then this effect is physically unobservable if the experiment is carried out locally, because the time derivative operator $\mathrm{d}/\mathrm{d}\tau$ with respect to the proper times has the eigenvalue

$$i\frac{\partial}{\partial\tau}\psi = \frac{i}{\sqrt{T}}\frac{\partial}{\partial t}\psi = \frac{E}{\sqrt{T}}\,\psi = E_c\,\psi\,. \tag{45}$$

All factors that go with $\sqrt{T}$ are unobservable since they can be absorbed in going to local, Cartesian coordinates.

It is highly instructive (and non-obvious) to convince oneself that the leading kinetic terms in the Dirac–Schwarzschild Hamiltonian (2) follow the $\sqrt{T}$ scaling.

This observation, in particular, implies that the gravitational Breit term

$$-\frac{3r_s}{8m}\left\{\vec{p}^2, \frac{1}{r}\right\}\,, \tag{46}$$

does not lead to an observable gravitational shift. At face value, one could otherwise assume that it induces a numerically large, $(1/n^2)$-dependent shift on hydrogen energy levels (where n is the principle quantum number), because the operator $1/r$, where r is the radial variable with respect to the gravitational center (e.g., the Earth), commutes, to an excellent approximation, with the momentum operator of the electron, and in fact, the difference of the operator $(1/r)\,\vec{p}^2$ and the anti-commutator $(1/2)\{r^{-1}, \vec{p}^2\}$ can be ignored altogether on the level of first-order perturbation theory. This is because one has $\langle\psi^+|r^{-1}\,\vec{p}^2|\psi\rangle = \frac{1}{2}\langle\psi^+|\{r^{-1}, \vec{p}^2\}|\psi\rangle$ for any reference state ψ. (The Hermitian adjoint, as opposed to the Dirac adjoint $\overline{\psi}$, is denoted as ψ^+.)

The kinetic terms from Eq. (2) read as follows,

$$H_{\mathrm{kin}} = m - \frac{r_s}{2\,r}\,m + \frac{\vec{p}^2}{2m} - \frac{3r_s}{8m}\left\{\vec{p}^2, \frac{1}{r}\right\}$$
$$\to m\left(1 - \frac{r_s}{2\,r}\right) + \left(1 - \frac{3}{2}\frac{r_s}{r}\right)\frac{\vec{p}^2}{2m}\,, \tag{47}$$

where we ignore the commutator and specialize the Hamiltonian to particles as opposed to anti-particles (i.e., we replace the Dirac β matrix by the unit matrix). For a central gravitational field, one has

$$T = 1 + 2\,\Phi = 1 - \frac{r_s}{r}\,, \qquad H = 1 - 2\,\Phi = 1 + \frac{r_s}{r}\,, \tag{48}$$

where $r_s = 2GM$. To first order in r_s, we can thus reformulate the gravitational dependence as follows,

$$H_{\mathrm{kin}} \sim \sqrt{T}\,m + \frac{\sqrt{T}}{H}\,\frac{\vec{p}^2}{2m} = \sqrt{T}\left(m + \frac{\vec{p}_c^2}{2m}\right)\,. \tag{49}$$

Here, we have transformed the momentum operator to local Cartesian coordinates, as follows,

$$p_c^j = -i\frac{\partial}{\partial x_c^j} = -i\frac{1}{\sqrt{H}}\frac{\partial}{\partial x^j} = \frac{1}{\sqrt{H}}p^j\,. \tag{50}$$

This implies that the gravitational Breit term does not contribute to an observable gravitational energy difference among atomic energy levels.

The Schrödinger Hamiltonian is completed by adding the Coulomb term

$$H_{\mathrm{coul}} = -\frac{Ze^2}{4\pi\epsilon\,\rho} = -\sqrt{\frac{T}{H}}\frac{Ze^2}{4\pi\,\rho} = -\sqrt{T}\frac{Ze^2}{4\pi\,\rho_c}\,, \tag{51}$$

where $\epsilon = \sqrt{H/T}$ is the gravitationally modified vacuum permittivity, $\rho = |\vec{\rho}|$ is the distance from the atomic nucleus, and $\rho_c = \sqrt{H}\,\rho$. It is instructive to compare the scaling outlined above to the relativistic formalism used in Sec. II B.

Adding the kinetic term from Eq. (49) and the Coulomb term given in Eq. (51), and subtracting the rest mass term, which is irrelevant for atomic transitions, one obtains the gravitationally modified Schrödinger Hamiltonian

$$H_S = \sqrt{T} \left(\frac{\vec{p}_c^2}{2m} - \frac{Z\alpha}{\rho_c} \right), \tag{52}$$

where $\alpha = e^2/(4\pi)$ is the fine-structure constant.

Interestingly, one could hypothesize about the physical consequences of the gravitational Breit term for high-precision atomic clocks [39, 40], which currently operate on a precision level of 10^{-18} or better, if the Breit term were to contribute to an observable energy difference and the Penrose conjecture were to hold in the renormalized form (B12). In this case, the renormalized gravitational energy difference (B12) among the different atomic levels involved in the atomic clock transition, in view of $r_s/r \sim 10^{-9}$ for the Earth, would result in gravitational collapse of the atomic state on a relative frequency level of 10^{-9}, which is the ratio of the gravitational Breit term to the leading nonrelativistic kinetic term in the atomic Hamiltonian $[\vec{p}^2/(2m)]$. This would prevent continuous interrogation of the atomic clock and thus make the experiments [39, 40] (and also the clock comparison, see Refs. [33, 34]) infeasible, because the hypothetical gravitational effect would limit the clock precision to a level of 10^{-9}. Indeed, the Yb$^+$ clock transitions described in Refs. [39, 40] involve atomic transitions with a change in the principal quantum number, and thus, the expectation value of the $\vec{p}^2$ operator becomes state dependent. This hypothetical consideration is included here in order to illustrate that care is required in the treatment of the gravitational terms; one can easily be fooled into obtaining excessively large effects if one does not carry through the analysis correctly (see also Refs. [3–8]).

B. Higher orders and broken $\sqrt{T}$ scaling

1. Overview

From this consideration, it becomes obvious that only gravitational effects on atomic transitions which go beyond the "common prefactor" $\sqrt{T}$ [see Eq. (44)], could lead to observable consequences (competing effects are discussed in Apps. B and C). We therefore attempt, for a central gravitational field, to analyze the leading effects which could contribute to quantum limitations of the EEP, in view of a breaking of the $\sqrt{T}$ scaling. There are three competing effects to compare and to analyze, *(i)* a first-order plain gravitational shift, obtained by expanding the Newtonian gravitational potential over the size of the atom, *(ii)* a second-order gravitational shift, again obtained on the basis of the Newtonian gravitational potential, *(iii)* commutator-induced shifts due to higher-order operators in the Dirac–Schwarzschild–

Coulomb Hamiltonian. A fourth effect, quite surprisingly, exists for diatomic molecules.

2. Gravitation and size of the atom

We denote by $\vec{R}$ the coordinate of the atomic nucleus with respect to the gravitational center, and by $\vec{\rho}$ the distance of the electron from the atomic nucleus. Then, if $\vec{\rho}$ denotes the vector from the gravitational center to the atomic electron, one has

$$V = -\frac{m \, r_s}{2 \, r} = m \, \Phi = -\frac{GmM}{r},$$
$$\frac{1}{r} = \frac{1}{|\vec{R} + \vec{\rho}|} = \frac{1}{R} - \frac{\vec{R} \cdot \vec{\rho}}{R^3} + \frac{3 \, (\vec{R} \cdot \vec{\rho})^2 - R^2 \, \rho^2}{2 \, R^5}$$
$$- \vec{\rho}^2 \, 4\pi \delta^{(3)}(\vec{R}) + \mathcal{O}(\rho^3), \tag{53}$$

where the Dirac-δ term can be ignored if the atom is sufficiently displaced from the point $\vec{R} = \vec{0}$, which can be safely assumed to be the case for practically important applications. One writes

$$V = V^{[0]} + V^{[1]} + V^{[2]}, \tag{54a}$$

$$V^{[0]} = -\frac{GmM}{R}, \tag{54b}$$

$$V^{[1]} = GmM \frac{\vec{R} \cdot \vec{\rho}}{R^3} \propto \Phi^2, \tag{54c}$$

$$V^{[2]} = -\frac{GmM}{2} \frac{3 \, (\hat{R} \cdot \vec{\rho})^2 - \vec{\rho}^2}{R^3} \propto \Phi^3. \tag{54d}$$

The term $V^{[0]}$ is absorbed in the scaling factor $\sqrt{T}$ which multiplies the mass term in $H_{\rm kin}$, as given in Eqs. (47) and (49). The expectation value of the leading correction $V^{[1]}$ vanishes on any atomic energy eigenstate, due to parity. However, as shown in the following, nontrivial effects can be expected for diatomic molecules. The effect scales as R^{-2} and thus is proportional to Φ^2, where $\Phi = -GM/R$ is the gravitational potential.

The first nonvanishing correction is due to the quadrupole term $V^{[2]}$, which scales with Φ^3. For an atom, $|\vec{\rho}| \sim a_0$ where a_0 is the Bohr radius. The induced shift is of order

$$\delta E^{(i)} = \langle V^{[2]} \rangle \sim \frac{G \, m \, M \, a_0^2}{R^3} = 8.99 \times 10^{-40} \, E_h, \tag{55}$$

where $E_h = \alpha^2 mc^2 \approx 27.2 \, {\rm eV}$ is the Hartree energy and the shift has been evaluated for the Earth ($M \to M_\oplus$, $R \to R_\oplus$). For other systems, see Table I. The effect is of first order in the gravitational potential and addresses point *(i)* listed above.

For completeness, we should point out that we use the following parameters: the Earth mass $M_+ = 5.974 \times 10^{24} \, {\rm kg}$, the Sun's mass $M_\odot = 1.989 \times 10^{30} \, {\rm kg}$, a typical white dwarf mass of $M_{\rm wd} = 1.4 \, M_\odot$, with a radius of $R_{\rm wd}$ being equal to the radius of the Earth, $R_{\rm wd} = R_\oplus =$

TABLE I. Order-of-magnitude estimate (rows 1, 2, 4, 5) and numerical values (remaining rows) of the quantum limitations of the EEP, for the effects $\delta E^{(i)}$, $\delta E^{(ii)}$, $\delta E^{(iii)}$ $\delta E^{(iv)}$ as described in the text [see Eqs. (55), (56), and (62)]. The shifts are evaluated for astrophysical objects of interest. The column labeled "Earth due to Sun" is included because, despite the large distance from the Earth to the Sun (about 146×10^9 m), the large solar mass of about $M_\odot = 1.989 \times 10^{30}$ kg could be assumed to lead to large gravitational shifts. However, because of the suppression of the gravitational effects by R^{-n}, with $n \geq 2$, the effects due to the Sun are numerically suppressed.

Effect	Earth	Earth Due to Sun	White Dwarf	Neutron Star
$\delta E^{(i)}/E_h$ [Eq. (55), estimate]	8.99×10^{-40}	2.50×10^{-47}	4.19×10^{-34}	2.72×10^{-26}
$\delta E^{(ii)}/E_h$ [Eq. (56), estimate]	1.17×10^{-44}	4.74×10^{-51}	2.55×10^{-33}	1.06×10^{-22}
$\delta E^{(ii)}/E_h$ [Eq. (60), hydrogen $2S$]	1.77×10^{-37}	7.13×10^{-44}	3.84×10^{-26}	1.59×10^{-15}
$\delta E^{(iii)}/E_h$ [Eq. (62), estimate]	4.79×10^{-44}	1.33×10^{-51}	2.23×10^{-38}	1.45×10^{-30}
$\delta E^{(iv)}/E_h$ [Eq. (68), estimate]	1.99×10^{-19}	1.26×10^{-22}	9.28×10^{-14}	1.89×10^{-8}
$\delta E^{(iv)}/E_h$ [Eq. (69), HF]	3.17×10^{-20}	2.02×10^{-23}	1.48×10^{-14}	3.01×10^{-9}
$\delta E^{(iv)}/E_h$ [Eq. (69), N_2]	8.89×10^{-19}	5.65×10^{-22}	4.14×10^{-13}	8.43×10^{-8}
$\delta E^{(iv)}/E_h$ [Eq. (69), Cl_2]	-1.32×10^{-18}	-8.41×10^{-22}	-6.17×10^{-13}	-1.25×10^{-7}

6.378×10^6 m, as well as a neutron star of mass $M_{\rm ns} = 2.8\, M_\odot$, and a radius of $R_{\rm ns} = 20$ km.

The second-order perturbation due to $V^{[1]}$, on an atomic state, can be expressed as

$$\delta E^{(ii)} = \left\langle V^{[1]} \frac{1}{(E-H)'} V^{[1]} \right\rangle$$
$$\sim \frac{G^2\, m\, M^2\, a_0^2}{\alpha^2\, c^2\, R^4} \sim 1.17 \times 10^{-44}\, E_h \,, \qquad (56)$$

where $[1/(E-H)']$ is the atomic reduced Green function, and the numerical value is obtained for a point on the surface of the Earth. We here assume that there are no quasi-degenerate levels which are displaced from the atomic reference state by an energy shift which is far less than a typical atomic energy level difference of $E - E_n \sim E_h \equiv \alpha^2\, m\, c^2$, where E is the reference-state energy, and E_n is the virtual-state energy. The Hartree energy is denoted as $E_h \approx 27.2$ eV. In the absence of such quasi-degenerate levels, the order-of-magnitude estimate $[1/(E-H)'] \sim 1/E_h$ is valid. One may consult Table I for numerical estimates of $\delta E^{(ii)}$ for other astrophysical systems. We have thus addressed point *(ii)* listed above.

A remark is in order. The estimate given above in Eq. (56) should be taken with a grain of salt, in part, because quasi-degenerate levels can otherwise alter the predictions quite drastically. E.g., for the hydrogen $1S$–$2S$ transition [31, 41], the $2P_{1/2}$ levels are displaced from the $2S$ state only by the Lamb shift, while the $2P_{3/2}$ levels are separated by the fine structure. With the following data [see Eq. (42) of [42]] for the $2S$–$2P_{1/2}$ Lamb shift energy interval $\mathcal{L}$ and the $2P_{3/2}$–$2P_{1/2}$ fine-structure interval $\mathcal{F}$,

$$\mathcal{L} = 1.61 \times 10^{-7}\, E_h \,, \qquad (57)$$
$$\mathcal{F} = 1.67 \times 10^{-6}\, E_h \,, \qquad (58)$$

we have [see Eq. (17) of [42]],

$$\left\langle z \frac{1}{(E-H)'} z \right\rangle = 3\, a_0^2 \left(\frac{1}{\mathcal{L}} - \frac{2}{\mathcal{F}} \right) . \qquad (59)$$

The estimates in the second row of Table I should thus be multiplied by a factor

$$3 \left(\frac{1}{\mathcal{L}} - \frac{2}{\mathcal{F}} \right) = 1.504 \times 10^7 \,, \qquad (60)$$

to obtain numbers for the hydrogen $2S$ state. The modified estimates, adjusted for the hydrogen $2S$ state, are given in the third row of Table I.

3. Fokker precession term

The Fokker precession term

$$H_{\rm FP} = \frac{3 r_s}{8m} \frac{\vec{\sigma} \cdot \vec{L}}{R^3} \qquad (61)$$

in the Dirac–Schwarzschild–Coulomb Hamiltonian (2) is proportional to $|\Phi|^3$, where $\Phi = -GM/r$ is the gravitational potential. This term is generated by the difference of the exact Foldy–Wouthuysen Hamiltonian, given in Eq. (2), and the approximate form (13), due to commutators of the momentum operators and the gravitational potential, while we had obtained the approximate form (13) by *ignoring* the commutators. It thus goes beyond the terms considered in Ref. [2], which exhibit the universal scaling with $\sqrt{T} = \sqrt{1 + 2\Phi}$, and leads to an energy shift of the order of

$$\delta E^{(iii)} = \langle H_{\rm FP} \rangle \sim \frac{\hbar^2 G M}{m R^3 c^2} = 4.79 \times 10^{-44}\, E_h \,. \qquad (62)$$

The numerical estimate is obtained for the Earth ($M = M_\oplus$ and $R = R_\oplus$). Again, one may consult Table I for numerical estimates of $\delta E^{(iii)}$ for other astrophysical systems. We have addressed point *(iii)* listed above.

TABLE II. Order-of-magnitude estimate (rows 1, 2, 4, 5) and numerical values (remaining rows) for the $C_n(M)$ coefficients for those gravitational shifts of atomic transitions which break the $\sqrt{T}$ scaling, as defined in Eq. (73).

Effect	Earth	Earth Due to Sun	White Dwarf	Neutron Star
$C_3(M)$ for $\delta E^{(i)}$ $[\hbar\omega_0 = E_h]$	8.99×10^{-40}	8.11×10^{-51}	4.14×10^{-51}	1.03×10^{-51}
$C_2(M)$ for $\delta E^{(ii)}$ $[\hbar\omega_0 = E_h]$	1.17×10^{-44}	2.24×10^{-53}	1.17×10^{-44}	1.19×10^{-39}
$C_2(M)$ for $\delta E^{(ii)}$ [hydrogen $2S$, $\omega_0 = \omega_{1S2S}$]	4.71×10^{-37}	8.99×10^{-46}	4.71×10^{-37}	4.79×10^{-32}
$C_3(M)$ for $\delta E^{(iii)}$ $[\hbar\omega_0 = E_h]$	4.79×10^{-44}	4.32×10^{-55}	2.20×10^{-55}	5.51×10^{-56}
$C_2(M)$ for $\delta E^{(iv)}$ $[\hbar\omega_0 = E_h]$	1.99×10^{-19}	5.98×10^{-25}	4.27×10^{-25}	2.13×10^{-25}
$C_2(M)$ for $\delta E^{(iv)}$ [HF, $\omega_0 = \omega_{\mathrm{ioni}}$]	1.41×10^{-19}	4.24×10^{-25}	3.03×10^{-25}	1.51×10^{-25}
$C_2(M)$ for $\delta E^{(iv)}$ [N_2, $\omega_0 = \omega_{\mathrm{ioni}}$]	1.55×10^{-18}	4.66×10^{-24}	3.33×10^{-24}	1.66×10^{-24}
$C_2(M)$ for $\delta E^{(iv)}$ [Cl_2, $\omega_0 = \omega_{\mathrm{ioni}}$]	-3.14×10^{-18}	-9.42×10^{-24}	-6.73×10^{-24}	-3.37×10^{-24}

4. Atoms and limit of vanishing Bohr radius

One might argue that the variation of the gravitational potential around the atomic center does not constitute a quantum limitation of the EEP, because it is simply given as the expectation value of a gravitational effect, evaluated on the atomic wave function. However, it leads to an observable frequency shift and to a deviation from the universal $\sqrt{T}$ scaling of the atomic transition frequencies. The effect would vanish if the electron could be perfectly localized, which however is incompatible with fundamental postulates of quantum mechanics. In particular, perfect localization of the electron's wave packet would be incompatible with Heisenberg's uncertainty principle. It is instructive to observe that the energy shifts $\delta E^{(i)}$ and $\delta E^{(ii)}$ vanish in the limit $a_0 \to 0$, which would correspond to the classical limit of a perfectly localizable electron. The energy shifts $\delta E^{(iii)}$, by contrast, is nonvanishing even in the limit a_0 and constitutes a genuine quantum correction to the EEP, due to the Fokker precession acting on the bound atomic electron.

5. Diatomic molecules

For a diatomic molecule, the situation is essentially more interesting because the expectation value

$$\delta E^{(iv)} = \langle V^{[1]} \rangle = \left\langle GmM \frac{\vec{R} \cdot \vec{\rho}}{R^3} \right\rangle \tag{63}$$

can be nonvanishing. It is known that diatomic molecules typically have nonvanishing electric dipole moments [43]. Indeed, it is known [44] that, e.g., hydrogen fluoride (HF) has a dipole moment of 1.82 D, where D denotes the Debye, which is a canonical unit of an atomic dipole moment, equal to $0.20819434 \, |e| \, \text{Å}$, where $|e|$ is the elementary charge. A calculation using GAUSSIAN 2.0 [45] reveals that the hydrogen fluoride ion (HF$^+$) has a dipole moment of 2.36 D (in units of Debye), which is measured with respect to the center-of-mass of the hydrogen fluoride molecule (by convention). However, the *electric*

dipole moment is of no significance when it comes to the evaluation of gravitational corrections.

Namely, for the evaluation of gravitational corrections, one should consider the fact that the mass of the atom is concentrated in the atomic nuclei. The two nuclei in a diatomic molecule are separated by the bond length. If the energetically highest molecular orbital is bonding, then the bond length will increase upon excitation into energetically higher states, with the maximum change reached for excitations close to the ionization threshold. An example is HF, which has a bond length of

$$\ell_{\mathrm{HF}} = 0.917 \, \text{Å}, \tag{64}$$

to be contrasted with HF$^+$, which has a bond length of

$$\ell_{\mathrm{HF^+}} = 1.001 \, \text{Å}, \tag{65}$$

according to Refs. [43, 44].

By contrast, if the energetically highest molecular orbital is anti-bonding, then the bond length will decrease upon excitation into energetically higher states, An example is CL$_2$, whose bond length decreases from

$$\ell_{\mathrm{CL_2}} = 1.99 \, \text{Å} \qquad \to \qquad \ell_{\mathrm{CL_2^+}} = 1.89 \, \text{Å} \tag{66}$$

upon ionization into CL$_2^+$ (see Ref. [43]). For N_2, the bond length changes according to

$$\ell_{\mathrm{N_2}} = 1.12 \, \text{Å} \qquad \to \qquad \ell_{\mathrm{N_2^+}} = 1.29 \, \text{Å}. \tag{67}$$

We can thus conclude that, in a diatomic molecule, if we hold the position of one of the nuclei (mass m_1) fixed to the origin, then there will be an energy correction of the form

$$\delta E^{(iv)} = \langle V^{[1]} \rangle = \left\langle GM \frac{m_2 \vec{R} \cdot \vec{L}}{R^3} \right\rangle$$
$$\sim \frac{G m_p M a_0}{R^2}. \tag{68}$$

Here, $\vec{L}$ is the bond length vector, m_2 is the mass of the respective other nucleus, while m_p is the proton mass. In

formulating the order-of-magnitude estimate, we use the proton mass (mass of the nucleus of the hydrogen atom) as a measure for m_2; of course, this assumption has to be adjusted according to the molecule under consideration.

The ionization energy of a diatomic molecule in a gravitational field thus changes according to

$$\delta E^{(iv)} = \frac{Gm_2 M \, \Delta \ell}{R^2} \qquad (69)$$

upon ionization, if the axis of the diatomic molecule is aligned along the $\vec{R}$ vector. Here, $\Delta \ell$ is the change in the bond length upon ionization. This is because directly under the ionization threshold, the bond length will asymptotically approach that of the ion.

According to the above considerations, given in Eqs. (64)—(67), one has

$$\Delta \ell_{\mathrm{HF}} = 0.084 \, \text{Å}, \qquad (70a)$$
$$\Delta \ell_{\mathrm{N_2}} = 0.17 \, \text{Å}, \qquad (70b)$$
$$\Delta \ell_{\mathrm{Cl_2}} = -0.10 \, \text{Å}. \qquad (70c)$$

Numerical estimates of the gravitational effects can be quite large for typical diatomic molecules, according to Table I. For absolute clarity, we should point out that, for a successful measurement of the gravitation frequency shift, the diatomic molecules need to be aligned with reference to the gravitational field; of course, the effect vanishes when averaged over an ensemble of unaligned molecules.

IV. MEASUREMENT OF THE HIGHER–ORDER SHIFTS

According to Table I, the dominant effects for either the hydrogen $1S$–$2S$ transition or molecular transitions are given by the shifts $\delta E^{(ii)}$ and $\delta E^{(iv)}$. It is instructive to study their dependence on the gravitational potential, and the measurability of the effects.

As evident from Eq. (56), the shift $\delta E^{(ii)}$ can be written as

$$\delta E^{(ii)} = \left(\frac{\Phi}{\Phi_0} \right)^4 C_4(M) \, (\hbar \omega_{1S2S}), \qquad (71)$$

where ω_{1S2S} is the unperturbed $1S$–$2S$ frequency, and $C(M)$ is a coefficient whose value depends on the mass of the gravitational center. The gravitational potential is $\Phi = -GM/R$, and we have normalized the potential with respect to $\Phi_0 = GM_\oplus / R_\oplus$, where $M_\oplus$ is the Earth mass, and $R_\oplus$ is the Earth's radius. Also, $\delta E^{(iv)}$ given in Eq. (68) can be written as

$$\delta E^{(iv)} = \left(\frac{\Phi}{\Phi_0} \right)^2 C_2(M) \, (\hbar \omega_{\mathrm{ioni}}), \qquad (72)$$

where ω_{ioni} is the angular unperturbed ionization frequency, and $C(M)$ [which may be different from the coefficient used in Eq. (71)] is a mass-dependent coefficient.

Let us assume that a general higher-order gravitational frequency shift, which limit the validity of the universal $\sqrt{T}$ scaling, can be written in the functional form

$$\delta E = \left(\frac{|\Phi|}{\Phi_0} \right)^n C_n(M) \, \hbar \omega_0, \qquad (73)$$

where, for the cases studied above, one would have either $n = 2, 3, 4$. The coefficient $C_n(M)$ depends on the mass of the gravitational center, while ω_0 is the unperturbed frequency.

We can thus write a gravitationally corrected transition energy E as

$$\begin{aligned} E &= \sqrt{T} \, \omega_0 + \delta E \\ &= \left(\sqrt{1 + 2\Phi} + |\Phi|^n C(M) \right) \hbar \omega_0. \end{aligned} \qquad (74)$$

In units with $\hbar = 1$, we have

$$E = \frac{\mathrm{d}\theta}{\mathrm{d}t}, \qquad \omega_0 = \frac{\mathrm{d}\theta}{\mathrm{d}\tau}, \qquad (75)$$

where t is the global coordinate time, and τ is the proper time measured by the local observer, while θ is the rotation angle of the oscillation. Then,

$$\frac{\mathrm{d}\tau}{\mathrm{d}t} = \sqrt{1 + 2\Phi} + |\Phi|^n C_n(M). \qquad (76)$$

Comparing two atomic clocks at different altitudes (points labeled 1 and 2 in the gravitational field), which is the essence of relativistic geodesy [46], one arrives at the result

$$\frac{\mathrm{d}\tau_1}{\mathrm{d}\tau_2} = \frac{\sqrt{1 + 2\Phi_1} + |\Phi_1|^n C_n(M)}{\sqrt{1 + 2\Phi_2} + |\Phi_2|^n C_n(M)}. \qquad (77)$$

We reemphasize that the numerical value of the coefficient $C_n(M)$, as well as the value of n, are not universal, but depend on the atomic system and the transition under study (see Table II). The prediction thus is that, if one expands this result in Φ_1 and Φ_2 to order n, then the coefficients of order less than n will agree with the expansion of the leading term $\sqrt{1 + 2\Phi_1}/\sqrt{1 + 2\Phi_2}$, while at order n, there will be an additional correction

$$\begin{aligned} \frac{\mathrm{d}\tau_1}{\mathrm{d}\tau_2} &\sim \left(\sum_{k=0}^{n} \binom{1/2}{k} (2\Phi_1)^k \right) \left(\sum_{k=0}^{n} \binom{1/2}{k} (2\Phi_2)^k \right)^{-1} \\ &\quad + C_n(M) \left(|\Phi_1|^n - |\Phi_2|^n \right), \end{aligned} \qquad (78)$$

which describes the deviation from Einstein's equivalence principle. Here,

$$\binom{n}{k} = \frac{\Gamma(n+1)}{\Gamma(k+1)\,\Gamma(n-k+1)} \qquad (79)$$

is the binomial coefficient. Terms of order $n + 1$ and higher in the gravitational potentials have been neglected in writing Eq. (78). Numerical results for the coefficient $C_n(M)$ are given in Table II. We use the ionization energies $6.12 \, \text{eV}$ for HF, $15.58 \, \text{eV}$ for $\mathrm{N_2}$, and $11.48 \, \text{eV}$ for $\mathrm{Cl_2}$, as well as the known $1S$–$2S$ frequency for hydrogen (see Ref. [41]).

V. CONCLUSIONS

Let us summarize the main results of the current, lengthy, paper. We shall proceed section by section.

In Sec. II, we derive generally applicable Hamiltonians for the combined gravitational-electromagnetic interaction in a central gravitational field, which add relativistic corrections to the leading-order (nonrelativistic) result [see Eqs. (4) and (5)]. Furthermore, we show that the interplay of the gravitationally modified Dirac equation, and the gravitationally modified vacuum permittivity and permeability, leads to a value of the fine-structure constant independent of gravity [see Eq. (17c)]. As a result, we confirm (see Ref. [2]) that atomic transition energies are (to an excellent approximation) compatible with the equivalence principle [see Eq. (18)]. We also derive a universal gravitational scaling for the electron's g factor, including the bound-state corrections, and the anomalous magnetic moment term [see Eq. (34)]. Only a careful consideration of the transformation of the magnetic-field components from global coordinates to a local Lorentz frame, restores the validity of the EEP [see Eq. (41)].

In Sec. III, we first discuss gravitational energy shifts which scale with the universal prefactor $\sqrt{T} = \sqrt{1 + 2\,\Phi}$. Our discussion culminates in Eq. (52), where we derive the gravitationally corrected Schrödinger–Coulomb Hamiltonian, to complement Eq. (18). Furthermore, we treat four effects which go beyond the universal prefactor $\sqrt{T}$, and which, therefore, in the language of Ref. [2], limit the compliance of transition frequencies with the Einstein equivalence principle. These effects are mainly caused by the non-deterministic nature of quantum mechanics, which prevents us from perfectly localizing an electron at a given point in time, as described by Heisenberg's uncertainty principle. Specifically, we have an energy correction $\delta E^{(i)}$, due to a quadrupole term in the gravitational field, given in Eq. (55), which leads to a nontrivial effect due to the nonvanishing extent of the quantum mechanical wave function. A second correction $\delta E^{(ii)}$ is due to a second-order effect involving the dipole expansion about the gravitational center of the atom, and $\delta E^{(iii)}$ is described by the Fokker precession term. One notices that the energy shift $\delta E^{(iii)}$ does not vanish in the limit $a_0 \to 0$. The effect thus does not require the gravitational field to change significantly over the dimension of the atom, at variance with a remark issued in the text following Eq. (12.13) of Ref. [9]. Then, for diatomic molecules, quite remarkably, the dipole term $\delta E^{(iv)}$ due to first-order perturbation theory involves the dipole expansion about the gravitational center of the atom; its expectation value does not vanish and leads to a direction-dependent energy shift. Numerical values for the energy shifts $\delta E^{(i)}$, $\delta E^{(ii)}$, $\delta E^{(iii)}$, and $\delta E^{(iv)}$, are given in Table I.

In Sec. IV, we discuss the measurability of the gravitational shifts in atomic-clock comparisons. One first observes that the energy shifts $\delta E^{(i)}$, $\delta E^{(ii)}$, $\delta E^{(iii)}$, and $\delta E^{(iv)}$, which limit the validity of the $\sqrt{T}$ scaling, have a

functional $|\Phi|^n$ dependence, where Φ is the gravitational potential. They thus lead to a correction term in the atomic-clock comparison, as given in in Eq. (77), which could in principle be measured in an accurate comparison of atomic clocks running at a place with different gravitational potentials. Equation (77) is one of the main results of the current paper. Data for the $C_n(M)$ coefficients, which enter Eq. (73), are given in Table II.

One should remember that the conclusions of Ref. [2] crucially depend on the approximation that commutator terms between the gravitational couplings and the kinetic operators in the Hamiltonian can be neglected. Only under this assumption can the fundamental $\sqrt{T}$ scaling of the atomic energy levels be derived. Here, we go beyond this approximation and quantify those effects which do not follow the universal $\sqrt{T}$ scaling. We reemphasize that the Fokker precession term does not vanish in the limit of a pointlike atom (vanishing Bohr radius), and leads to a manifest deviation of the gravitational modification of atomic transition frequencies from the fundamental $\sqrt{T}$ scaling, which is otherwise crucial in establishing the compatibility of high-precision spectroscopy experiments with the equivalence principle [2].

The tiny gravitational corrections beyond the $\sqrt{T}$ scaling should be compared to effects due to space-time non-commutativity [47–49] (see App. B), and a conceivable limitation of the achievable accuracy due to a gravitationally induced collapse of the wave function (Penrose conjecture, see Refs. [50–52], see App. C). The conclusion is that under reasonable assumptions, they do not preclude the measurability of the quantum corrections outlined in Eqs. (77) and (73), as explained in detail in App. B 3 and App. C 3. In view of seemingly unstoppable progress in high-precision spectroscopy [53], the effects could be of phenomenological relevance sooner than otherwise expected.

Appendix A: Theoretical Background

1. Dirac Hamiltonian and Hermiticity

We set, with Ref. [14],

$$T = w^2, \qquad H = v^2, \qquad \mathrm{d}s^2 = w^2 \mathrm{d}t^2 - v^2 \mathrm{d}\vec{r}^2. \quad \text{(A1)}$$

It is known from the literature (see, e.g., Refs. [9, 14, 54]) that the Hamiltonian obtained from the variation of the fully relativistic curved-space action of a Dirac particle is not Hermitian [see Eq. (11) of Ref. [14]]. It reads as

follows,

$$\mathcal{H} = \frac{w}{v}\vec{\alpha}\cdot\vec{p} - \frac{\mathrm{i}}{2v}\,\vec{\alpha}\cdot\vec{\nabla}w - \frac{\mathrm{i}w}{v^2}\vec{\alpha}\cdot\vec{\nabla}v + \beta m w\,. \quad \text{(A2)}$$

Let us carry out the transformation which leads to a Hermitian operator, in great detail. One sets

$$H_0 = \frac{w}{v}\vec{\alpha}\cdot\vec{p}\,. \quad \text{(A3)}$$

Then,

$$\begin{aligned}
X &= v^{3/2}H_0 v^{-3/2} - \frac{1}{2}\left\{\vec{\alpha}\cdot\vec{p},\frac{w}{v}\right\}\\
&= v^{3/2}\frac{w}{v}v^{-3/2}\vec{\alpha}\cdot\vec{p} + v^{3/2}\frac{w}{v}\left[\vec{\alpha}\cdot\vec{p},v^{-3/2}\right] - \frac{w}{v}\vec{\alpha}\cdot\vec{p} - \frac{1}{2}\left[\vec{\alpha}\cdot\vec{p},\frac{w}{v}\right]\\
&= v^{3/2}\frac{w}{v}\left[-\mathrm{i}\vec{\alpha}\cdot\left(-\frac{3}{2}v^{-5/2}\right)\vec{\nabla}v\right] - \frac{1}{2}\left(-\mathrm{i}\frac{1}{v}\vec{\alpha}\cdot\vec{\nabla}w + \left[-\mathrm{i}\left(-\frac{w}{v^2}\right)\vec{\alpha}\cdot\vec{\nabla}v\right]\right)\\
&= \frac{3\mathrm{i}w}{2v^2}\vec{\alpha}\cdot\vec{\nabla}v + \frac{\mathrm{i}}{2v}\vec{\alpha}\cdot\vec{\nabla}w - \frac{\mathrm{i}w}{2v^2}\vec{\alpha}\cdot\vec{\nabla}v = \frac{\mathrm{i}w}{v^2}\vec{\alpha}\cdot\vec{\nabla}v + \frac{\mathrm{i}}{2v}\vec{\alpha}\cdot\vec{\nabla}w\,.
\end{aligned} \quad \text{(A4)}$$

Hence, one obtains the relativistic and Hermitian Dirac–Schwarzschild Hamiltonian [14],

$$H_{\mathrm{DS}} = v^{3/2}\,\mathcal{H}\,v^{-3/2} = \frac{1}{2}\left\{\vec{\alpha}\cdot\vec{p},\frac{w}{v}\right\} + \beta m w\,. \quad \text{(A5)}$$

The original Hamiltonian $\mathcal{H}$ can thus be written as follows,

$$\mathcal{H} = v^{-3/2}\,H_{\mathrm{DS}}\,v^{3/2}\,. \quad \text{(A6)}$$

This relation, in particular, implies that $\mathcal{H}$ and H_{DS} have the same eigenvalues. In order to see this, consider an eigenfunction Ψ of H_{DS}, with $H_{\mathrm{DS}}\,\Psi = E\,\Psi$. The corresponding eigenstate of $\mathcal{H}$ is $\Phi = v^{-3/2}\,\Psi$, with the same energy eigenvalue E. Hence, $\mathcal{H}$ and H_{DS} can be used interchangeably in eigenvalue perturbation theory, a fact which has implicitly been used in Eq. (13) of Ref. [54] and elucidated in greater detail in Refs. [14]. The equivalence of the eigenvalues also is used throughout the current paper.

The Hermitian adjoint of $\mathcal{H}$ is

$$\mathcal{H}^+ = v^{3/2}\,H_{\mathrm{DS}}\,v^{-3/2} = v^3\,\mathcal{H}\,v^{-3}\,, \quad \text{(A7)}$$

and thus, not equal to $\mathcal{H}$ itself. Rather, we have the relation $\mathcal{H}^+\,v^3 = v^3\,\mathcal{H}$. The relation (A7) is reminiscent of pseudo–Hermiticity, a property which has been discussed by Pauli [55] and recently used in the analysis of a number of quantum systems [56–63].

Let us now consider the a general matrix element $\langle\psi|v^3|\phi\rangle$ between general states ψ and ϕ which fulfill the time-dependent Schrödinger equation $\mathcal{H}\psi = \mathrm{i}\partial_t\psi$ and $\mathcal{H}\phi = \mathrm{i}\partial_t\phi$, for $\mathcal{H}$ (not H_{DS}!),

$$\begin{aligned}
\mathrm{i}\partial_t\langle\psi|v^3|\phi\rangle &= \langle\psi|v^3|\mathrm{i}\partial_t\phi\rangle - \langle\mathrm{i}\partial_t\psi|v^3|\phi\rangle\\
&= \langle\psi|v^3|\mathcal{H}\,\phi\rangle - \langle\mathcal{H}\psi|v^3|\phi\rangle\\
&= \langle\psi|v^3\,\mathcal{H}|\phi\rangle - \langle\psi|\mathcal{H}^+\,v^3|\phi\rangle = 0\,, \quad \text{(A8)}
\end{aligned}$$

where we have used Eq. (A7). Hence, we have shown that the generalized scalar product $\langle\psi|v^3|\phi\rangle$ is conserved under the time evolution induced by $\mathcal{H}$. This makes perfect sense in a metric $\mathrm{d}s^2 = w^2\mathrm{d}t^2 - v^2\mathrm{d}\vec{r}^2$, where $|\mathrm{d}s| = v\,|\mathrm{d}\vec{r}|$ for $\mathrm{d}t = 0$.

2. Alternative form of the Dirac Hamiltonian

In order to make contact with the literature, let us try to compare the Dirac–Schwarzschild Hamiltonian to the result given in Eq. (42) of Ref. [64], which is formulated using a general potential $U_+ = U_- = U = -G\,M/r$ [see Eq. (2) of Ref. [64]], where we set the contribution of the chameleon field discussed in Ref. [64] to zero. First of all, an important identity is

$$\{A,\{A,B\}\} = 2\{A^2,B\} - [A,[A,B]]\,. \quad \text{(A9)}$$

Here, we use this identity for $B = U$ and $A = \vec{\nabla}$, and obtain for general U,

$$\{\vec{\nabla}, \{\vec{\nabla}, U\}\} = 2\{\vec{\nabla}^2, U\} - \vec{\nabla}^2(U) = 2U\vec{\nabla}^2 + 2\vec{\nabla}^2 U - \vec{\nabla}^2(U)$$
$$= 2U\vec{\nabla}^2 + 2\vec{\nabla}[\vec{\nabla}, U] + 2\vec{\nabla} U \cdot \vec{\nabla} - \vec{\nabla}^2(U)$$
$$= 2U\vec{\nabla}^2 + 2\vec{\nabla}[\vec{\nabla}, U] + 2[\vec{\nabla}, U] \cdot \vec{\nabla} + 2U\vec{\nabla}^2 - \vec{\nabla}^2(U)$$
$$= 2U\vec{\nabla}^2 + 2[\vec{\nabla}, [\vec{\nabla}, U]] + 2[\vec{\nabla}, U] \cdot \vec{\nabla} + 2[\vec{\nabla}, U] \cdot \vec{\nabla} + 2U\vec{\nabla}^2 - \vec{\nabla}^2(U)$$
$$= 4U\vec{\nabla}^2 + 4\vec{\nabla}(U) \cdot \vec{\nabla} + \vec{\nabla}^2(U). \tag{A10}$$

The result given in Eq. (42) of Ref. [64] can then be rewritten as follows, under the identification $\beta = \gamma^0$,

$$H_3 = \beta \left(m - \frac{1}{2m}\vec{\nabla}^2 + mU \right) + \frac{\beta}{2m} \left(-3U\vec{\nabla}^2 - 3\vec{\nabla}(U) \cdot \vec{\nabla} - \frac{3}{4}\vec{\nabla}^2(U) \cdot \vec{\nabla} \right) - \frac{\beta}{4m} i\vec{\Sigma} \cdot [3\vec{\nabla}U \times \vec{\nabla}]$$
$$= \beta \left(m - \frac{1}{2m}\vec{\nabla}^2 - \frac{GmM}{r} \right) - \frac{3\beta}{8m}\{\vec{\nabla}, \{\vec{\nabla}, U\}\} + \frac{3\beta}{4m}\vec{\Sigma} \cdot \left[\frac{GM\vec{r}}{r^3} \times (-i\vec{\nabla}) \right]$$
$$= \beta \left(m + \frac{\vec{p}^2}{2m} - \frac{GmM}{r} \right) + \frac{3\beta}{8m} \left\{ \left\{ -\frac{GM}{r}, \vec{p} \right\}, \vec{p} \right\} + \frac{3\beta GM}{4mr^3}\vec{\Sigma} \cdot \vec{r} \times \vec{p}$$
$$= \beta \left(m + \frac{\vec{p}^2}{2m} - \frac{mr_s}{2r} \right) - \frac{3\beta}{16m} \left\{ \left\{ \frac{r_s}{r}, \vec{p} \right\}, \vec{p} \right\} + \frac{3\beta r_s}{8mr^3}\vec{\Sigma} \cdot \vec{r} \times \vec{p}$$
$$= \beta \left(m + \frac{\vec{p}^2}{2m} - \frac{mr_s}{2r} \right) - \frac{3\beta}{8m} \left\{ \frac{r_s}{r}, \vec{p}^2 \right\} + \frac{3\beta\pi r_s}{4m}\delta^{(3)}(\vec{r}) + \beta\frac{3r_s\vec{\Sigma} \cdot \vec{L}}{8mr^3}. \tag{A11}$$

Thus, the result given in Ref. [64], upon setting the chameleon field to zero, is seen to be equivalent to the Dirac–Schwarzschild Hamiltonian [14]. However, it is also clear that the result given in Ref. [64] concerns a (chameleon-field inspired generalization of) the Dirac–Schwarzschild Hamiltonian, but does not consider the Coulomb-field terms which must be added to obtain the Dirac–Schwarzschild–Coulomb Hamiltonian discussed in Sec. II. We also mention the necessity of considering the relativistic $\vec{p}^4$ correction, depending on the approximations used in a particular treatment of the problem.

Appendix B: Penrose Conjecture

1. Theoretical foundations

The Copenhagen interpretation of quantum mechanics and the pertinent collapse of the wave function still give rise to interesting questions about the foundations of physical theory, as discussed by Penrose [50–52]. The Penrose conjecture implies that gravity yanks objects back into a single location, without any need to invoke observers or parallel universes. The gravitationally induced effects envisaged by the Penrose conjecture should be compared to the quantum effects discussed in Sec. III of this article.

In Fig. 5 of Ref. [52], Penrose conjectures that collapse of the wave function to one of two possible states is induced on a time scale

$$t_C \sim \frac{\hbar}{E_G}, \tag{B1}$$

where E_G is the gravitational self-energy of the difference between the two mass distributions, which, notably, is not equal to the difference of their gravitational self-energies.

According to the an (unnumbered) equation on p. 595 of Ref. [50], the relevant expression is

$$E_G = -G \int d^3x \int d^3y \frac{[\rho(\vec{x}) - \rho'(\vec{x})] \, [\rho(\vec{y}) - \rho'(\vec{y})]}{|\vec{x} - \vec{y}|}, \tag{B2}$$

where $\rho(\vec{r})$ and $\rho'(\vec{r})$ are the two mass distributions.

Let us confront this expression with the well-known Colella–Overhauser–Werner experiment [65–68], where, according to the experimental description in Ref. [66], neutrons are separated across an interferometer with a side length of about $2.5\,\text{cm}$, and an opening angle of $22.1°$. During the experiment, the neutrons are "gravitationally bound to the Earth". It is important to analyze the predictions of the Penrose conjecture for this experiment, because a conceivable collapse of the wave would otherwise preclude the observation of interference fringes in the experiment [66].

Let us denote the mass distribution of the Earth by $\rho_\oplus(\vec{r})$. We associate the neutron wave function with a mass distribution $m_n f(\vec{r} - \vec{r}_n)$, where m_n is the neutron mass and f is a properly normalized sampling function, centered about the origin, and $\vec{r}_n$ is a point on the "lower" arm of the quantum interferometer. The other state, which is part of the superposition and is centered around the "higher" arm of the interferometer, has a mass distribution given by the sum of the mass distri-

bution of the Earth, $\rho_\oplus(\vec{r})$, and a neutron wave function with a mass distribution $m_n\, f(\vec{r} - \vec{r}_n - \vec{h}s)$, where m_n is the neutron mass, and $\vec{h}$ is the vector that describes the height difference of the "elevation" of the neutrons in the gravitational field of the Earth. In this case,

$$\rho(\vec{r}) = \rho_\oplus(\vec{r}) + m_n\, f(\vec{r} - \vec{r}_n)$$
$$= \rho_\oplus(\vec{r}) + \widetilde{\rho}(\vec{r})\,, \qquad \text{(B3a)}$$

$$\rho'(\vec{r}) = \rho_\oplus(\vec{r}) + m_n\, f(\vec{r} - \vec{r}_n - \vec{h})$$
$$= \rho_\oplus(\vec{r}) + \widetilde{\rho}'(\vec{r})\,, \qquad \text{(B3b)}$$

$$\rho(\vec{r}) - \rho'(\vec{r}) = m_n\, [f(\vec{r} - \vec{r}_n) - f(\vec{r} - \vec{r}_n - \vec{h})]\,, \quad \text{(B3c)}$$

where $\rho_\oplus(\vec{r})$ is the mass density of the Earth, and m_n is the neutron mass, while f is normalized according to $\int \mathrm{d}^3 r\, f(\vec{r}) = 1$. One might assume that $f \sim |\psi|^2$, where ψ is the quantum mechanical wave function.

In this case, the expression (B2) can be written as the sum of three terms, two of which correspond to the (negative values of) self-energy integrals S and S', and a third (interaction) integral I,

$$E_G = -\,S - S' + I\,, \qquad \text{(B4a)}$$

$$S = G \int \mathrm{d}^3 x \int \mathrm{d}^3 y\, \frac{\widetilde{\rho}(\vec{x})\, \widetilde{\rho}(\vec{y})}{|\vec{x} - \vec{y}|}\,, \qquad \text{(B4b)}$$

$$S' = G \int \mathrm{d}^3 x \int \mathrm{d}^3 y\, \frac{\widetilde{\rho}'(\vec{x})\, \widetilde{\rho}'(\vec{y})}{|\vec{x} - \vec{y}|}\,, \qquad \text{(B4c)}$$

$$I = 2G \int \mathrm{d}^3 x \int \mathrm{d}^3 y\, \frac{\widetilde{\rho}(\vec{x})\, \widetilde{\rho}'(\vec{y})}{|\vec{x} - \vec{y}|}\,. \qquad \text{(B4d)}$$

The easiest integral to approximate in this case is

$$I \sim 2G\, m_n^2 \int \mathrm{d}^3 x \int \mathrm{d}^3 y\, \frac{\delta^{(3)}(\vec{x})\, \delta^{(3)}(\vec{y} - \vec{h})}{|\vec{x} - \vec{y}|}$$
$$= 2\frac{G\, m_n^2}{|\vec{h}|}\,, \qquad \text{(B5)}$$

which is the gravitational interaction energy of two neutrons, a distance $h = |\vec{h}| \sim 2.5\,\mathrm{cm}$ apart (in the experiment described in Ref. [66]). Newton's gravitational constant is denoted as G.

In order to estimate the order-of-magnitude of the gravitational self-energies $S = S'$, we need a measure of the spread of the mass distribution f, which enters the modulus $|\vec{x} - \vec{y}|$ in the integrals for S and S' [see Eqs. (B4b) and (B4c)]. We estimate the length scale of the mass distribution to be equal to the de Broglie wavelength of the neutron, which, for the experiment [66], is equal to $\lambda = 1.445\,\text{Å}$. One obtains

$$S = S' \sim \frac{Gm_n^2}{\lambda}\,. \qquad \text{(B6)}$$

A numerical evaluation, using experimental parameters given in Ref. [66], leads to

$$S = S' \approx 1.3 \times 10^{-54}\,\mathrm{J}\,, \qquad I \approx 1.5 \times 10^{-62}\,\mathrm{J}\,. \quad \text{(B7)}$$

We notice that the sign of the energy E_G defined in Eq. (B4a) is not a priori determined by the formalism used and depends on details of the mass distribution. It is obtained as a negative quantity if the formula is applied to the experimental configuration used in Ref. [66]. This problem could be remedied by replacing E_G by its modulus $|E_G|$ in Eq. (B1). Otherwise, one might argue that it is somewhat counter-intuitive that smaller Compton wavelengths λ (which occur at higher energies) in the self-energy integrals S and S' (not in the interaction integral I) induce a faster gravitational collapse of the wave function.

Finally, for the experimental configuration described in Ref. [66], the (modulus of the) time t_C is obtained to be of the order of

$$|t_C| \sim 10^{18}\,\mathrm{s}\,, \qquad \text{(B8)}$$

which is longer than the age of the Universe. Hence, the Penrose conjecture as given in Eq. (B2) predicts a collapse time for the gravitational interference experiment [66] which is so long that the effect can safely be neglected in the analysis of the experiment.

One should supplement an estimate concerning atomic spectroscopy. Indeed, for atomic states, one can easily estimate that the gravitational self-energy integrals of the mass distributions associated with the atomic wave functions [69] are of the order of

$$E_G \sim G\, \frac{m^2}{a_0} \sim 1.0 \times 10^{-54}\,\mathrm{J}\,, \qquad \text{(B9)}$$

where m is the electron mass, and a_0 is the Bohr radius. The numerical value of the self-energy integral (B9) is so small that gravitationally induced collapse of the wave function can be safely ignored for high-precision spectroscopy, and also, for the analysis of the gravitational shifts discussed in Secs. III and IV.

2. Alternative forms

In an alternative version of the Penrose conjecture, Diósi [70, 71] has conjectured that gravitationally induced wave function collapse occurs over a time scale $t_C \sim \hbar/E_G'$, where the modified gravitational self-energy E_G' is given by the full mass distributions, and can be written as the sum of two interaction integrals $\mathcal{I}$ and $\mathcal{I}'$, and one self-energy integral $\mathcal{S}_\oplus$,

$$E_G' = G \int \mathrm{d}^3 x \int \mathrm{d}^3 y\, \frac{\rho(\vec{x})\, \rho'(\vec{y})}{|\vec{x} - \vec{y}|} = \mathcal{S} + \mathcal{S}' + \mathcal{S}_\oplus\,, \qquad \text{(B10a)}$$

$$\mathcal{I} = G \int \mathrm{d}^3 x \int \mathrm{d}^3 y\, \frac{\rho_\oplus(\vec{x})\, \widetilde{\rho}(\vec{y})}{|\vec{x} - \vec{y}|}\,, \qquad \text{(B10b)}$$

$$\mathcal{I}' = G \int \mathrm{d}^3 x \int \mathrm{d}^3 y\, \frac{\rho_\oplus(\vec{x})\, \widetilde{\rho}'(\vec{y})}{|\vec{x} - \vec{y}|}\,, \qquad \text{(B10c)}$$

$$\mathcal{S}_\oplus = G \int \mathrm{d}^3 x \int \mathrm{d}^3 y\, \frac{\rho_\oplus(\vec{x})\, \rho_\oplus(\vec{y})}{|\vec{x} - \vec{y}|}\,. \qquad \text{(B10d)}$$

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Here, we neglect the term that does not involve $\rho_\oplus(\vec{x})$. In formulating this expression, we have again used the fact that the neutrons in the Colella–Overhauser–Werner experiments [66] are particles "bound to the Earth". However, a surprising observation can be made if we take Eq. (B10a) literally. The expression $\mathcal{S}_\oplus$, given in Eq. (B10d), is the gravitational self-energy of the Earth,

$$E_\oplus = \frac{3}{5}\,\frac{G\,M_\oplus^2}{R_\oplus} = 2.2 \times 10^{32}\,\mathrm{J}\,. \qquad (B11)$$

This huge self-energy would induce any gravitational collapse of a wave packet separated in the gravitational field of the Earth, on a time scale of $10^{-67}\,\mathrm{s}$.

A much more intuitively sensible expression is obtained if, instead of the product of the two mass distributions, we use in the self-energy integral in Eq. (B10a) the difference of the two mass distributions, $\delta\rho(\vec{y}) = \rho'(\vec{y}) - \rho(\vec{y})$. Let us therefore consider the renormalized integral

$$E_G'' = G \int \mathrm{d}^3x \int \mathrm{d}^3y\, \frac{\rho(\vec{x})\,[\rho'(\vec{y}) - \rho(\vec{y})]}{|\vec{x} - \vec{y}|} \equiv \mathcal{T}\,,$$
$$\mathcal{T} \approx G \int \mathrm{d}^3x \int \mathrm{d}^3y\, \frac{\rho_\oplus(\vec{x})\,[\widetilde{\rho}'(\vec{y}) - \widetilde{\rho}(\vec{y})]}{|\vec{x} - \vec{y}|}$$
$$= m_n\, g\, h\,, \qquad (B12)$$

which is just the gravitational energy difference of the two wave packet contributions into which the neutron beam is being split in the Colella–Overhauser–Werner experiments.

A numerical evaluation, with $h = \sin(22.1°)\times 2.5\,\mathrm{cm}$, adapted to the experiment [66], leads to a value of $t_c \approx 6.8 \times 10^{-7}\,\mathrm{s}$ for the wave function collapse time, if formula (B12) is used. This result has to be compared to the flight time of the neutrons in the interferometric apparatus. Using the de Broglie relation with a neutron wavelength $\lambda = 1.445\,\mathring{A}$, one can convert the neutron momentum $|\vec{p}_n| = m\,|\vec{v}_n| = h/\lambda$ into a classical velocity $|\vec{v}_n|$, and, for interferometer arms of a length of around $2.5\,\mathrm{cm}$, to a flight time of about $t_F \approx 9.1 \times 10^{-6}\,\mathrm{s}$. Because $t_C \sim t_F$, the observation of interference fringes in the Colella–Overhauser–Werner experiments [66] pressures the parameters of the modified self-energy integral E_G''. If gravitationally induced wave function collapse were to occur, then we would see a smearing of the fringes. According to Ref. [72], it would easily be possible to increase the arm length of the gravitational interferometer, to test the renormalized form (B12) of the conjecture.

3.   Brief summary

For systems of practical interest, such as atomic and molecular bound states, the original form of the Penrose conjecture [50–52], given in Eq. (B2), predicts very long collapse times for quantum-mechanical wave functions, due to gravitational effects. These are typically long even when compared to the age of the Universe [see Eq. (B8)]. Under reasonable assumptions, the collapse of the wave function can thus be neglected in the discussion of gravitational shifts or line broadenings involving quantum mechanical energy levels in bound systems. Notably, the collapse time, when converted to frequency units, is smaller than the gravitational shifts of energy levels which could lead to a quantum limitation of the EEP.

By contrast, the alternative form of the Penrose conjecture proposed by Diósi [70, 71] [see Eq. (B10a)] fails basic consistency considerations in regard to the Colella–Overhauser–Werner [65–68] experiment, where a neutron wave packet is being split in a gravitational field. Indeed, if the conjecture were to hold in the form proposed by Diósi [70, 71], then collapse times would be so short that the interference fringes in the Colella–Overhauser–Werner experiment [65–68] would disappear.

An interesting incentive for further study might be given by the renormalized form (B12) of the Penrose conjecture, which is proposed here. The observation of interference fringes in the Colella–Overhauser–Werner experiment [65–68] pressures the renormalized form of the Penrose conjecture. However, it leads to predictions which could be tested in a modified form of the Colella–Overhauser–Werner experiment [65–68], with a larger arm length for the gravitational interferometer. This proposal could lead to interesting future studies.

Appendix C: Space–Time Noncommutativity

1.   Theoretical foundations

We shall attempt to compare the parametric estimates for the limitation of the Einstein equivalence principle, due to quantum effects (see Sec. III), to the effects that would otherwise be induced by space-time noncommutativity [47, 48, 73]. The essence of the noncommutative geometry is to promote space-time coordinates to operators, which fulfill the commutation relations [see Eq. (1.1) of Ref. [47]],

$$[\hat{x}_\mu, \hat{x}_\nu] = \mathrm{i}\,\theta_{\mu\nu}\,. \qquad (C1)$$

The energy scale of space-time noncommutativity is the upper limit for the applicability of ordinary quantum field theory. Hence, it is crucial to compare the magnitude of the effects induced by space-time noncommutativity to any conceivable limitations of the Einstein equivalence principle.

In general, one assumes that the parameters $\theta_{\mu\nu}$ are related to the mass scale Λ_{NC} of noncommutativity as in

$$\theta_{\mu\nu} \sim \frac{\hbar^2}{\Lambda_{\mathrm{NC}}^2\,c^2}\,, \qquad (C2)$$

where we use full SI mksA units. The original idea of Ref. [47] was to conjecture that $\Lambda_{\mathrm{NC}}\,c^2$ should be com-

mensurable with the Planck energy, i.e., that its associated reduced Compton wavelength is equal to the Planck length ℓ_P,

$$\frac{\hbar}{\Lambda_{NC}\, c} = \ell_P \,. \tag{C3}$$

We recall that the Planck length ℓ_P is given by

$$\ell_P = \sqrt{\frac{\hbar G}{c^3}} = 1.616 \times 10^{-35}\, \mathrm{m} \,. \tag{C4}$$

So, according to Ref. [47], $\Lambda_{NC}\, c^2$ should assume a numerical value of the order of the Planck energy E_p, i.e., the Planck mass m_P multiplied by c^2,

$$\Lambda_{NC}\, c^2 \sim m_P\, c^2 = E_p = 1.22 \times 10^{28}\, \mathrm{eV} \,. \tag{C5}$$

The authors of Ref. [48] go a different route and use Lamb shift data in order to derive a lower bound on Λ_{NC}. To this end, they define a vector $\vec{\theta}$ by the relation $\theta^i = \epsilon^{ijk}\,\theta^{jk}$, and assume that upon a suitable rotation of the coordinate system, they can set $\theta^3 = \theta$, where θ is a dimensionless scalar parameter.

According to Eq. (3.2) of Ref. [48], the relative energy change δE, due to space-time noncommutativity, of a hydrogen transition energy E which involves a transition with a change of the principle quantum number, is of order

$$\frac{\delta E}{E} = \alpha^2 \frac{m^2}{\Lambda_{NC}^2} \,. \tag{C6}$$

In Ref. [48], the authors argue that, since theory and experiment in hydrogen agree to a level of $10^{-13} \ldots 10^{-14}$ (see Refs. [38, 74]), one can derive a bound for the noncommutativity parameter θ, Specifically, according to the unnumbered equation following Eq. (4.6) of Ref. [48], one has

$$\frac{\theta}{\lambda_e^2} = \frac{m^2}{\Lambda_{NC}^2} \lesssim 10^{-7}\,\alpha \,, \qquad \Lambda_{NC} \gtrsim 10^4\,\frac{\mathrm{MeV}}{c^2} = 10\,\frac{\mathrm{GeV}}{c^2} \,. \tag{C7}$$

This bound is derived based on a comparison of Lamb shift experiments and theory. Here, Λ_{NC} is the mass scale of noncommutativity of space-time. The final numerical result for the bound on Λ_{NC} given in the unnumbered equation following Eq. (4.6) of Ref. [48] obviously contains a typographical error; a numerical verification leads to values for Λ_{NC} on the order of GeV, not TeV.

The latest derived bounds on Λ_{NC} (for a summary, see Ref. [49]) significantly improve over the paper [48]. In Sec. IV.B of Ref. [75], the authors arrive at a bound on the order of

$$\Lambda_{NC} \gtrsim \Lambda_P = 20\,\frac{\mathrm{TeV}}{c^2} = 2 \times 10^4\,\frac{\mathrm{GeV}}{c^2} \,, \tag{C8}$$

which improves the bound originally derived in Ref. [48] by more than three orders of magnitude, and leads to a bound of

$$\frac{\delta E}{E} \lesssim \alpha^2 \frac{m^2}{\Lambda_P^2} = 3.47 \times 10^{-20} \,. \tag{C9}$$

Yet, on the other hand, if we assume the order-of-magnitude estimate (C5) to be valid (i.e., a scale of noncommutativity commensurable with the Planck scale), then the relative change of an atomic (hydrogen) transition frequency is of order [see Eq. (C6)]

$$\frac{\delta E}{E} \lesssim \alpha^2 \frac{m^2}{m_P^2} = 9.32 \times 10^{-50} \,. \tag{C10}$$

Note that this estimate in independent of the gravitational environment of the atom; it thus holds independently for the gravitational field of the Earth, where its effect is suppressed in comparison to quantum limitations of the Einstein equivalence principle (EEP), and also, for much more intense gravitational fields. In the latter case, of course, it is evidently suppressed in comparison to the quantum gravitational effects.

2. Quantum optical experiments

Recently [49, 76], a quantum optical experimental scheme has been devised whose aim is to dramatically improve the bounds currently available for Λ_{NC}, with the aim of approaching the Planck scale. The essential idea is to explore the noncommutative algebra with the help of a radiation-pressure interaction of a micro-mechanical actuator, interacting with a laser beam inside a high-finesse cavity. Specifically, the opto-mechanical effect is probed multiple times after the passing of the reference laser beam through a electro-optic modulator (EOM) which changes the polarization direction. In this case, a sequence of four radiation-pressure interactions leads to an evolution operator of the form [see Eq. (4) of Ref. [76]]

$$\xi = \mathrm{e}^{\mathrm{i}\lambda n_L P_m}\, \mathrm{e}^{-\mathrm{i}\lambda n_L X_m}\, \mathrm{e}^{-\mathrm{i}\lambda n_L P_m}\, \mathrm{e}^{\mathrm{i}\lambda n_L X_m} \tag{C11}$$

where λ measures the optical path, n_L is the number of laser photons. The dimensionless mechanical momentum and position operators are $P_m = p/p_0$, and $X_m = x/x_0$, where $p_0 = \sqrt{\hbar m \omega_m}$, and $x_0 = \sqrt{\hbar/(m \omega_m)}$, where ω_m is the mechanical resonance frequency. Very slight deviations of the commutation relations among the X_m and P_m from the canonical form $[X_m, P_p] = \mathrm{i}$ could then be measured using interferometric techniques. It is argued in Refs. [49, 76] that, using a high-finesse cavity with $\mathcal{F} \sim 10^5$, one could constrain Λ_{NC} to values approaching the Planck scale in a challenging experiment, which would nevertheless be feasible with currently available technologies.

3. Brief summary

The original idea of Seiberg and Witten (see Ref. [47]) was to introduce a noncommutativity scale of the order of the Planck length [see Eq. (C3)], the underlying hypothesis being that conventional quantum field theory breaks down for length scales smaller than the Planck length.

We can consult Ref. [48] for an analysis of the effects of the noncommutativity of space-time on bound-state energy levels. If the original estimate given in Eq. (C5) holds, then the effects of space-time noncommutativity are extremely tiny [see Eq. (C10)] and, notably, smaller than the gravitational shifts discussed in Secs. III and IV.

One can use spectroscopic data (see Ref. [48]) or astrophysical data from the Planck mission (see Ref. [49]) in order to formulate bounds on the noncommutativity scale Λ_{NC} [see Eqs. (C7) and (C8)]. The bound (C9) is less strict than the bound (C10), the latter being based on the Planck-scale hypothesis [47]. So, in an extreme case, the effects of noncommutativity might exceed those discussed in Secs. III and IV.

However, the original estimate given in Eqs. (C3) and (C9) is well motivated, and recent proposals for ultra-precise quantum optical interference experiments [49, 76] might allow for a drastic improvement of the bounds for Λ_{NC}, possibly approaching the Planck scale. In view of Eqs. (C3) and (C9), it is indicated to assume that the effects of noncommutativity should be smaller than the gravitational shifts discussed in Secs. III and IV. Finally, we note that the quantum limitations discussed in the current article do not require us to consider neither space-time quantization nor any quantization of the gravitational interaction itself, a process which could otherwise lead to further (very tiny) limitations of the applicability of the equivalence principle [77].

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