

## Isospin Splittings in the Light-Baryon Octet from Lattice QCD and QED

Sz. Borsanyi,<sup>1</sup> S. Dürr,<sup>1,2</sup> Z. Fodor,<sup>1,2,3</sup> J. Frison,<sup>4,5,†</sup> C. Hoelbling,<sup>1</sup> S. D. Katz,<sup>3,6</sup> S. Krieg,<sup>1,2</sup> Th. Kurth,<sup>1</sup>  
L. Lellouch,<sup>4,5</sup> Th. Lippert,<sup>2</sup> A. Portelli,<sup>4,5,7,\*</sup> A. Ramos,<sup>4,5,‡</sup> A. Sastre,<sup>4,5</sup> and K. Szabo<sup>1</sup>

(Budapest-Marseille-Wuppertal Collaboration)

<sup>1</sup>*Department of Physics, Wuppertal University, Gausstrasse 20, D-42119 Wuppertal, Germany*

<sup>2</sup>*IAS/JSC, Forschungszentrum Jülich, D-52425 Jülich, Germany*

<sup>3</sup>*Institute for Theoretical Physics, Eötvös University, Pázmány Peter sétány 1/A, H-1117 Budapest, Hungary*

<sup>4</sup>*Aix-Marseille Université, CNRS, CPT, UMR 7332, 13288 Marseille, France*

<sup>5</sup>*Université de Toulon, CNRS, CPT, UMR 7332, 83957 La Garde, France*

<sup>6</sup>*MTA-ELTE Lendület Lattice Gauge Theory Research Group, H-1117 Budapest, Hungary*

<sup>7</sup>*School of Physics and Astronomy, University of Southampton, Southampton SO17 1BJ, United Kingdom*

(Received 5 July 2013; published 17 December 2013)

While electromagnetic and up-down quark mass difference effects on octet baryon masses are very small, they have important consequences. The stability of the hydrogen atom against beta decay is a prominent example. Here, we include these effects by adding them to valence quarks in a lattice QCD calculation based on  $N_f = 2 + 1$  simulations with five lattice spacings down to 0.054 fm, lattice sizes up to 6 fm, and average up-down quark masses all the way down to their physical value. This allows us to gain control over all systematic errors, except for the one associated with neglecting electromagnetism in the sea. We compute the octet baryon isomultiplet mass splittings, as well as the individual contributions from electromagnetism and the up-down quark mass difference. Our results for the total splittings are in good agreement with experiment.

DOI: [10.1103/PhysRevLett.111.252001](https://doi.org/10.1103/PhysRevLett.111.252001)

PACS numbers: 14.20.-c, 11.15.Ha, 12.38.Gc, 13.40.Dk

The existence and stability of atoms and ordinary matter rely heavily on the fact that neutrons are slightly more massive than protons. The difference in the mass of these two particles has been measured very precisely and is only 0.14% of their average mass [1]. Although it has yet to be shown from first principles, we believe that this tiny difference results from the competition between electromagnetic (EM) effects proportional to the fine structure constant  $\alpha \equiv e^2/(4\pi)$  and mass isospin breaking effects proportional to the mass difference of up and down quarks  $\delta m \equiv m_u - m_d$ . Here, we study this issue in the light-baryon octet. In particular, we compute mass splittings in the nucleon ( $N$ ),  $\Sigma$ , and  $\Xi$  isospin multiplets using lattice QCD, to which we add QED in the valence quark sector. Although one would also have to account for QED contributions from sea quarks to have a complete calculation, these effects are suppressed, as discussed below. Moreover, the approach taken here allows us to use a very rich set of QCD gauge configurations that we have already generated [2–4]. Eliminating the uncertainty associated with neglecting QED sea-quark contributions would require performing completely new simulations, implementing reweighting techniques [5,6], or using EM current insertion methods [7] and including quark-disconnected contributions. Such a computation is beyond the scope of the present work.

Because mass and EM isospin symmetry breaking corrections are small and of comparable size, it is legitimate

to expand the standard model in powers of  $\delta m$  and  $\alpha$ , assuming  $O(\delta m) \sim O(\alpha)$  [8]. This expansion is expected to converge very rapidly, with each subsequent order contributing  $\sim 1\%$  of the previous one. Given the size of other uncertainties in our calculation, we can safely work at leading order in this expansion, i.e., at  $O(\delta m, \alpha)$ .

*The physical point.*—In the absence of weak interactions and for energies smaller than the charm-anticharm threshold, the standard model of quarks has five parameters that must be fixed by comparison to experiment. Here, we trade these parameters for observables which are particularly sensitive to them: (1) the lattice spacing  $a$  for the mass of the decuplet baryon  $\Omega^-$ —alternatively, the isospin averaged  $\Xi$  mass—as in Ref. [9], (2) the average  $u$ - $d$  mass  $m_{ud}$  for  $M_{\pi^+}^2$ , (3) the strange mass  $m_s$  for  $M_{K^*}^2 \equiv (M_{K^+}^2 + M_{K^0}^2 - M_{\pi^+}^2)/2$ , (4)  $\delta m$  for the mass-squared difference  $\Delta M_K^2 \equiv M_{K^+}^2 - M_{K^0}^2$ , and (5) bare  $\alpha$  for its renormalized value because it does not renormalize in our quenched QED calculation. The *physical point* is then reached by tuning these observables to their physical values given in Ref. [1], while taking the continuum  $a \rightarrow 0$  and infinite-volume  $L \rightarrow \infty$  limits.

*Separating EM and  $\delta m$  contributions.*—In addition to computing the total splittings, it is interesting to separate them into a contribution coming from  $\delta m$  and one coming from QED. We define the EM contribution by setting  $\delta m = 0$  via  $\Delta M^2 = M_{uu}^2 - M_{dd}^2 = 0$ , with all other

parameters tuned to their physical values. Here,  $M_{\bar{q}q}$  is the mass of a neutral meson  $\bar{q}q$ ,  $q = u, d$ , whose propagator includes only quark-connected diagrams. Using the  $\chi$ PT results of Ref. [10], it is straightforward to show that the difference of these mesons' squared masses is  $\Delta M^2 = 2B_2\delta m + O(\alpha m_{ud}, \delta m m_{ud}, \alpha \delta m, \alpha^2)$ , where  $B_2$  is the  $N_f = 2$  quark condensate parameter. Close to the physical point,  $O(m_{ud})$  can be counted like  $O(\delta m)$ . Thus, our definition of the EM contribution differs from any other valid one by corrections of the size of next-to-leading order (NLO) isospin breaking terms, which are one order higher than the one to which we work here. To obtain the contribution from  $\delta m$ , we set  $\alpha = 0$  and all other parameters to their physical values. In particular, the physical value of  $\Delta M^2$  is obtained from the analysis of  $\Delta M_K^2$  briefly described below and by computing the value of  $\Delta M^2$  corresponding to the physical  $\Delta M_K^2$ . This analysis and its implications for Dashen's theorem [11] and  $m_{u,d}$ , which are very interesting in their own right, will be discussed elsewhere [12].

*Simulation details and parameters.*—We start from our 47, isospin symmetric,  $N_f = 2 + 1$ , QCD ensembles, obtained from simulations with pion masses down to 120 MeV, lattice sizes up to 6 fm, five lattice spacings down to 0.054 fm, and more than 1000 trajectories each [4]. To these ensembles, we add QED gauge degrees of freedom in a way which has now become standard [13–15]. For each QCD gauge configuration, we generate an EM field  $A_\mu(x)$  defined on the links, using the noncompact EM action (in Coulomb gauge) and the methods detailed in Ref. [14]. The gauge potential is then exponentiated as  $U_\mu^{\text{QED}}(x) = \exp[iqeA_\mu(x)]$ . Unlike the QCD links, our QED links undergo no smearing before being coupled to quarks. Similarly, we have not added a clover improvement term for the  $U(1)$  field. The  $U(1)$  fields are then multiplied with the  $SU(3)$  gauge variable on each link and inserted into the Wilson-Dirac operator associated with the quark of charge  $q$  before inversion. The resulting quark propagators are combined into meson and baryon two-point functions. The extended sources and sinks used are the same as in Refs. [3,4].

For most of our  $SU(3)$  ensembles, we have generated two valence data sets, which include QED with the physical value of  $\alpha$ . In the first set (set 1), the bare, valence  $u, d$ , and  $s$  quark masses are individually tuned so that their partially conserved axial current values approximately reproduce the corresponding ensemble's light and strange sea-quark partially conserved axial current masses. Thus, we subtract the  $\alpha/a$  divergences in the valence bare quark masses, which come from the EM self-energy, as described in Ref. [15]. In the second set (set 2), we choose  $m_d$  to be slightly more massive than in the first set so that  $\Delta M^2$  scatters around its physical value from ensemble to ensemble. We have one additional valence data set (set 3) in which  $\alpha$  is varied. The latter includes a point with  $\alpha \sim 2\alpha^{\text{ph}}$  and  $\Delta M^2 \simeq \Delta M^{2,\text{ph}}$ , a

second with  $\alpha \sim \alpha^{\text{ph}}/4$  and a similar  $\Delta M^2$ , and a third with  $\alpha \sim 0$  and  $\Delta M^2 \simeq 0$ . The superscript ph indicates that we are referring to the physical value of a quantity. We have 74 valence points in total, which are shown in the  $M_{\bar{u}u}^2 - M_{\bar{d}d}^2$  plane in Fig. 1. This rich collection of data allows us to gain full control over the dependence of the splittings on all of the relevant parameters.

*Analysis of meson and baryon correlators.*—The time dependence of the  $\pi^+$ ,  $K^+$ ,  $K^0$ , and the  $\Omega^-$  or  $\Xi$  two-point functions is fitted, in the asymptotic regime, to a hyperbolic cosine and an exponential, respectively. For the isospin multiplets whose splittings we wish to determine, we perform a simultaneous, correlated fit to the two-point functions of the two members of the multiplet in which we replace the individual hadron mass parameters by their average and their difference. The time ranges for correlator fits are determined after a systematic study of the goodness of fit as a function of initial and final fitting times. The choices made here are very similar to those of Refs. [3,4].

*Interpolating to the physical point and determining the individual EM and  $\delta m$  contributions.*—Having determined the isospin splittings and relevant hadron masses in lattice units for each of our QCD plus QED data sets, we have to convert them to physical units and extrapolate them to the continuum and infinite-volume limits. We also must interpolate the splittings to the physical mass point, as well as to the mass and EM isospin limits.

We determine the five lattice spacings simultaneously from a combined fit of the data with  $\Delta M^2 \simeq 0$ , for the isospin symmetric observable  $aM_{\Omega^-}$ , or, alternatively,  $aM_{\Xi}$ , using the techniques of Refs. [3,4,9]. The isospin mass splitting  $\Delta M_X$  of a hadron  $X$  is naturally described by the leading order isospin expansion

$$\Delta M_X = A_X \alpha + B_X \Delta M^2, \quad (1)$$

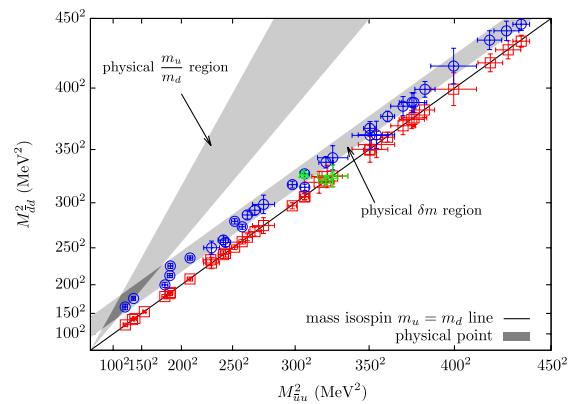


FIG. 1 (color online). Valence data sets plotted in the  $M_{\bar{d}d}^2$  vs  $M_{\bar{u}u}^2$  plane. The red squares (set 1) lie along the mass isospin line  $M_{\bar{u}u}^2 = M_{\bar{d}d}^2$ , and the blue circles (set 2) are scattered around an estimate of the  $\Delta M^{2,\text{ph}}$  region, obtained from the results of Refs. [1,28]. The green triangles (set 3) are points in which  $\alpha$  is varied away from its physical value. For clarity, points with  $M_\pi > 450$  MeV are not shown.

where  $\Delta M^2$  substitutes for  $\delta m$ . The coefficients  $A_X$  and  $B_X$  still depend on the isospin symmetric parameters of the theory, e.g.,  $m_{ud}$  or  $m_s$ . We find that their dependences on these parameters are well described by a linear expansion in  $M_{\pi^+}^2$  and in  $M_{K^X}^2$  for the range of masses retained below.

We must also account for discretization and finite-volume (FV) effects. The latter are particularly important because of the presence of the massless photon. Using techniques from Ref. [16] and performing appropriate asymptotic expansions, it is straightforward to show that the leading finite-volume term in scalar and spinor QED is proportional to  $1/L$ . We find these corrections to be generically large. For instance, in boxes with  $L = 1.6$ – $2.6$  fm, which is the largest range of sizes considered in all but the preliminary work of Ref. [17] on pseudoscalar masses, the correction to  $\Delta_{\text{QED}}M_{\Xi}$ , the QED contribution to  $\Delta M_{\Xi} \equiv M_{\Xi^0} - M_{\Xi^-}$ , ranges from 123% to 76%. This is illustrated in Fig. 2. In our calculation,  $L$  extends up to 6 fm, where the figure indicates a 36% FV correction. While still large, our corrections are sufficiently small that they may be described with a low-order polynomial in  $1/L$ . This is confirmed by the data in Fig. 2, which show no sensitivity to terms beyond linear order in  $1/L$ . The same is true of our results for  $\Delta M_N \equiv M_p - M_n$ , which have a slope in  $1/L$  which is compatible with that of  $\Delta_{\text{QED}}M_{\Xi}$ , but with larger statistical errors. Not surprisingly, the slope in  $\Delta M_{\Sigma} \equiv \Delta_{[\Delta_{I_3=2}]M_{\Sigma}} = M_{\Sigma^+} - M_{\Sigma^-}$  is consistent with zero: the absolute values of the two particles' charges are equal.

Concerning discretization effects, the improvement of the QCD action implies  $O(\alpha_s a, a^2)$  corrections to  $A_X$  and  $B_X$ . However, due to the lack of improvement in the QED sector, discretization effects on  $A_X$  are  $O(a)$ . In our

analysis, we include  $O(a)$  QED discretization effects to  $A_X$  as well as  $O(\alpha_s a, a^2)$  QCD ones to  $B_X$ .

Combining all of this information yields a nine parameter description of each of the mass splittings. In the notation of Eq. (1), this corresponds to

$$A_X = a_0^X + a_1^X[M_{\pi}^2 - (M_{\pi}^{\text{ph}})^2] + a_2^X[M_{K^X}^2 - (M_{K^X}^{\text{ph}})^2] + a_3^X a + a_4^X \frac{1}{L}, \quad (2)$$

$$B_X = b_0^X + b_1^X[M_{\pi}^2 - (M_{\pi}^{\text{ph}})^2] + b_2^X[M_{K^X}^2 - (M_{K^X}^{\text{ph}})^2] + b_3^X f(a), \quad (3)$$

where the  $a_i^X$  and  $b_i^X$  are the parameters and  $f(a) = \alpha_s a$  or  $a^2$ , alternatively. For each splitting, among the nine possible parameters, we have retained all combinations which are such that adding one more dependence to the fit causes the associated parameter to be consistent with zero within one standard deviation.

*Error estimation.*—Our analysis methodology makes no assumptions beyond those of the fundamental theory, except for the isospin symmetry which is maintained in the sea and whose consequences we discuss below. However, the analysis does depend on several choices that can be sources of systematic uncertainties.

To deal with these uncertainties, we proceed with the method put forward in Ref. [9]. More specifically, we consider the following variations in our analysis procedure. For the time ranges of the correlator fits, we consider two initial fit times, one for which we expect negligible excited state contributions and a second, more aggressive one. This estimates the uncertainty due to contributions from excited states. Regarding the choice of scale setting quantities, we consider two possibilities: the mass of the  $\Omega^-$  and that of the isospin averaged  $\Xi$ . To estimate the uncertainty associated with the truncation of the Taylor expansion used to interpolate these two masses to physical  $M_{\pi^+}$ , we vary the fit ranges by excluding all data with pion mass above 400 and 450 MeV. To estimate part of this same uncertainty for the isospin splittings, we consider cuts at  $M_{\pi^+} = 450$  and 500 MeV, since their  $M_{\pi^+}^2$  dependence is very mild. These cuts also provide an estimate of the uncertainty associated with FV corrections, as our simulations keep  $LM_{\pi} \sim 4$ , implying cuts on  $1/L$  as low as  $1/L < 100$  MeV. Part of the uncertainty associated with the continuum extrapolation is determined by considering either  $\alpha_s a$  or  $a^2$  discretization errors. Finally, to estimate any additional uncertainty arising from the truncation of these expansions, we consider the result of replacing either  $A_X$  or  $B_X$  by Padé expressions. These are obtained by considering that the expansions of  $A_X$  and  $B_X$  in Eqs. (2) and (3) are the first two terms of a geometric series which we resum. This resummation is not applied to the FV corrections. Instead, we try adding a  $1/L^2$  term to either the Taylor or Padé forms.

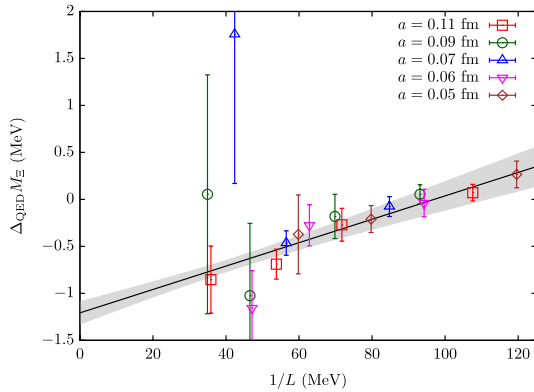


FIG. 2 (color online). Example of FV corrections to  $\Delta_{\text{QED}}M_{\Xi}$ , plotted as a function of  $1/L$ . The dependence of the lattice results on all other variables has been subtracted using a fit of the type described in the text. Results with a same  $1/L$  and  $a$  are averaged because they show no systematic residual dependence on the other simulation parameters, in particular, on quark mass. The linear fit in  $1/L$ , which is performed for points with  $M_{\pi^+} \leq 500$  MeV, has a  $\chi^2/\text{DOF} = 59/67$ . It is plotted as a solid curve, with its  $1\sigma$  band.

TABLE I. Isospin breaking mass differences in MeV for members of the baryon octet. The first error is statistical, and the second is systematic. As discussed in the text, we guesstimate the QED quenching uncertainties on the EM contributions to be  $O(10\%)$ . Propagating the uncertainty in  $\Delta_{\text{QED}}M_K^2$  yields an  $O(4\%)$  error on the  $\delta m$  contributions. The quenching uncertainties on the total splittings can then be obtained by adding those of the EM and  $\delta m$  contributions in quadrature. These guesstimates are not included in the results.

$X$	$\Delta M_X$	$\Delta_{\text{QED}}M_X$	$\Delta_{\text{QCD}}M_X$
$N$	$-0.68(39)(36)$	$1.59(30)(35)$	$-2.28(25)(7)$
$\Sigma$	$-7.84(87)(72)$	$0.08(12)(34)$	$-7.67(79)(105)$
$\Xi$	$-7.16(76)(47)$	$-1.29(15)(8)$	$-5.87(76)(43)$

In all cases, we find the coefficient of this term to be consistent with zero.

These variations lead to  $2^7 = 128$  different fits for each of the isospin splittings and parameter combinations. Correlating these with the 128 fits used to determine  $\Delta M^{2,\text{ph}}$  and allowing various parameter combinations but discarding fits with irrelevant parameters, we obtain between 64 and 256 results for each observable. The central value of a splitting is then the mean of these results, weighted by the  $p$ -value. The systematic error is the standard deviation. Because we account for all correlations, these fit qualities are meaningful. The whole procedure is repeated for 2000 bootstrap samples, and the statistical error is the standard deviation of the weighted mean over these samples. We have also checked that the results are changed only negligibly (far less than the calculated errors) if they are weighted by 1 instead of by the  $p$ -value.

The  $\delta m$  corrections that we do not include in the sea are NLO in isospin breaking and can safely be neglected. The neglected  $O(\alpha)$  sea-quark contributions break flavor  $SU(3)$ . Moreover, large- $N_c$  counting indicates that they are  $O(1/N_c)$ . Combining the two suppression factors yields an estimate  $(M_\Sigma - M_N)/(N_c M_N) \approx 0.09$ . A smaller estimate is obtained by supposing that these corrections are typical quenching effects [18] that are  $SU(3)$  suppressed, or by using [19] the NLO  $\chi$ PT results of Ref. [10]. However, in the absence of direct quantitative evidence, it is safer to assume that the EM contributions to the splittings carry an  $O(10\%)$  QED quenching uncertainty.

*Final results and discussion.*—Combining the methods described above, we obtain our final results for the total octet baryon isospin splittings  $\Delta M_N$ ,  $\Delta M_\Sigma$ , and  $\Delta M_\Xi$  defined above. These results, together with those obtained for the EM and  $\delta m$  contributions, are summarized in Table I. We also plot them in Fig. 3, with the experimental values for the full splittings. Our results are compatible with experiment.

Concerning the separation into  $\delta m$  and EM contributions, there exist very few determinations of these quantities up to now. In the review [20], hadron EM splittings were estimated using a variety of models and Cottingham’s formula

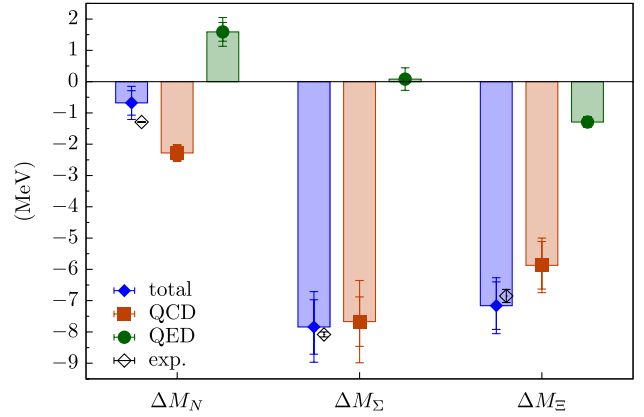


FIG. 3 (color online). Results for the isospin mass splittings of the octet baryons (total) and the individual contributions to these splittings from the mass difference  $m_u - m_d$  (QCD) and from EM (QED). The bands denote the size of these results. The error bars are the statistical and total uncertainties (statistical and systematic combined in quadrature). For comparison, the experimental values for the total splittings are also displayed.

for the nucleon. These estimates are compatible with our results within  $\sim 1.5\sigma$ . The EM nucleon splitting has recently been reevaluated with Cottingham’s formula in Ref. [21], yielding a result which is in better agreement with ours.  $\Delta M_N$  has further been studied with sum rules in Ref. [22].

Besides the entirely quenched, pioneering work of Ref. [23], ours is the only one in which the baryon octet isospin splittings are fully computed. The only other lattice calculation of the full nucleon splitting is presented in Ref. [24]. Like ours, it implements QED only for valence quarks. While their  $\Delta_{\text{QCD}}M_N$  agrees very well with ours, agreement is less good for the EM contribution and total splitting, which they find to be  $0.38(7)$  and  $-2.1(7)$  MeV, respectively. That study was performed in rather small volumes with a limited set of simulation parameters, making an estimate of systematic errors difficult. The few other lattice calculations consider only the  $\delta m$  contributions to the baryon splittings, in  $N_f = 2$  [7,25] and  $N_f = 2 + 1$  [26,27] simulations. The results of Refs. [25–27] rely on imprecise phenomenological input to fix  $m_u/m_d$  or  $(m_u - m_d)$ . The estimate for  $\Delta_{\text{QED}}M_K^2$  of Ref. [28] is used directly in Refs. [25,27] and that of Ref. [29], indirectly in Ref. [26]. The most recent  $N_f = 2$  calculation [7] actually determines  $\Delta_{\text{QED}}M_K^2$  in quenched QED, as we do here for  $N_f = 2 + 1$ .  $\Delta_{\text{QCD}}M_N$  is computed in Refs. [7,25,26], while all three QCD splittings are obtained in Ref. [27]. The latter is also true in Ref. [30], where  $N_f = 2 + 1$  lattice results are combined with  $SU(3)$   $\chi$ PT and phenomenology. Agreement with our results is typically good. In all of these calculations, the range of parameters explored is smaller than in ours, making it more difficult to control the physical limit.

L. L. thanks Heiri Leutwyler for enlightening discussions. We also thank Jérôme Charles and Marc Knecht

for helpful conversations. Computations were performed using the PRACE Research Infrastructure Resource JUGENE at FZ Jülich, with further HPC resources provided by GENCI-[IDRIS/CCRT] (Grant No. 52275) and FZ Jülich, as well as using clusters at Wuppertal and CPT. This work was supported in part by the OCEVU Labex (ANR-11-LABX-0060) and the A\*MIDEX Project (ANR-11-IDEX-0001-02) funded by the “Investissements d’Avenir” French government program managed by the ANR, by CNRS Grants GDR No. 2921 and PICS No. 4707, by EU Grants FP7/2007-2013/ERC No. 208740 and No. MRTN-CT-2006-035482 (FLAVIANet), and by DFG Grants No. FO 502/2 and No. SFB-TR 55.

\*Corresponding author.

a.portelli@soton.ac.uk

†Present address: School of Physics and Astronomy, University of Edinburgh, Edinburgh EH9 3JZ, United Kingdom.

‡Present address: NIC, DESY Platanenallee 6, D-15738 Zeuthen, Germany.

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