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SU(3) flavour symmetry breaking and charmed states

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By extending the SU(3) flavour symmetry breaking expansion from up, down and strange sea quark masses to partially quenched valence quark masses we propose a method to determine charmed quark hadron masses including possible QCD isospin breaking effects. Initial results for some open charmed pseudoscalar meson states and singly and doubly charmed baryon states are encouraging and demonstrate the potential of the procedure. Essential for the method is the determination of the scale using singlet quantities, and to this end we also give here a preliminary estimation of the recently introduced Wilson flow scales.

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1. Motivation and Strategy

At present there is considerable interest in open charm masses. While much is known about $C = 1$ charmed meson masses and singly charmed baryon masses, the situation is far less clear for doubly charmed quark baryons (i.e. $C = 2$ or ccq with $q = u$, d, s). Here many masses are unknown, but as stable states in QCD they must exist (presently only some candidate states are seen by the SELEX Collaboration [1], but not by BaBar [2], or BELLE [3]). Also there are possible relations to tetraquark states. For example in the $n_c \to \infty$, [4], $m_c \to \infty$ limit we expect the relation $M(cc\overline{u}\overline{d}) \approx M_{\Xi_{cc}^{++}} + M_{\Lambda_c^+} - M_{D^0} - (M_{D^{*+}} + M_{D^0})/4$, [5].

The charm quark, c is considerably heavier than the up u, down d and strange s quarks, which has hampered its direct simulation using lattice QCD. However as the available lattice spacings become finer, this is becoming less of an obstacle. The sea quarks in present day $n_f = 2+1$ flavour dynamical lattice simulations consist of two mass degenerate (i.e. $m_u = m_d$) light flavours u, d and a heavier flavour s. Their masses are typically larger than the 'physical' masses necessary to reproduce the experimental spectrum. How can we usefully approach the 'physical' u, d, s quark masses? One possibility suggested in [6] is to consider an $SU(3)$ flavour breaking expansion from a point m_0 on the flavour symmetric line keeping the average quark mass $\overline{m} = (m_u + m_d + m_s)/3$ constant ($= m_0$). This not only significantly reduces the number of expansion coefficients allowed, but the expansion coefficients remain the same whether we consider $m_u \neq m_d$ or $m_u = m_d$. Thus we can also find the pure QCD contribution to isospin breaking effects with just one $n_f = 2+1$ numerical simulation.

The $SU(3)$ flavour breaking expansion can also be extended to valence quark masses, i.e. the quarks making up the meson or baryon have not necessarily the same mass as the sea quarks. The valence quarks are called 'Partially Quenched' or PQ quarks in distinction to the sea or dynamical sea quarks. We call the 'Unitary Limit' when the masses of the valence quarks coincide with the sea quarks. PQ determinations have the advantage of being cheap compared to dynamical simulations and including them allows a better determination of the expansion coefficients over a wider range of quark masses. (This was the strategy pursued in [7].) In addition because the charm quark, c is much heavier than the u, d and s quarks, it contributes little to the dynamics of the sea and so we can regard the charm quark as a PQ quark.

2. Method

We presently only consider hadrons which lie on the outer ring of their associated multiplet and not the central hadrons. (So we need not consider either any mixing or numerical evaluation of quark–line disconnected correlation functions.) The $SU(3)$ flavour symmetry breaking expansion for the pseudoscalar mesons with valence quarks a and b up to cubic or NNLO terms in the quarks masses is given by

$$\begin{aligned} M^2(a\overline{b}) = \; & M_{0\pi}^2 + \alpha(\delta\mu_a + \delta\mu_b) \\ & + \beta_0 \tfrac{1}{6}(\delta m_u^2 + \delta m_d^2 + \delta m_s^2) + \beta_1(\delta\mu_a^2 + \delta\mu_b^2) + \beta_2(\delta\mu_a - \delta\mu_b)^2 \\ & + \gamma_0 \delta m_u \delta m_d \delta m_s + \gamma_1(\delta\mu_a + \delta\mu_b)(\delta m_u^2 + \delta m_d^2 + \delta m_s^2) \\ & + \gamma_2(\delta\mu_a + \delta\mu_b)^3 + \gamma_3(\delta\mu_a + \delta\mu_b)(\delta\mu_a - \delta\mu_b)^2 \, , \end{aligned} \tag{2.1}$$

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with $\delta\mu_q = \mu_q - \overline{m}$, $q = a, b, \ldots \in \{u, d, s, c\}$ being valence quarks of arbitrary mass, μ_q and $\delta m_q = m_q - \overline{m}$, $q \in \{u, d, s\}$ being sea quarks. (These have the automatic constraint $\delta m_u + \delta m_d + \delta m_s = 0$.) Note that we have some mixed sea/valence mass terms. The unitary limit occurs when $\delta\mu_q \to \delta m_q$. The expansion coefficients are $M^2_{0\pi}(\overline{m})$, $\alpha(\overline{m})$, ... so if $\overline{m}$ is held constant then we have constrained fits to the numerical data. In particular a $n_f = 2+1$ flavour simulation, when $\delta m_u = \delta m_d \equiv \delta m_l$ is enough to determine the expansion coefficients. We now use the PQ (and unitary) data to determine the expansion coefficients (i.e. αs, βs, γs). This in turn leads to a determination of the 'physical' quark masses δm_u^*, δm_d^*, δm_s^* and $\delta\mu_c^*$ by fitting to e.g. $M^{\rm exp}_{\pi^+}(u\overline{d})$, $M^{\rm exp}_{K^+}(u\overline{s})$ and $M^{\rm exp}_{\eta_c}(c\overline{c})$. We can now describe pseudoscalar open charm states with the same wavefunction (and hence expansion) $\mathscr{M} = \overline{q}\gamma_5 c$ ($q = u,\ d,\ s$) i.e. $D^0(c\overline{u})$, $D^+(c\overline{d})$ and $D_s^+(c\overline{s})$. Using δm_u^*, δm_d^*, δm_s^* and $\delta\mu_c^*$ gives estimates of their physical masses.

Similarly for the baryon octet the same procedure can be applied. We have the $SU(3)$ flavour symmetry breaking expansion

$$\begin{aligned}
M^2(aab) \;=\; & M^2_{0N} + A_1(2\delta\mu_a + \delta\mu_b) + A_2(\delta\mu_b - \delta\mu_a) \\
& + B_0 \tfrac{1}{6}(\delta m_u^2 + \delta m_d^2 + \delta m_s^2) + B_1(2\delta\mu_a^2 + \delta\mu_b^2) + B_2(\delta\mu_b^2 - \delta\mu_a^2) + B_3(\delta\mu_b - \delta\mu_a)^2 \\
& + C_0 \delta m_u \delta m_d \delta m_s + [C_1(2\delta\mu_a + \delta\mu_b) + C_2(\delta\mu_b - \delta\mu_a)](\delta m_u^2 + \delta m_d^2 + \delta m_s^2) \\
& + C_3(\delta\mu_a + \delta\mu_b)^3 + C_4(\delta\mu_a + \delta\mu_b)^2(\delta\mu_a - \delta\mu_b) \\
& + C_5(\delta\mu_a + \delta\mu_b)(\delta\mu_a - \delta\mu_b)^2 + C_6(\delta\mu_a - \delta\mu_b)^3 \,,
\end{aligned} \tag{2.2}$$

(so for example $M_p = M(uud)$). Again we use PQ (and unitary) data to first determine the expansion coefficients (i.e. the As, Bs, Cs). We can then describe charm states with the same nucleon like wavefunction and hence same expansion. For example for single open charm ($C = 1$) states we have $\Sigma_c^{++}(uuc)$, $\Sigma_c^0(ddc)$, $\Omega_c^0(ssc)$ which all have the wavefunction $\mathscr{B} = \varepsilon(q^T C\gamma_5 c)q$ ($q = u$, d, s) while for double open charm ($C = 2$) states we have $\Xi_{cc}^{++}(ccu)$, $\Xi_{cc}^{+}(ccd)$, $\Omega_{cc}^{+}(ccs)$ which all have the wavefunction $\mathscr{B} = \varepsilon(c^T C\gamma_5 q)c$ ($q = u,\ d,\ s$). In both cases using δm_u^*, δm_d^*, δm_s^* and $\delta\mu_c^*$ gives estimates of these physical masses.

3. Lattice details

We use a tree level Symanzik gluon action and an $O(a)$ improved clover fermion action, including mild stout smearing [8]. Thus the quark mass is given by

$$m_q = \frac{1}{2}\left(\frac{1}{\kappa_q} - \frac{1}{\kappa_{0c}}\right), \tag{3.1}$$

where κ_q is the hopping parameter, κ_0 is the hopping parameter along the symmetric line with κ_{0c} being its chiral limit. We shall consider two lattice spacings ($\beta = 5.50$ on $32^3 \times 64$ lattices and preliminary results for $\beta = 5.80$ on $48^3 \times 96$ lattices).

We shall now briefly mention here our progress in defining and determining the scale using singlet quantities, collectively denoted here by X_S. There are many possibilities such as pure gluon quantities like the r_0 Sommer scale: $X_{r_0} = 1/r_0$, or the $\sqrt{t_0}$ [9], w_0 [10] scales based on the Wilson gauge action flow: $X_{t_0} = 1/\sqrt{t_0}$, $X_{w_0} = 1/w_0$, or quantities constructed using fermions. One simple possibility in this case is to take the 'centre of mass' of the hadron octet. In all these cases it can

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easily be shown that linear terms in δm_q are absent, [6]. We then have from eqs. (2.1), (2.2) in the unitary limit (with $\overline{\delta m^2} = (\delta m_u^2 + \delta m_d^2 + \delta m_s^2)/3$)

$$X_\pi^2 = \tfrac{1}{6}(M_{K^+}^2 + M_{K^0}^2 + M_{\pi^+}^2 + M_{\pi^-}^2 + M_{\overline{K}^0}^2 + M_{K^-}^2) = M_{0\pi}^2 + \left(\tfrac{1}{2}\beta_0 + 2\beta_1 + 3\beta_2\right)\overline{\delta m^2} + \ldots, \quad (3.2)$$

and

$$X_N^2 = \tfrac{1}{6}(M_p^2 + M_n^2 + M_{\Sigma^+}^2 + M_{\Sigma^-}^2 + M_{\Xi^0}^2 + M_{\Xi^-}^2) = M_{0N}^2 + \tfrac{1}{2}(B_0 + B_1 + B_3)\overline{\delta m^2} + \ldots. \quad (3.3)$$

In the left panel of Fig. 1 we plot various singlet quantities $(a_S X_S)^2$ for $S = t_0,\ w_0,\ \pi,\ \rho,\ N$. It is

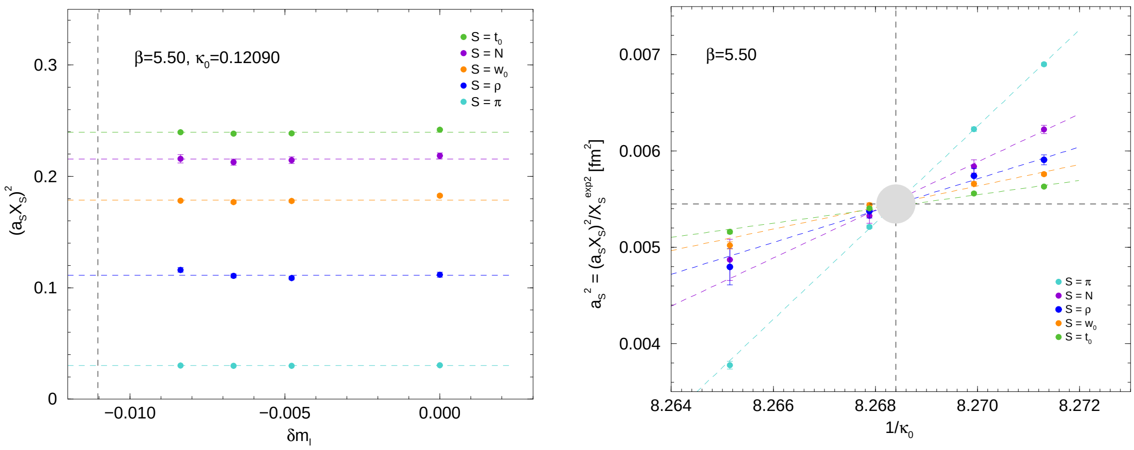

Figure 1: Left panel: $(a_S X_S)^2$ for $S = t_0$, N, w_0, ρ and π along the unitary line, from the symmetric point $\delta m_l = 0$ down to the physical point $\delta m_l^* = (\delta m_u^* + \delta m_d^*)/2$ (vertical dashed line) together with constant fits (for $\beta = 5.50$, $\kappa_0 = 0.12090$). Right panel: Values of a_S^2 for $S = \pi$, N, ρ, w_0 and t_0 using eq. (3.4) for κ_0 values on the symmetric line from $\kappa_0 = 0.12090$ to $\kappa_0 = 0.12099$, for $\beta = 5.50$, together with quadratic fits. The crossing of the horizontal and vertical dashed lines and circle gives an estimate for the common scale.

apparent that the constancy $(a_S X_S)^2$ holds over the complete range from the symmetric point down to the physical point. Using this enables us to use $X_S^{\rm exp}$ to determine the lattice spacing by

$$a_S^2 = \frac{(a_S X_S)^2}{X_S^{\rm exp\,2}}. \quad (3.4)$$

We shall define our lattice spacing here using $S = N$: a_N. Of course depending on how well we have chosen our initial κ_0 point, using a different singlet quantity (i.e. $S \neq N$) will give a slightly different lattice spacing. More ambitiously we can vary κ_0 to try to find a point where we have a common scale. We have initiated a programme to investigate this. In the right panel of Fig. 1 we plot a_S^2 again for $S = \pi$, N, ρ, w_0, t_0 against various κ_0. The crossing of the a_S^2s for $S = \pi$, N and ρ give an estimation of the common scale as $a \approx 0.074(2)$ fm. We can now adjust $X_{t_0}^{\rm exp}$, $X_{w_0}^{\rm exp}$ to also cross at this point to find a preliminary estimate for these 'intermediate scales' of $\sqrt{t_0}^{\rm exp} \approx 0.153(7)$ fm, $w_0^{\rm exp} \approx 0.179(6)$ fm.

Practically it is numerically advantageous to form dimensionless ratios (within a multiplet): $\widetilde{M}^2 \equiv M^2/X_S^2$ and re-write eqs. (2.1), (2.2) in terms of $\widetilde{\alpha} \equiv \alpha/M_{0\pi}^2, \ldots$ and $\widetilde{A}_i \equiv A_i/M_{0N}^2, \ldots$ in the expansions. About $\sim O(80)$ PQ and unitary masses are used to determine these expansion coefficients and hence the 'physical' quark masses δm_u^*, δm_d^*, δm_s^* and $\delta \mu_c^*$ as described in section 2.

4. Results and Conclusions

We now discuss our results. In Fig. 2 left panel, we show the diagonal pseudoscalar mesons

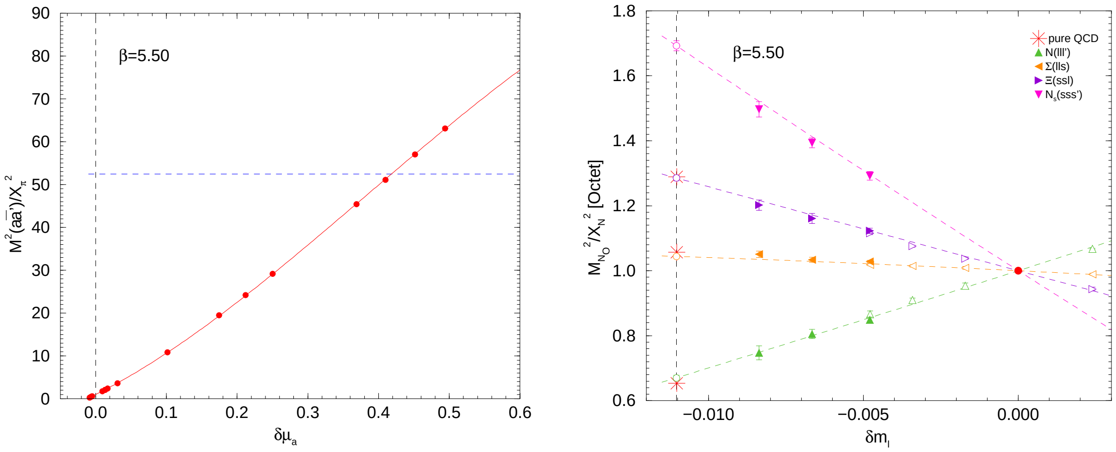

Figure 2: Left panel: $\widetilde{M}^2(a\bar{a}') = M^2(a\bar{a}')/X_\pi^2$ versus $\delta\mu_a$ for $\beta = 5.50$, together with the fit from eq. (2.1). The vertical dashed line represents the symmetric point, while the horizontal dashed line is the physical value of $\widetilde{M}^2_{\eta_c}$. Right panel: 'fan' plot for the baryon octet, from the symmetric point $\delta m_l = 0$ to the physical point $\delta m_l^* = (\delta m_u^* + \delta m_d^*)/2$ (vertical dashed line and stars) for $\beta = 5.50$. The filled triangles are from $32^3 \times 64$ sized lattices, while the open triangles are from $24^3 \times 48$ sized lattices (not used in the fits). The fits are again given from eq. (2.1).

$\widetilde{M}^2(a\bar{a}')$ (to avoid a three dimensional plot) versus $\delta\mu_a$ together with the fit from eq. (2.1) (using the prime notation a' to mean a distinct quark from a but degenerate in mass). The horizontal dashed line represents the physical value of $\widetilde{M}^2_{\eta_c}$, the intersection with the fit curve gives a determination of $\delta\mu_c^*$. In the right panel we show a 'fan' plot of $\widetilde{M}^2_N$, $\widetilde{M}^2_\Sigma$, $\widetilde{M}^2_\Xi$ and $\widetilde{M}^2_{N_s}$ against δm_l, together with the fit using eq. (2.1). Note that the scales involved are rather different, for the unitary masses $|\delta m_l| \sim 0.01$ and the LO terms in eq. (2.1) or (2.2) dominate, [6], while for the PQ masses (reaching up to the charm masses) we have $\delta\mu_a \sim 0.4$ but still with rather moderate curvature.

In Fig. 3 we show $D^0(c\bar{d})$, $D^+(c\bar{d})$ and $D_s^+(c\bar{s})$ against our a_N^2 lattice spacings (left panel) and their mass differences (right panel). These mass differences in particular are sensitive to unknown QED effects (the present computation is for pure QCD only). As we currently have only two lattice spacings (and are also increasing their statistics) the results are to be regarded as preliminary and we do not presently attempt a continuum extrapolation. However there do not seem to be strong scaling violations present.

In Figs. 4 and 5 we show the $C = 1$ and $C = 2$ charmed baryons (from the spin $1/2$ 20-plet). Again while we do not see significant lattice effects in either case, we gain an impression that those present are a little larger for the doubly charmed baryons than for the singly charmed mesons.

In conclusion we note that we have developed a method to determine some open charm states using a precise $SU(3)$ flavour symmetry breaking expansion enabling u, d, s quarks to approach the physical point while the c quark is treated as PQ. The expansion appears to be highly convergent. The method can be extended to other states. In a $2+1$ world there is no Σ^0 - Λ^0 mixing, but the determined coefficients can be used to compute $\Sigma^0(uds)$ - $\Lambda^0(uds)$ mixing, [12]. Therefore

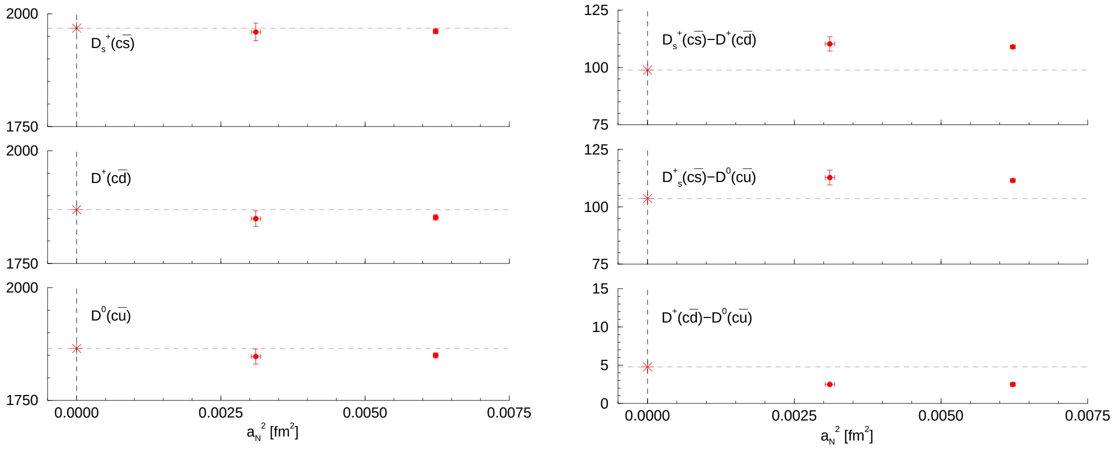

Figure 3: Left panel: $D^0(c\bar{u})$, $D^+(c\bar{d})$ and $D_s^+(c\bar{s})$. Right panel: $D^+(c\bar{d}) - D^0(c\bar{u})$, $D_s^+(c\bar{s}) - D^0(c\bar{u})$ and $D_s^+(c\bar{s}) - D^+(c\bar{d})$ mass splittings. (All values in MeV.) The experimental values are given as red stars. To guide the eye, we extend these values as horizontal dashed lines.

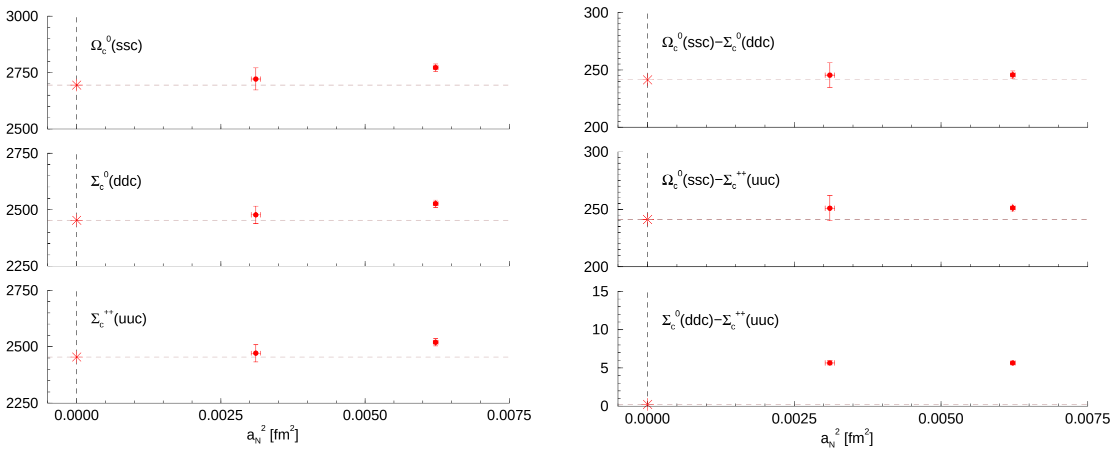

Figure 4: Left panel: $\Sigma_c^{++}(uuc)$, $\Sigma_c^0(ddc)$, $\Omega_c^0(ssc)$. Right panel: $\Sigma_c^0(ddc) - \Sigma_c^{++}(uuc)$, $\Omega_c^0(ssc) - \Sigma_c^{++}(uuc)$, $\Omega_c^0(ssc) - \Sigma_c^0(ddc)$ mass splittings.

computing e.g. Σ_c^+ - Λ_c^+, Ξ_c^0 - $\Xi_c^{\prime 0}$ mixing is possible. Furthermore the method can be applied to the baryon decuplet and QED effects can be introduced, [13].

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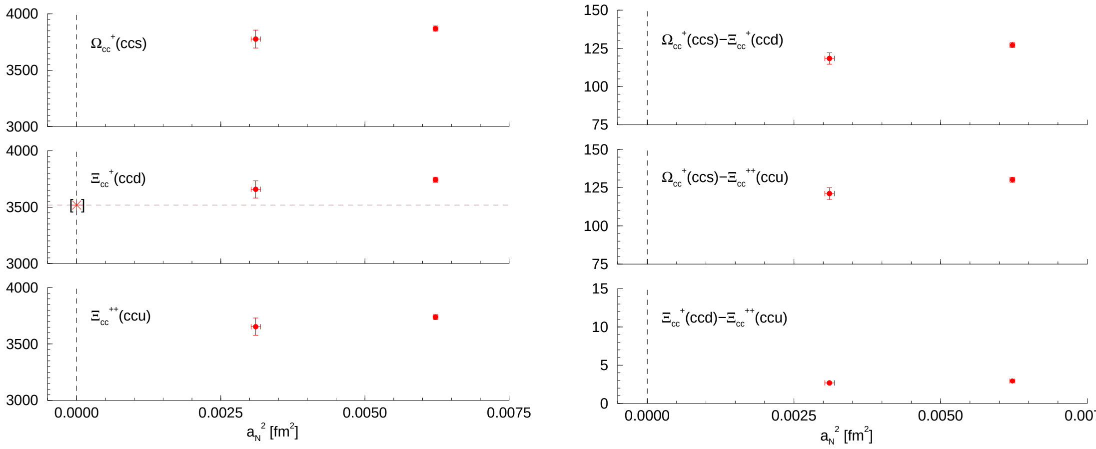

Figure 5: Left panel: $\Xi_{cc}^{+}(ccd) - \Xi_{cc}^{++}(ccu)$. The SELEX Collaboration result, [1], for Ξ_{cc}^{+} is shown as a red star. Right panel: $\Omega_{cc}^{+}(ccs) - \Xi_{cc}^{++}(ccu)$, $\Omega_{cc}^{+}(ccs) - \Xi_{cc}^{+}(ccd)$ mass splittings.

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