Lattice QCD Calculations and α_{s}

Andreas S. Kronfeld Fermilab 11 February 2011 Workshop on Precision Measurements of α_s Max-Planck-Insitut für Physik, München





Requirements for α_s Determinations

- A dimensionless quantity, R, sensitive to QCD at a (range of) short distance(s), Q^{-1} ;
 - if not dimensionless, use Q to make it so; then $R = \mathcal{R}(\alpha_s(Q_s)) + o((\Lambda_{QCD}/Q)^r)$.
- A theoretical framework—or at least a notion—to separate short-distance scales from Λ_{QCD} (and other long-distance scales).
- An N^{*n*}LO/N^{*n*}LL calculation of $\mathcal{R}(\alpha_s(Q_s))$; recall α_s^{-1}
- Measurements of R over a range of Q large enough to control power-law effects, $(\Lambda_{QCD}/Q)^r$.
- Control of non-QCD physics at scales probed by *Q* (*e.g.*, electroweak or new physics).
- A measurement of Q—usually a *calibration*, in contrast to *event counting* for R.



$$(Q) \approx 2\beta_0 \ln(Q/\Lambda_s).$$

Tevatron α_s from Inclusive-Single-Jet Production CDF, <u>arXiv:hep-ex/0108034</u>

- $Q = E_T$, $R = E_T^3 d\sigma/dE_T \propto \alpha_s^2$ @ LO.
- Factorization; \mathcal{R} to NLO [Ellis & Sexton].
- 33 independent E_T bins; range $\times 8$.
- $\alpha_s = 0.1178 \pm 0.0022 \pm 0.0082 \pm 0.0085$:
 - errors from R (stats+norm), \mathcal{R}, Q .
- Calibration measurement of *Q*!!!
- Quark substructure for $E_T > 250 \text{ GeV}$?



α_s from Lattice QCD

- How is *R* "measured"?
- What's Q?
- Frameworks for scale separation.
- Perturbative calculations of $\mathcal{R}(\alpha_s(Q_s))$ at NNLO or N³LO.
- How many "measurements"?
- Extrapolate from computer to QCD.
- How is *Q* calibrated?



• Compute *R* from QCD functional integral.

• $Q = a^{-1}$ (lattice), Q, $2m_Q$, L^{-1} (box).

• Symanzik EFT, OPE, duality....

• Lattice perturbation theory ($Q = a^{-1}$); continuum perturbation theory (else).

• Several to numerous.

• Discretization; unphysical quark masses.

• Ultimately hadron masses: Q = (Qa/Ma)M.

5

Outline

• Introduction: How to Determine α_s

• Lattice Gauge Theory in a Nutshell

• Overview of Lattice QCD α_s Methods

From Computer to QCD

Summary & Outlook





Lattice Gauge Theory in a Nutshell

Lattice Gauge Theory

- Invented to understand asymptotic freedom without the need for gauge-fixing and ghosts [Wilson, <u>hep-lat/0412043</u>].
- Gauge symmetry on a spacetime lattice:
 - mathematically rigorous definition of QCD functional integrals;

$$\langle \bullet \rangle = \frac{1}{Z} \int \mathcal{D}U \mathcal{D}\Psi \mathcal{D}$$

- enables theoretical tools of statistical mechanics in quantum field theory and provides a basis for constructive field theory.
- Lowest-order strong coupling expansion demonstrates confinement.

K. Wilson, <u>PRD 10 (1974) 2445</u>

 $\nabla \bar{\Psi} \exp(-S)[\bullet]$

Numerical Lattice QCD

- Nowadays "lattice QCD" usually implies a numerical technique.
- Integrate the functional integral on a $N_3^3 \times N_4$ lattice (spacing *a*) numerically:

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- Finite lattice: can evaluate integrals on a computer; dimension ~ 10^8 , using *importance sampling*.
- Healthy research field to devise MC algorithms.





 $L = N_{s}a$

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 $L = N_{s}a$

- Some compromises:
 - finite human lifetime \Rightarrow Wick rotate to Euclidean time: $x^4 = ix^0$;
 - finite memory \Rightarrow finite space volume & finite time extent; nonzero lattice spacing;
 - finite CPU power \Rightarrow light quarks heavier than up and down; nonzero lattice spacing.
- The first introduces no error, but can be an obstacle (*e.g.*, fragmentation functions).
- Finite volume unimportant for stable hadrons.
- Continuum and chiral limits are crucial when calibrating physical units (*i.e.*, computing mass spectrum), but for α_s recall $\delta M \Rightarrow \delta \alpha_s = \frac{1}{2}\beta_0 \alpha_s^2 \delta M$.

Some Jargon

• QCD observables (quark integrals by hand):

$$\langle \bullet \rangle = \frac{1}{Z} \int \mathcal{D}U \prod_{f=1}^{n_f} \det(\not D + m_f) \exp\left(-S_{\text{gauge}}\right) \left[\bullet\right]$$
sea vale

- Quenched means replace det with 1.
- Unquenched means not to do that.
- Partially quenched (usually) doesn't mean " n_f too small", but $m_{val} \neq m_{sea}$, or $D_{val} \neq D_{sea}$ ("mixed action").



ence: $(D + m)^{-1}$

(Obsolete.)



- Staggered quarks, with rooted determinant, $O(a^2)$.
- Wilson quarks, O(a):
 - twisted mass term—auto O(a) improvement $\Rightarrow O(a^2)$;
 - tree or nonperturbatively O(a) improved $\Rightarrow O(a^2)$.
- Ginsparg-Wilson (domain wall or overlap), $O(a^2)$:
 - $D\gamma_5 + \gamma_5 D = 2aD^2$ implemented w/ sign(D_W).



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- Many numerical simulations with sea quarks are called (perhaps misleadingly) "full QCD."
 - $n_f = 2$: with same mass, omitting strange sea;
 - $n_f = 3$: may (or may not) imply 3 of same mass;
 - $n_f = 2 + 1$: strange sea + 2 as light as possible for up and down;
 - $n_f = 2 + 1 + 1$: add charmed sea to 2 + 1.
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From the Computer to QCD

The QCD Lagrangian

• SU(3) gauge symmetry and $1 + n_f + 1$ parameters:

$$\mathcal{L}_{\text{QCD}} = \frac{1}{g_0^2} \operatorname{tr}[F_{\mu\nu}F^{\mu\nu}] - \sum_f \bar{\Psi}_f (\not{D} + m_f) \Psi_f + \frac{i\theta}{32\pi^2} \varepsilon^{\mu\nu\rho\sigma} \operatorname{tr}[F_{\mu\nu}F_{\rho\sigma}$$

- Observable CP violation $\propto \vartheta = \theta \arg \det m_f$ (if all masses nonvanishing):
 - neutron electric-dipole moment sets limit $\vartheta \leq 10^{-11}$.

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m_{Ω} or Y(2S-1S) or f_{π} or r_1 or

 m_{π} , m_K , m_{Ds} or $m_{J/\psi}$, m_{Bs} or m_Y ,

 $\theta = 0.$

Systematic Uncertainties and Effective Field Theories ASK, <u>hep-lat/0205021</u>

• Multi-scale problem: m_u , m_s , m_π , m_K , Λ_{QCD} , m_c , m_b , m_t ; Q^2 ; a^{-1} ; L^{-1} .



Most conveniently handled with effective field theories.

Scale	Effective field theory	Small parameter	Physics	
a^{-1}	Symanzik EFT	Λa	Discretization errors: $o((\Lambda a)^n)$	
тq	HQET	Λ/m_Q	Nearly static heavy quark	
	NRQCD	<i>p/m</i> _Q ~ <i>v</i>	Slowly orbiting QQ	
$m_q, m_{\rm PS}$	Chiral PT (χPT)	$(m_{\rm PS}/4\pi f_\pi)^2 \sim m_q/\Lambda$	Chiral symmetry constrains pion cloud	
L^{-1}	Lüscher EFT, χ PT	$\exp(-m_{\pi}L)$, $(\Lambda L)^{-1}$	Self-energy "around the world"	

Symanzik EFT (outgrowth of Callan-Symanzik equation) provides a framework for

- "improving" the action;
- guiding the continuum limit.
- Chiral perturbation theory removes the (too massive, too compact) pion cloud of the computer, and replaces it with the real one: $m_q \rightarrow m_u$.
 - Some recent work (PACS-CS, BMW) has m_q so close to m_d that χ PT isn't needed.

Symanzik Effective Field Theory K. Symanzik, NPB **226** (1983) 187, ibid. 205; P. Weisz, NPB **212** (1983) 1; NPB **236** (1984) 397

• Illustrate with pure gauge theory. Classically,

$$\mathcal{L}_{\text{LGT}} \approx \frac{1}{g_0^2} \left\{ \text{tr} F_{\mu\nu} F^{\mu\nu} + a^2 \mathcal{K}_1 \text{tr} [D_\mu F_{\mu\nu} D^\mu F^{\mu\nu}] + a^2 \mathcal{K}_1 \right\}$$

• Symanzik formalizes this idea to include radiative corrections:

$$\mathcal{L}_{\text{LGT}} \doteq \frac{1}{g^2} \left\{ \text{tr} F_{\mu\nu} F^{\mu\nu} + a^2 \mathcal{K}_1(g^2) \, \text{tr} [D_\mu F_{\mu\nu} D^\mu F^{\mu\nu}] \right\}$$

- Consider these operators to be renormalized, *i.e.*, with power divergences subtracted off.
- Structure established in perturbation theory and believed to hold nonperturbatively.
- Symanzik provides a "continuum-QCD description" of lattice QCD's discretization effects.

 $a^2 \mathcal{K}_2 \operatorname{tr}[F^{\nu}_{\mu} F^{\rho}_{\nu} F^{\mu}_{\rho}] + a^2 \mathcal{K}_3 \operatorname{tr}[D^{\mu} F_{\mu\nu} D_{\rho} F^{\rho\nu}] + \cdots \}$

 $+a^2 \mathcal{K}_2(g^2) \operatorname{tr}[F^{\nu}_{\mu} F^{\rho}_{\nu} F^{\mu}_{\rho}] + \operatorname{redundant} + \cdots \}$

Fermions and Chiral Symmetry

• Lattice fermions coexist uneasily with axial symmetries:

Discretization	$U_V(1)$	$SU_V(n_f)$	$SU_A(n_f)$	U _A (1)
Ginsparg-Wilson*				magic
Wilson			broken, o(a)	broken, a/a
Staggered [†]		Γ_4	$U_A(n_r)$	broken, a/a
Rooted staggered		$SU(n_f) \subset SU(4n_f)$		broken, a/a

* symmetries exact for overlap; domain-wall fermions break axial symmetries at $o(exp(-mL_5))$

[†] with n_r staggered fermion fields, the number of physical species $n_f = 4n_r$

- If the lattice action is ultra-local, then there is either a 16-fold replication of species (naive), the axial symmetries are explicitly broken (Wilson), or a compromise (staggered/Susskind).
- Lattice-artifact chiral-symmetry breaking still treatable with chiral perturbation theory.

- Broad consensus that (unrooted) staggered, Wilson, domain-wall, & overlap all yield QCD.
- To reduce the 4-fold replication of staggered species (aka "tastes"), one can replace sea

$$\det_{\mathbf{4}} \left(D_{\text{stag}} + m \right) \to \left[\det_{\mathbf{4}} \left(D_{\text{stag}} + m \right) \right]^{1/4}$$

• Weak coupling suggests, and numerical simulation corroborates, that staggered fermions have a "taste" basis in which

$$D_{\text{stag}} + m \doteq \begin{pmatrix} \not D + m & a\Delta \\ & \not D + m \\ & a\Delta & \not D + m \\ & a\Delta & & \not D + m \end{pmatrix},$$

where $a\Delta$ leads to discretization errors of $o(a^2)$.

• This structure suggests that the fourth root yields one species in the continuum limit.

- Rooting violates unitarity at nonzero $a \neq 0$, but if SU(4) emerges as a "phantom" symmetry, it provides a "safe house" for these effects, *cf.* scalar and longitudinal gluon polarizations.
- Numerical evidence that these effects can be handled with "rooted staggered chiral perturbation theory"; for example, $n_r = 0.28(2)(3)$ [MILC, arXiv:0710.1118 [hep-lat]].
- Concerns remain along two lines of reasoning:
 - UV: perhaps rooted sea leads to anomalous dimension -1 for $a\Delta$;
 - IR: symmetries of the 't Hooft vertex incompatible with rooting.
- Assuming correctness, uncertainties from rooting are part of chiral extrapolation error bar.
- Everyone agrees that calculations with rooted staggered sea should be repeated with other formulations of sea quarks.

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no evidence

wrong derivation

2+1 Sea Quarks!



HPQCD, MILC, Fermilab Lattice, <u>hep-lat/0304004</u>

- *a* = 0.12 & 0.09 fm;
- $O(a^2)$ improved: asqtad;
- FAT7 smearing;
- $2m_l < m_q < m_s;$
- π , K, Y(2S-1S) input.

Predictions Fermilab Lattice, MILC, HPQCD, <u>hep-ph/0408306</u>, <u>hep-lat/0411027</u>, <u>hep-lat/0506030</u>



22

Hadron Spectrum

2000 1500 ___Σ* M[MeV] 000 experiment 500 **⊸**−K width QCD ₫ - π 0

QCD postdicts the low-lying hadron masses

e.g., BMW Collaboration: <u>Science **322** (2008) 1224</u>



Light Quark Masses

- The nonzero pion (kaon) mass is very sensitive to the light (strange) masses.
- Chiral perturbation theory predicts *ratios* of masses, but not the overall scale.

Lattice QCD	MILC	<u>RBC</u>	BMW	HPQCD	
$\overline{m}_u(2 \text{ MeV})$	1.9 ± 0.2	2.24 ± 0.35	2.15 ± 0.11		
$\overline{m}_u(2 \text{ MeV})$	4.6 ± 0.3	4.65 ± 0.35	4.79 ± 0.14		
$\overline{m}_s(2 \text{ MeV})$	88 ± 5	97.6 ± 6.2	95.5 ± 1.9	92.4 ± 1.5	
$\overline{m}_c(\overline{m}_c)$				1268 ± 9	

• Competitive results for *m_s* from elsewhere?

Pertinent Synopsis

- The spectrum results suggest that the calibration step is understood:
 - Continuum limit under control: 3–5 different lattice spacings—up to ×3;
 - Chiral extrapolation under control;
 - Finite-volume effects small (as expected for masses of stable particles);
 - Several groups (MILC, PACS-CS, BMW) with 2+1 spectrum and few % errors.
- Influential results: matrix elements for flavor physics (aids search for NP in B decays and mixing), thermodynamics (early universe, heavy ions), chiral condensate (Nambu's pion), nucleon sigma term (relevant to DM search), nucleon structure (parton densities), nucleon interactions (neutron stars)

goldplated

Methods for α_{s}

Matching

- Lattice perturbation theory is completely well-defined.
- Compute a renormalized (*e.g.*, BPHZ) coupling α_R (= R) with lattice and dimensional regulators.
- Equate $\alpha_{\rm R} = \alpha_{\rm R}$, obtaining $\bar{\alpha}^{-1}(\mu) = \alpha_0^{-1} \bar{C}_0(\mu a) + \cdots$; asymptotically, $\Lambda_{\overline{\rm MS}} = \Lambda_0 \exp\left[\bar{C}_0(1)/2\beta_0\right]$.
- Theory of power effects is Symanzik EFT.
- Range of $Q = a^{-1}$ limited.
- With standard lattice actions, asymptopia is too far away and convergence is too slow to be useful.

Lattice Perturbation Theory

- The lattice gauge field is $U_{\mu}(x) = \operatorname{Pexp}\left[ag_0 \int_x^{x+ae_{\mu}} \mathrm{d}s A_{\mu}(x+sae_{\mu})\right]$.
- In the perturbation expansion, the second-order part of U_{μ} leads to an extra-gluon vertex, suppressed by *a*.
- These vertices lead to tadpole diagrams. Pre-factors of *a* are cancelled by inverse powers from UV divergent loop integrals.
- Tadpoles lead to large coefficients of α_s and explain the bad behavior of the previous slide.
- These cancel in various "tadpole-improved" combinations of short-distance coefficients.
- A further key to making lattice perturbation theory viable is to eliminate g₀, for example, by re-expanding short-distance quantities in a (quasi-)renormalized coupling.

Lepage and Mackenzie, PRD 48 (1992) 2250

Small Wilson Loops

- Wilson loop $W(\mathcal{P}) = \operatorname{Re} \langle \operatorname{trexp} \oint_{\mathcal{P}} dz \cdot A \rangle$ has UV singularities.
- Creutz ratios $\chi(N_1, M_1, N_2, M_2) = \frac{W(N_1 \times M_1)W(N_2 \times M_2)}{W(N_2 \times M_1)W(N_1 \times M_2)}$ cancels these, but still has UV behavior.
- Tadpole-improved Wilson loops: cancel sides.
- OPE/Symanzik: $W_{N \times M} = Z_{N \times M}(\alpha_s) + a^4 \mathcal{K}_{N \times M}(\alpha_s) \alpha_s \operatorname{tr} G_{\mu\nu} G^{\mu\nu}$ so some condensate information must be accounted for.
- $R = -\ln W$, $-\ln \chi$; Q = d/a, with d estimated via BLM.
- Range of Q at present is $\sim 6 = 1.8/0.3$.
- \mathcal{R} to NNLO.

HPQCD, arXiv:0807.1687; Maltman, arXiv:0807.2020

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Adler Function

• Vacuum polarization at space-like momentum transfer—ideal for Euclidean field theory:

$$\mathsf{FT}\langle J_{\mu}(x)J_{\nu}(0)\rangle = \left(\delta_{\mu\nu}Q^2 - Q_{\mu}Q_{\nu}\right)$$

- Let $\Pi = \Pi_V^{(0)} + \Pi_V^{(1)} + \Pi_A^{(0)} + \Pi_A^{(1)}$ and $R(Q^2) = D(Q^2) = -Q^2 \, d\Pi/dQ^2$, which has a continuum limit. Use nonsinglet currents.
- Operator product expansion (OPE):

$$R(Q^2) = \mathcal{R}\left(\alpha_s(Q^2)\right) + \frac{\bar{m}^2}{Q^2}\mathcal{R}_m\left(Q^2\right) + \frac{\bar{m}$$

known to N³LO in continuum pQCD. (Cited JLQCD publication uses NNLO.)

• Compute $R(Q^2)$ for $a \ll Q^{-1} \ll \Lambda_{QCD}$, take continuum limit, extract α_s .

JLQCD, <u>arXiv:1002.0371</u>

 $\Pi_{I}^{(1)}(Q^{2}) + Q_{\mu}Q_{\nu} \Pi_{I}^{(0)}(Q^{2})$

 $(\alpha_s(Q^2)) + \text{condensates}$

Moments of the Charmonium Correlator Bochkarev & de Forcrand, hep-lat/9505025; HPQCD+KIT, arXiv:0805.2999

• Similar idea, but now J is a $\bar{c}c$ current; in particular $m_c \bar{c} \gamma^5 c$. Take moments:

$$G_n = a \sum_t t^n a^3 \sum_{\boldsymbol{x}} m_c^2 \langle \bar{c} \boldsymbol{\gamma}^5 c(\boldsymbol{x}, t) \bar{c} \boldsymbol{\gamma}^5 c(\boldsymbol{0}) \rangle = \frac{\mathcal{R}_a \left(\alpha_s(2m_c) \right)}{[\bar{m}_c(2m_c)]^{n-4}} + o\left((m_c a)^2 \right) + o\left((\Lambda/2m_c)^2 \right)$$

where \mathcal{R}_n is computed in continuum PT; known to NNLO.

- Use $G_4 = \mathcal{R}_4$ for α_s ; others for m_c (and cross checks).
- Moments correspond to derivatives of the Fourier transformed correlator at $q^2 = 0$, where the charmed quarks are far off shell, so the relevant short distance is $Q = (2m_c)^{-1}$.
- Virtuality depends on *n*.
- Continuum power effects from OPE.

Other Such Quantities

- The theme of the previous two methods can be generalized.
- Other examples include the static-quark potential (or force).
- In general, they require $a^{-1} \gg Q \gg \Lambda_{QCD}$, or at least $a^{-1} \gg Q \& 2Q \gg \Lambda_{QCD}$.
- A key advantage is that you can take the CL data from the lattice paper, and carry out your own α_s analysis [Maltman, <u>arXiv:0807.2020</u>].
- A disadvantage is that Q will be limited, though not more so than many determinations from high-energy scattering.

Schrödinger Functional Wolff, <u>NPB **265** (1986) 506, 567</u>; Lüscher, Narayanan, Weisz, Wolff, <u>NPB **384** (1992) 168</u>

- QCD in a can (well, on a 3-torus), typically $L^3 \times 2L$, $Q = L^{-1}$.
- Apply boundary conditions at caps, filling the can with some sort of chromodynamic muck. Femtoscale hadronization?!
- Parton-hadron duality says energy in can, for $Q \gg \Lambda_{QCD}$, can be computed with partons, *i.e.*, with perturbation theory.
- Actually, $R^{-1} = -L^{-1} d \ln Z(A_{\Omega})/dA_{\Omega}$ (removing an additive UV divergence; A_{Ω} = boundary potential).
- Vary $Q = L^{-1}$ over potentially *enormous* range: $\times 10^3$ [<u>Alpha</u>].
- No theory of effects suppressed by of $(L\Lambda_{QCD})^s$.

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Running with 4 Flavors

Sommer, Tekin, Wolff [Alpha], arXiv:011.2332

Summary & Outlook

Selected $\alpha_s(M_Z)$ Results from Lattice QCD

$lpha_{\overline{ extsf{MS}}}^{(5)}(M_Z)$	R	Q range	\mathcal{R}	sea	collab	when
0.1170(12)		3		2+1 √stag	HPQCD	<u>2005</u>
0.1183(8)	Wilson loops	7	NNLO			<u>2008</u>
0.1192(11)					Maltman	<u>2008</u>
0.1174(12)		1–2		2+1 √stag	HPQCD + KIT	<u>2008</u>
0.1183(7)	QQ correlator	3–6	ININLO			<u>2010</u>
0.1181(3)(+14/-12)	Adler	5	NNLO	2+1 overlap	JLQCD	<u>2010</u>
0.1205(8)(5)(+0/-17)	Schrödinger	80	asymptote	2+1 Wilson	PACS-CS	<u>2009</u>
$\Lambda_{\overline{\rm MS}}^{(2)} = 245(23) \frac{0.5 \text{ fm}}{r_0} \text{ MeV}$		270	asymptote	2 Wilson	Alpha	<u>2004</u>
0.1xxx(y)	Schrodinger	1000	asymptote	2+1+1 Wilson		<u>2012</u>

• Superseded; re-analysis.

Click on year to find paper.

Has $\alpha_s(M_Z)$ from Lattice QCD Changed?

- In 1992, one of the first lattice QCD results reported $\alpha_s(M_Z) = 0.107 \pm 0.004$.
- Attracted some interest.
- One-loop matching $\alpha_0/W_{1\times 1}$ to $\alpha_{\overline{MS}}^{(0)}(5 \text{ MeV})$, two-loop running to M_Z .
- Quenched approximation, so scale not clear.
- Focus on charmonium splittings for Q, argued insensitive to quenching.
- Potential-model argument to justify a correction for $n_f = 0$ running between 0.75–5.0 GeV.
- NNLO PT & restoring sea quarks could both easily explain 2σ shift.

<u>mea culpa</u>

- Many determinations of α_s from lattice QCD are & will be available.
- No important error from experiment.
- Transparent theory.
- Small uncertainties.
- Tempting to use lattice QCD α_s as input for high-energy scattering to:
 - understand QCD;
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Homework

- MILC, ETMC, others are generating ensembles of gauge fields with 2+1+1 sea quarks:
 - α_s calculations will be repeated here, tested perturbativity of charmed threshold.
- Other methods that can exploit continuum PT will appear.
- Your homework:
 - study and familiarize yourself with lattice QCD error budgets;
 - ask why unfamiliar items are included;
 - ask why expected items are left out.