Excited state energies and scattering phase shifts from lattice QCD with the stochastic LapH method

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Outline

- project goals:
 - comprehensive survey of QCD stationary states in finite volume
 - hadron scattering phase shifts, decay widths
- preliminary results for 20 channels I = 1, S = 0
 - correlator matrices of size 100×100
 - large number of extended single-hadron operators
 - attempt to include all needed 2-hadron operators
- preliminary results for $I = \frac{1}{2}, S = 1, T_{1u}$
- very preliminary results for $I = 0, S = 0, A_{1u}^+$
- I = 1 *P*-wave $\pi\pi$ scattering phase shifts and width of ρ

Extended operators for single hadrons

• quark displacements build up orbital, radial structure



definite momentum p, irreps of little group of p

Two-hadron operators

 our approach: superposition of products of single-hadron operators of definite momenta

 $c^{I_{3a}I_{3b}}_{\boldsymbol{p}_a\lambda_a;\;\boldsymbol{p}_b\lambda_b}\;B^{I_aI_{3a}S_a}_{\boldsymbol{p}_a\Lambda_a\lambda_ai_a}\;B^{I_bI_{3b}S_b}_{\boldsymbol{p}_b\Lambda_b\lambda_bi_b}$

- fixed total momentum $p = p_a + p_b$, fixed $\Lambda_a, i_a, \Lambda_b, i_b$
- group-theory projections onto little group of p and isospin irreps
- restrict attention to certain classes of momentum directions
 - on axis $\pm \widehat{x}, \pm \widehat{y}, \pm \widehat{z}$
 - planar diagonal $\pm \widehat{x} \pm \widehat{y}, \ \pm \widehat{x} \pm \widehat{z}, \ \pm \widehat{y} \pm \widehat{z}$
 - cubic diagonal $\pm \widehat{oldsymbol{x}} \pm \widehat{oldsymbol{y}} \pm \widehat{oldsymbol{z}}$
- efficient creating large numbers of two-hadron operators
- generalizes to three, four, ... hadron operators

Testing our two-meson operators

- (left) $K\pi$ operator in T_{1u} $I = \frac{1}{2}$ channels
- (center and right) comparison with localized $\pi\pi$ operators

$$\begin{aligned} &(\pi\pi)^{A_{1g}^+}(t) &= \sum_{\boldsymbol{x}} \pi^+(\boldsymbol{x},t) \ \pi^+(\boldsymbol{x},t), \\ &(\pi\pi)^{T_{1u}^+}(t) &= \sum_{\boldsymbol{x},k=1,2,3} \Big\{ \pi^+(\boldsymbol{x},t) \ \Delta_k \pi^0(\boldsymbol{x},t) - \pi^0(\boldsymbol{x},t) \ \Delta_k \pi^+(\boldsymbol{x},t) \Big\} \end{aligned}$$



• less contamination from higher states in our $\pi\pi$ operators

Quark line diagrams

- temporal correlations involving our two-hadron operators need
 - slice-to-slice quark lines (from all spatial sites on a time slice to all spatial sites on another time slice)
 - sink-to-sink quark lines



isoscalar mesons also require sink-to-sink quark lines



• solution: the stochastic LapH method!

Stochastic estimation of quark propagators

- do not need exact inverse of Dirac matrix K[U]
- use noise vectors η satisfying $E(\eta_i) = 0$ and $E(\eta_i \eta_j^*) = \delta_{ij}$
- Z_4 noise is used $\{1, i, -1, -i\}$
- solve $K[U]X^{(r)} = \eta^{(r)}$ for each of N_R noise vectors $\eta^{(r)}$, then obtain a Monte Carlo estimate of all elements of K^{-1}

$$K_{ij}^{-1} \approx \frac{1}{N_R} \sum_{r=1}^{N_R} X_i^{(r)} \eta_j^{(r)}$$

- variance reduction using noise dilution
- dilution introduces projectors

$$\begin{split} P^{(a)}P^{(b)} &= \delta^{ab}P^{(a)}, \qquad \sum_{a} P^{(a)} = 1, \qquad P^{(a)\dagger} = P^{(a)} \\ \bullet \mbox{ define } & \eta^{[a]} = P^{(a)}\eta, \qquad X^{[a]} = K^{-1}\eta^{[a]} \end{split}$$

to obtain Monte Carlo estimate with drastically reduced variance

$$K_{ij}^{-1} \approx \frac{1}{N_R} \sum_{r=1}^{N_R} \sum_{a} X_i^{(r)[a]} \eta_j^{(r)[a]*}$$

Correlators and quark line diagrams

baryon correlator

 $C_{l\bar{l}} \approx \frac{1}{N_R} \sum_{r} \sum_{d_A d_B d_C} \mathcal{B}_l^{(r)[d_A d_B d_C]}(\varphi^A, \varphi^B, \varphi^C) \mathcal{B}_{\bar{l}}^{(r)[d_A d_B d_C]}(\varrho^A, \varrho^B, \varrho^C)^*$

express diagrammatically



meson correlator



More complicated correlators

• two-meson to two-meson correlators (non isoscalar mesons)



Quantum numbers in toroidal box

- periodic boundary conditions in cubic box
 - not all directions equivalent ⇒ using J^{PC} is wrong!!



- label stationary states of QCD in a periodic box using irreps of cubic space group even in continuum limit
 - zero momentum states: little group O_h
 - $A_{1a}, A_{2ga}, E_a, T_{1a}, T_{2a}, \quad G_{1a}, G_{2a}, H_a, \qquad a = g, u$ • on-axis momenta: little group C_{4v}

xis momenta: intie group C_{4v}

 $A_1, A_2, B_1, B_2, E, G_1, G_2$

• planar-diagonal momenta: little group C_{2v}

 $A_1, A_2, B_1, B_2, \quad G_1, G_2$

cubic-diagonal momenta: little group C_{3v}

 $A_1, A_2, E, \quad F_1, F_2, G$

• include G parity in some meson sectors (superscript + or -)

Spin content of cubic box irreps

• numbers of occurrences of Λ irreps in J subduced

		J	A_1		A_2	E	T_1	T_2	
		0	1	-	0	0	0	0	
		1	0)	0	0	1	0	
		2	0)	0	1	0	1	
		3	0)	1	0	1	1	
		4	1		0	1	1	1	
		5	0)	0	1	2	1	
		6	1		1	1	1	2	
		7	0)	1	1	2	2	
J	G_1	. (G_2	H		J	G_{1}	$G_1 = G_2$	H
$\frac{1}{2}$	1		0	0		$\frac{9}{2}$	1	0	2
$\frac{3}{2}$	0		0	1		$\frac{11}{2}$	1	1	2
$\frac{5}{2}$	0		1	1		$\frac{13}{2}$	1	2	2
$\frac{7}{2}$	1		1	1		$\frac{15}{2}$	1	1	3

Common hadrons

• irreps of commonly-known hadrons at rest

Hadron	Irrep	Hadron	Irrep	Hadron	Irrep
π	A^{1u}	K	A_{1u}	η,η^\prime	A_{1u}^+
ρ	T_{1u}^+	ω,ϕ	T^{1u}	K^*	T_{1u}
a_0	A_{1g}^+	f_0	A_{1g}^+	h_1	T^{1g}
b_1	T_{1g}^+	K_1	T_{1g}	π_1	T^{1u}
N, Σ	G_{1g}	Λ, Ξ	G_{1g}	Δ, Ω	H_{g}

Ensembles and run parameters

- plan to use three Monte Carlo ensembles
 - $(32^3|240)$: 412 configs $32^3 \times 256$, $m_\pi \approx 240$ MeV, $m_\pi L \sim 4.4$
 - $(24^3|240)$: 584 configs $24^3 \times 128$, $m_\pi \approx 240$ MeV, $m_\pi L \sim 3.3$
 - $(24^3|390)$: 551 configs $24^3 \times 128$, $m_\pi \approx 390$ MeV, $m_\pi L \sim 5.7$
- anisotropic improved gluon action, clover quarks (stout links)
- QCD coupling $\beta = 1.5$ such that $a_s \sim 0.12$ fm, $a_t \sim 0.035$ fm
- strange quark mass $m_s = -0.0743$ nearly physical (using kaon)
- work in $m_u = m_d$ limit so SU(2) isospin exact
- generated using RHMC, configs separated by 20 trajectories
- stout-link smearing in operators $\xi = 0.10$ and $n_{\xi} = 10$
- LapH smearing cutoff $\sigma_s^2 = 0.33$ such that
 - $N_v = 112$ for 24^3 lattices
 - $N_v = 264$ for 32^3 lattices
- source times:
 - 4 widely-separated t₀ values on 24³
 - 8 t_0 values used on 32^3 lattice

Excited states from correlation matrices

• in finite volume, energies are discrete (neglect wrap-around)

 $C_{ij}(t) = \sum_{n} Z_i^{(n)} Z_j^{(n)*} e^{-E_n t}, \qquad Z_j^{(n)} = \langle 0 | O_j | n \rangle$

- not practical to do fits using above form
- define new correlation matrix $\widetilde{C}(t)$ using a single rotation

 $\widetilde{C}(t) = U^{\dagger} C(\tau_0)^{-1/2} C(t) C(\tau_0)^{-1/2} U$

- columns of U are eigenvectors of $C(\tau_0)^{-1/2} C(\tau_D) C(\tau_0)^{-1/2}$
- choose τ_0 and τ_D large enough so $\widetilde{C}(t)$ diagonal for $t > \tau_D$
- effective energies $\widetilde{m}_{\alpha}^{\text{eff}}(t) = \frac{1}{\Delta t} \ln \left(\frac{\widetilde{C}_{\alpha\alpha}(t)}{\widetilde{C}_{\alpha\alpha}(t + \Delta t)} \right)$

tend to N lowest-lying stationary state energies in a channel

• 2-exponential fits to $\widetilde{C}_{\alpha\alpha}(t)$ yield energies E_{α} and overlaps $Z_{i}^{(n)}$

$I = 1, S = 0, T_{1u}^+$ channel

- effective energies $\widetilde{m}^{\mathrm{eff}}(t)$ for levels 0 to 24
- energies obtained from two-exponential fits



$I = 1, S = 0, T_{1u}^+$ energy extraction, continued

- effective energies $\widetilde{m}^{\mathrm{eff}}(t)$ for levels 25 to 49
- energies obtained from two-exponential fits



Level identification

- level identification inferred from Z overlaps with probe operators
- analogous to experiment: infer resonances from scattering cross sections
- keep in mind:
 - probe operators \overline{O}_i act on vacuum, create a "probe state" $|\Phi_i\rangle$, Z's are overlaps of probe state with each eigenstate
 - have limited control of "probe states" $Z_j^{(n)} = \langle \Phi_j | n \rangle$
 - ideal to be ρ , single $\pi\pi$, and so on
 - use of small-a expansions to characterize probe operators
 - use of smeared guark, gluon fields
 - field renormalizations
 - mixing is prevalent
 - identify by dominant probe state(s) whenever possible

Level identification

overlaps for various operators



Identifying quark-antiquark resonances

- resonances: finite-volume "precursor states"
- probes: optimized single-hadron operators
 - analyze matrix of just single-hadron operators $O_i^{[SH]}$ (12 × 12)
 - perform single-rotation as before to build probe operators $O_m^{\prime [SH]} = \sum_i v_i^{\prime (m)*} O_i^{[SH]}$
- obtain Z' factors of these probe operators

Staircase of energy levels

• stationary state energies $I = 1, S = 0, T_{1u}^+$ channel on $(32^3 \times 256)$ anisotropic lattice

Summary and comparison with experiment

- right: energies of $\overline{q}q$ -dominant states as ratios over m_K for $(32^3|240)$ ensemble (resonance precursor states)
- Ieft: experiment

Bosonic $I = 1, S = 0, A_{1u}^-$ channel

- finite-volume stationary-state energies: "staircase" plot
- $32^3 \times 256$ lattice for $m_\pi \sim 240 \text{ MeV}$
- use of single- and two-meson operators only
- blue: levels of max ovelaps with SH optimized operators

A1um 1

Bosonic $I = 1, S = 0, E_u^+$ channel

- finite-volume stationary-state energies: "staircase" plot
- $32^3 \times 256$ lattice for $m_\pi \sim 240$ MeV
- use of single- and two-meson operators only
- blue: levels of max ovelaps with SH optimized operators

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Bosonic $I = 1, S = 0, T_{1q}^{-}$ channel

- finite-volume stationary-state energies: "staircase" plot
- $32^3 \times 256$ lattice for $m_{\pi} \sim 240$ MeV
- use of single- and two-meson operators only
- blue: levels of max ovelaps with SH optimized operators

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Bosonic $I = 1, S = 0, T_{1u}^-$ channel

- finite-volume stationary-state energies: "staircase" plot
- $32^3 \times 256$ lattice for $m_\pi \sim 240$ MeV
- use of single- and two-meson operators only
- blue: levels of max ovelaps with SH optimized operators

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- kaon channel: effective energies $\widetilde{m}^{\text{eff}}(t)$ for levels 0 to 8
- results for $32^3 \times 256$ lattice for $m_\pi \sim 240 \text{ MeV}$
- two-exponential fits

- effective energies $\widetilde{m}^{\mathrm{eff}}(t)$ for levels 9 to 17
- results for $32^3 \times 256$ lattice for $m_\pi \sim 240 \text{ MeV}$
- two-exponential fits

- effective energies $\widetilde{m}^{\mathrm{eff}}(t)$ for levels 18 to 23
- dashed lines show energies from single exponential fits

- finite-volume stationary-state energies: "staircase" plot
- $32^3 \times 256$ lattice for $m_{\pi} \sim 240$ MeV
- use of single- and two-meson operators only
- blue: levels of max ovelaps with SH optimized operators

kaon T1u 32

- Lowest level diagonalized correlator fit
- $32^3 \times 256$ lattice for $m_{\pi} \sim 240$ MeV
- use of single- and two-meson operators only

- Second level diagonalized correlator fit
- $32^3 \times 256$ lattice for $m_{\pi} \sim 240$ MeV
- use of single- and two-meson operators only

- Third level diagonalized correlator fit
- $32^3 \times 256$ lattice for $m_{\pi} \sim 240$ MeV
- use of single- and two-meson operators only

- Fourth level diagonalized correlator fit
- $32^3 \times 256$ lattice for $m_{\pi} \sim 240$ MeV
- use of single- and two-meson operators only

- Fifth level diagonalized correlator fit
- $32^3 \times 256$ lattice for $m_{\pi} \sim 240$ MeV
- use of single- and two-meson operators only

Preliminary $I = 0, S = 0, A_{1u}^+$ Results

- Lowest level diagonalized correlator fit
- $32^3 \times 256$ lattice for $m_{\pi} \sim 240$ MeV
- use of single-meson operators only

Preliminary $I = 0, S = 0, A_{1u}^+$ Results

- Second level diagonalized correlator fit
- $32^3 \times 256$ lattice for $m_{\pi} \sim 240$ MeV
- use of single-meson operators only

Scattering phase shifts from finite-volume energies

• correlator of two-particle operator σ in finite volume

Bethe-Salpeter kernel

• $C^{\infty}(P)$ has branch cuts where two-particle thresholds begin

- momentum quantization in finite volume: cuts \rightarrow series of poles
- C^L poles: two-particle energy spectrum of finite volume theory

Phase shift from finite-volume energies (con't)

 finite-volume momentum sum is infinite-volume integral plus correction *F*

 define the following quantities: A, A', invariant scattering amplitude iM

Phase shifts from finite-volume energies (con't)

• subtracted correlator $C_{\rm sub}(P) = C^L(P) - C^{\infty}(P)$ given by

sum geometric series

$$C_{\rm sub}(P) = A \mathcal{F}(1 - i\mathcal{M}\mathcal{F})^{-1} A'.$$

• poles of $C_{\text{sub}}(P)$ are poles of $C^L(P)$ from $\det(1 - i\mathcal{MF}) = 0$

Phase shifts from finite-volume energies (con't)

- work in spatial L³ volume with periodic b.c.
- total momentum $P = (2\pi/L)d$, where d vector of integers
- masses m_1 and m_2 of particle 1 and 2
- calculate lab-frame energy E of two-particle interacting state in lattice QCD
- boost to center-of-mass frame by defining:

$$egin{array}{rcl} E_{
m cm} &=& \sqrt{E^2-oldsymbol{P}^2}, & \gamma=rac{E}{E_{
m cm}}, \ oldsymbol{q}_{
m cm}^2 &=& rac{1}{4}E_{
m cm}^2-rac{1}{2}(m_1^2+m_2^2)+rac{(m_1^2-m_2^2)^2}{4E_{
m cm}^2}, \ oldsymbol{u}^2 &=& rac{L^2oldsymbol{q}_{
m cm}^2}{(2\pi)^2}, & oldsymbol{s}=\left(1+rac{(m_1^2-m_2^2)}{E_{
m cm}^2}
ight)oldsymbol{d} \end{array}$$

• *E* related to *S* matrix (and phase shifts) by $det[1 + F^{(s,\gamma,u)}(S-1)] = 0,$

where F matrix defined next slide

Phase shifts from finite-volume energies (con't)

• F matrix in JLS basis states given by

$$F_{J'm_{J'}L'S'a';\ Jm_{J}LSa}^{(\boldsymbol{s},\boldsymbol{\gamma},\boldsymbol{u})} = \frac{\rho_{a}}{2} \delta_{a'a} \delta_{S'S} \bigg\{ \delta_{J'J} \delta_{m_{J'}m_{J}} \delta_{L'L} \bigg\}$$

 $+ W_{L'm_{L'}; Lm_{L}}^{(s,\gamma,u)} \langle J'm_{J'} | L'm_{L'}, Sm_{S} \rangle \langle Lm_{L}, Sm_{S} | Jm_{J} \rangle \bigg\},$ • total angular mom *J*, *J'*, orbital mom *L*, *L'*, intrinsic spin *S*, *S'*

- a, a' channel labels
- $\rho_a = 1$ distinguishable particles, $\rho_a = \frac{1}{2}$ identical

 $W_{L'm_{L'};\ Lm_{L}}^{(s,\gamma,u)} = \frac{2i}{\pi\gamma u^{l+1}} \mathcal{Z}_{lm}(s,\gamma,u^{2}) \int d^{2}\Omega \ Y_{L'm_{L'}}^{*}(\Omega) Y_{lm}^{*}(\Omega) Y_{Lm_{L}}(\Omega)$

- Rummukainen-Gottlieb-Lüscher (RGL) shifted zeta functions Z_{lm} defined next slide
- $F^{(s,\gamma,u)}$ diagonal in channel space, mixes different J, J'
- recall S diagonal in angular momentum, but off-diagonal in channel space

RGL shifted zeta functions

• compute Z_{lm} using

$$\begin{aligned} \mathcal{Z}_{lm}(\boldsymbol{s},\gamma,u^2) &= \sum_{\boldsymbol{n}\in\mathbb{Z}^3} \frac{\mathcal{Y}_{lm}(\boldsymbol{z})}{(\boldsymbol{z}^2 - u^2)} e^{-\Lambda(\boldsymbol{z}^2 - u^2)} \\ &+ \delta_{l0}\gamma \pi e^{\Lambda u^2} \left(2uD(u\sqrt{\Lambda}) - \Lambda^{-1/2} \right) \\ &+ \frac{i^l\gamma}{\Lambda^{l+1/2}} \int_0^1 dt \left(\frac{\pi}{t}\right)^{l+3/2} e^{\Lambda t u^2} \sum_{\substack{\boldsymbol{n}\in\mathbb{Z}^3\\\boldsymbol{n}\neq 0}} e^{\pi i \boldsymbol{n} \cdot \boldsymbol{s}} \mathcal{Y}_{lm}(\boldsymbol{w}) \ e^{-\pi^2 \boldsymbol{w}^2/(t\Lambda)} \end{aligned}$$

where

$$\boldsymbol{z} = \boldsymbol{n} - \gamma^{-1} \begin{bmatrix} \frac{1}{2} + (\gamma - 1)s^{-2}\boldsymbol{n} \cdot \boldsymbol{s} \end{bmatrix} \boldsymbol{s},$$

$$\boldsymbol{w} = \boldsymbol{n} - (1 - \gamma)s^{-2}\boldsymbol{s} \cdot \boldsymbol{n}\boldsymbol{s}, \qquad \mathcal{Y}_{lm}(\mathbf{x}) = |\mathbf{x}|^l Y_{lm}(\widehat{\mathbf{x}})$$

$$D(x) = e^{-x^2} \int_0^x dt \ e^{t^2} \qquad \text{(Dawson function)}$$

- choose $\Lambda \approx 1$ for convergence of the summation
- integral done Gauss-Legendre quadrature, Dawson with Rybicki

P-wave $I = 1 \pi \pi$ scattering

- for *P*-wave phase shift $\delta_1(E_{\rm cm})$ for $\pi\pi I = 1$ scattering
- \bullet define $w_{lm} = \frac{\mathcal{Z}_{lm}(\boldsymbol{s}, \boldsymbol{\gamma}, u^2)}{\boldsymbol{\gamma} \pi^{3/2} u^{l+1}}$

\boldsymbol{d}	Λ	$\cot \delta_1$
(0,0,0)	T_{1u}^{+}	$\operatorname{Re} w_{0,0}$
(0,0,1)	A_1	$\operatorname{Re} w_{0,0} + \frac{2}{\sqrt{5}} \operatorname{Re} w_{2,0}$
		$\operatorname{Re} w_{0,0} - \frac{1}{\sqrt{5}} \operatorname{Re} w_{2,0}$
(0,1,1)	A_1^+	Re $w_{0,0} + \frac{1}{2\sqrt{5}}$ Re $w_{2,0} - \sqrt{\frac{6}{5}}$ Im $w_{2,1} - \sqrt{\frac{3}{10}}$ Re $w_{2,2}$,
	B_1^+	Re $w_{0,0} - \frac{1}{\sqrt{5}}$ Re $w_{2,0} + \sqrt{\frac{6}{5}}$ Re $w_{2,2}$,
	B_2^+	Re $w_{0,0} + \frac{1}{2\sqrt{5}}$ Re $w_{2,0} + \sqrt{\frac{6}{5}}$ Im $w_{2,1} - \sqrt{\frac{3}{10}}$ Re $w_{2,2}$
(1,1,1)	A_1^+	Re $w_{0,0} + 2\sqrt{\frac{6}{5}}$ Im $w_{2,2}$
	E^+	${ m Re}\; w_{0,0} - \sqrt{rac{6}{5}} { m Im}\; w_{2,2}$

Finite-volume $\pi\pi I = 1$ energies

- $\pi\pi$ -state energies for various d^2
- dashed lines are non-interacting energies, shaded region above inelastic thresholds

Pion dispersion relation

- boost to cm frame requires aspect ratio on anisotropic lattice
- aspect ratio ξ from pion dispersion

$$(a_t E)^2 = (a_t m)^2 + \frac{1}{\xi^2} \left(\frac{2\pi a_s}{L}\right)^2 d^2$$

• slope below equals $(\pi/(16\xi))^2$, where $\xi = a_s/a_t$

$I = 1 \ \pi \pi$ scattering phase shift and width of the ρ

- preliminary results $32^3 \times 256$, $m_{\pi} \approx 240$ MeV
- additional collaborator: Ben Hoerz (Dublin)

References

- S. Basak et al., *Group-theoretical construction of extended baryon operators in lattice QCD*, Phys. Rev. D **72**, 094506 (2005).
- S. Basak et al., *Lattice QCD determination of patterns of excited baryon states*, Phys. Rev. D **76**, 074504 (2007).
- C. Morningstar et al., *Improved stochastic estimation of quark propagation with Laplacian Heaviside smearing in lattice QCD*, Phys. Rev. D **83**, 114505 (2011).
- C. Morningstar et al., *Extended hadron and two-hadron operators of definite momentum for spectrum calculations in lattice QCD*, Phys. Rev. D **88**, 014511 (2013).

Conclusion

- goal: comprehensive survey of energy spectrum of QCD stationary states in a finite volume
- stochastic LapH method works very well
 - allows evaluation of all needed quark-line diagrams
 - source-sink factorization facilitates large number of operators
 - last_laph software completed for evaluating correlators
- analysis software sigmond urgently being developed
- analysis of 20 channels I = 1, S = 0 for $(24^3|390)$ and $(32^3|240)$ ensembles nearing completion
- can evaluate and analyze correlator matrices of unprecedented size 100×100 due to XSEDE resources
- study various scattering phase shifts also planned
- infinite-volume resonance parameters from finite-volume energies → need new effective field theory techniques