# supersymmetric insights 

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(1) Supersymmetric Hotspots

- the raise of supersymmetry
- the particle spectrum
- the consequences
- constructing a sym-theory
(2) PHMC-Algorithm
- the path-integral
- polynomial approximation
- evaluating the trajectory
(3) Action Improvements

- speed improvements
- signal improvements
(4) Matrix Inversions
- the reason why
- conjugate gradient algorithm
- krylov spaces
- matrix deflation
- domain decomposition


## why supersymmetry?

- aim of investigations: constructing a theory with only one symmetry-group and delivering the standard model by symmetry breaking
- generators of the $\mathcal{P}$ oincaré and Lie-Group $\mathcal{I}$ :

$$
\begin{aligned}
& {\left[P^{\mu}, P^{\nu}\right]=0} \\
& {\left[M^{\mu \nu}, P^{\rho}\right]=} \\
& \begin{aligned}
{\left[M^{\mu \nu}, M^{\rho \sigma}\right] } & =i\left(\eta^{\nu \rho} P^{\mu}-\eta^{\mu \rho} P^{\nu}\right) \quad \leftrightarrow \quad M^{\mu \sigma}+\eta^{\mu \sigma} M^{\nu \rho} \\
& \left.-\eta^{\mu \rho} M^{\nu \sigma}-\eta^{\nu \sigma} M^{\mu \sigma}\right)
\end{aligned}
\end{aligned}
$$

- $\rightarrow$ non-trivial it is impossible (no-go theorem from Coleman \& Mandula '67)


## to crack this theorem

- extend the algebra by anti-commutating vectors instead of commutating ones Golfand \& Likhtman ('71)

$$
\begin{aligned}
{[\text { even, even] }} & =\text { even } \\
\text { \{odd, odd }\} & =\text { even } \\
{[\text { even, odd] }} & =\text { odd }
\end{aligned}
$$

- this so called $\mathbb{Z}_{2}$ graded algebra is the only one, consistent with reIQFT


## the majorana-spinors $Q_{\alpha}$

- anti-commuting values are associated with fermionic degrees of freedom $\rightarrow$ generators are majorana/weyl-spinors.

$$
\begin{aligned}
& \text { self-conjugated complex/real dirac spinors } \\
& \qquad \psi_{M}^{C}=\psi_{M}
\end{aligned}
$$

- with commutation- and anticommutation relations

$$
\begin{gathered}
\left\{Q_{\alpha}, \bar{Q}_{\dot{\beta}}\right\}=2 \sigma_{\alpha \dot{\beta}}^{\mu} P_{\mu} \\
\left\{Q_{\alpha}, Q_{\beta}\right\}=\left\{\bar{Q}_{\dot{\alpha}}, \bar{Q}_{\dot{\beta}}\right\}=\left[Q_{\alpha}, P_{\mu}\right]=\left[\bar{Q}_{\dot{\alpha}}, P_{\mu}\right]=0 \\
{\left[Q_{\alpha}, M_{\mu \nu}\right]=\sigma_{\mu \nu \alpha}^{\beta} Q_{\beta} \quad\left[\bar{Q}^{\dot{\alpha}}, M_{\mu \nu}\right]=\bar{\sigma}_{\mu \nu \dot{\beta}}^{\dot{\alpha}} Q^{\dot{\beta}}}
\end{gathered}
$$

## the particle spectrum

- defining the Pauli-Lubanski-Vector $W_{\mu}$

$$
\begin{aligned}
& W_{\mu}=\frac{1}{2} \epsilon_{\mu \nu \rho \sigma} P^{\nu} M^{\rho \sigma}, \quad X^{\mu}=Q \sigma^{\mu} \bar{Q} \\
& Y:=W^{\mu}-\frac{1}{4} X^{\mu}, \quad\left[Y_{\mu}, Y_{\nu}\right]=i m \epsilon^{\mu \nu \sigma} Y^{\sigma}, \quad\left(\frac{Y}{m}\right)=y(y+1) \\
& (\mathrm{m}, 0) \longrightarrow \text { skalares Teilchen } \\
& (\mathrm{m}, 1 / 2)
\end{aligned}
$$

## the particle spectrum



## the consequences

- solution for the hierarchy-problem
- fewer divergencies
- local supersymmetry $\phi_{i}^{\prime}(x)=U_{i}^{j} \phi_{j}(x) \rightarrow U_{i}^{j}(x) \phi_{j}(x)$ $\rightarrow$ SUGRA (with ART in the low energy limit)
- TOE's only consistent with space-time supersymmetry
- quark confinement
- breaking electroweak interaction is a consequence of supersymmetry breaking





## Wess-Zumino-Model '74

- take the action-functional

$$
S[\phi]=\int d^{4} x \mathcal{L}(\phi, \partial \phi)
$$



- calculate the invariance under variation of the Poincaré-Group $\mathcal{P}$

$$
\delta S[\phi]=\int d^{4} x \delta \mathcal{L}
$$

- with the extension

$$
\left(x_{1}, x_{2}, x_{3}, x_{4}, \theta^{1}, \theta^{2}, \bar{\theta}_{\dot{1}}, \bar{\theta}_{\dot{2}}\right)
$$

- and transformations

$$
\theta \rightarrow \theta+\eta, \quad \bar{\theta} \rightarrow \bar{\theta}+\bar{\eta} \quad x^{\mu} \rightarrow x^{\mu}+a^{\mu}-i \eta \sigma^{\mu} \bar{\theta}+i \theta \sigma^{\mu} \bar{\eta}
$$

## the continuums lagrangian

- equation of motion should be invariant under supersymmetric transformations

$$
\frac{\partial}{\partial x_{\mu}}\left(\frac{\partial \mathcal{L}}{\partial\left(\partial \phi / \partial x_{\mu}\right)}\right)-\frac{\partial \mathcal{L}}{\partial \phi}=0
$$

- the simplest supersymmetric $\mathcal{L}$ agrangian for the chiral multiplet

$$
\mathcal{L}_{\text {chiral }}=\mathcal{L}_{\text {scalar }}+\mathcal{L}_{\text {fermion }}=-\partial^{\mu} \phi^{*} \partial_{\mu} \phi-i \psi^{t} \bar{\sigma}^{\mu} \partial_{\mu} \psi
$$

- the interaction between fermion- and boson-fields should be yukawa-like and renormalisable. the product $\phi^{\dagger} \phi$ leads to a vektor-superfield
- Super-Yang-Mills with symmetry breaking term

$$
\mathcal{L}=\mathcal{L}_{S Y M}+m \bar{\lambda} \lambda
$$

## on-shell action/Curci-VEnEZIANo lattice action ('87)

- ...further constructions and restrictions...
- leads to the euclidean on-shell continuum-action

$$
S_{S Y M}=\int d^{4} x\left\{\frac{1}{4} F_{\mu \nu}^{a} F_{\mu \nu}^{a}+\frac{1}{2} \bar{\lambda}^{a} \gamma^{\mu} \nabla_{\mu} \lambda^{a}\right\}
$$

- putting it on the lattice leads to $S_{l a t}=S_{g}+S_{f}$ with

$$
\begin{aligned}
S_{g}[U]= & \beta \sum_{x} \sum_{\mu \nu}\left[1-\frac{1}{N_{c}} \operatorname{Re} \operatorname{Tr} U_{\mu \nu}\right] \\
S_{f}[U, \bar{\lambda}, \lambda]= & \frac{1}{2} \sum_{x} \bar{\lambda}(x) \lambda(x)+ \\
& \frac{\kappa}{2} \sum_{x} \sum_{\mu}\left[\bar{\lambda}(x+\hat{\mu}) V_{\mu}(x)\left(r+\gamma_{\mu}\right) \lambda(x)\right. \\
& \left.\quad+\bar{\lambda}(x) V_{\mu}^{T}(x)\left(r-\gamma_{\mu}\right) \lambda(x+\hat{\mu})\right]
\end{aligned}
$$

## some comments on $Q$ and $V$-matrix

- by defining the $Q$-Matrix

$$
Q_{y, x}[U] \equiv \delta_{y x}-\kappa \sum_{\mu}\left[\delta_{y, x+\hat{\mu}}\left(1+\gamma_{\mu}\right) V_{\mu}(x)+\delta_{y+\hat{\mu}}\left(1-\gamma_{\mu}\right) V_{\mu}^{T}(y)\right]
$$

- we can write $S_{f}$ more compactly as

$$
S_{f}=\frac{1}{2} \sum_{x y} \bar{\lambda}(x) Q_{x, y} \lambda(y)=\frac{1}{2} \sum_{x y} \lambda^{T}(x) \mathcal{C} Q_{x, y} \lambda(y)
$$

- the adoint matrices have the form

$$
\left[V_{\mu}(x)\right]_{a b} \equiv 2 \operatorname{Tr}\left[U_{\mu}^{\dagger}(x) T^{a} U_{\mu}(x) T^{b}\right]
$$

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## multi-bosonic representation

- it's not feasible to simulate Grassmann fields directly, because $e^{-S_{F}}=e^{-\bar{\phi} D \phi}$ is not positive $\rightarrow$ poor importance sampling
- we therefore integrate out the fermion fields to obtain the fermion determinant

$$
\int[d \lambda] e^{-S_{f}}=\int[d \lambda] e^{-\frac{1}{2} \bar{\lambda} Q \lambda}= \pm \sqrt{\operatorname{det} Q}
$$

- questions concerning the $\pm$-sign $\rightarrow$ ask Jair
- now we turn around - that thing is calles "bosonification", with $\sqrt{\operatorname{det} Q}=\left[\operatorname{det}\left(Q^{\dagger} Q\right)\right]^{\frac{1}{4}}$. In QCD you have

$$
\operatorname{det}\left(Q^{\dagger} Q\right)=\int\left[d \phi^{\dagger} d \phi\right] \exp \left(-\sum_{x y} \phi_{y}^{\dagger}\left[Q^{\dagger} Q\right]_{y x}^{-1} \phi_{x}\right)
$$

## polynomial approximation

- use the approximation


$$
\lim _{n \rightarrow \infty} P_{n}(x)=\left[\frac{1}{x}\right]^{\frac{1}{4}} \quad \forall x \in[\epsilon, \lambda]
$$

## keep in mind the condition number

$$
\sqrt{\lambda / \epsilon}
$$

- choose the polynom

$$
P\left(\tilde{Q}^{2}\right)=c_{0}\left(\tilde{Q}-\rho_{1}\right)\left(\tilde{Q}-\rho_{2}\right) \ldots\left(\tilde{Q}-\rho_{n}\right)\left(\tilde{Q}-\rho_{n}^{*}\right) \ldots\left(\tilde{Q}-\rho_{1}^{*}\right)
$$

- so in our simulation, we have

$$
\sqrt{\operatorname{det} Q}=\left[\operatorname{det}\left(Q^{\dagger} Q\right)\right]^{\frac{1}{4}}=\int\left[d \phi^{\dagger} d \phi\right] \exp \left(-\sum_{x y} \phi_{y}^{\dagger}\left(P\left(\tilde{Q}^{2}\right)\right)_{y x} \phi_{x}\right)
$$

## the hamiltonian

- update the field globally
- takes large steps through configuration space
- we introduce a fictitious Hamiltonian

$$
H[P, U, \phi]=\frac{1}{2} \sum_{x \mu j} P_{x \mu j}^{2}+S_{g}[U]+S_{f}[U, \phi]
$$

- the action plays the role of a fictitious potential
- HMC-Markov-Chain alternates two Markov-Steps:

Molecular Dynamics Monte Carlo and Moment Refreshment (together they are ergodic)

## equations of motion

- these are the hamilton equations of motion

$$
\frac{d P_{x \mu j}}{d \tau}=-D_{x \mu j} S, \quad \frac{d U_{x \mu}}{d \tau}=i P_{x \mu j} U_{x \mu}
$$

- to update of momenta and fields

$$
U_{x \mu}^{\prime}=\exp \left\{\sum_{j} i 2 T_{j} P_{x \mu j} \Delta \tau\right\} U_{x \mu}, \quad P_{x \mu j}^{\prime}=P_{x \mu j}-D_{x \mu j} S[U, \phi] \Delta \tau
$$

- you have to derive the fermionic derivative $\left(\left[D_{x \mu j} V_{\mu}\right]_{a b}=2 f_{b j c}\left[V_{\mu}\right]_{a c}\right)$

$$
\begin{aligned}
& D_{x \mu j} S_{f}[U, \phi]= \\
& \sum_{k=0}^{n-1}\left(\phi_{1, a}^{(k)}(x)\left(D_{x \mu j} \tilde{Q}\right) \phi_{2, b}^{(k) \dagger}(y)\right)+\sum_{k=0}^{n-1}\left(\phi_{2, a}^{(k)}(x)\left(D_{x \mu j} \tilde{Q}\right) \phi_{1, b}^{(k) \dagger}(y)\right)
\end{aligned}
$$

## integrators

- Leapfrog integrator

$$
T_{t o t}(\Delta \tau)=T_{P}\left(\frac{\Delta \tau}{2}\right) T_{U}(\Delta \tau) T_{P}\left(\frac{\Delta \tau}{2}\right)
$$

- Sexton-Weingarten integrator

$$
T_{g e s}(\Delta \tau)=T_{U}\left(\frac{\Delta \tau}{6}\right) T_{P}\left(\frac{\Delta \tau}{2}\right) T_{U}\left(\frac{2 \Delta \tau}{3}\right) T_{P}\left(\frac{\Delta \tau}{2}\right) T_{U}\left(\frac{\Delta \tau}{6}\right)
$$

- higher order Leapfrog integrator with multiple timescales

$$
T_{i}\left(\Delta \tau_{i}\right)=T_{S_{i}}\left(\frac{\Delta \tau_{i}}{2}\right)\left\{T_{i-1}\left(\Delta \tau_{i-1}\right)\right\}^{N_{i}} T_{S_{i}}\left(\frac{\Delta \tau_{i}}{2}\right)
$$

- higher order Sexton-Weingarten integrator with multiple timescales

$$
T_{i}\left(\Delta \tau_{i}\right)=T_{S_{i}}\left(\frac{\Delta \tau_{i}}{6}\right)\left\{T_{i-1}\left(\frac{\Delta \tau_{i-1}}{2}\right)\right\}^{N_{i-1}} T_{S_{i}}\left(\frac{2 \Delta \tau_{i}}{3}\right)\left\{T_{i-1}\left(\frac{\Delta \tau_{i-1}}{2}\right)\right\}^{N_{i-1}} T_{S_{i}}\left(\frac{\Delta \tau_{i}}{6}\right)
$$

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## speed improvements

- two-step polynomial $\frac{1}{x} \equiv P_{n_{1}, n_{2}}(x)=P_{n_{1}}^{\prime}(x) P_{n_{2}}^{\prime \prime}(x)$ with noisy correction


$$
\frac{\mathrm{e}^{\eta^{\dagger} P_{n_{2}}^{\prime \prime}(\tilde{Q}) \eta}}{\int \mathcal{D}[\eta] \mathrm{e}^{\dagger^{\dagger} P_{n_{2}}^{\prime \prime}(\tilde{Q}) \eta}}
$$

- even-odd preconditioning ( $\tilde{Q}=Q \gamma_{5}$ )

$$
\begin{array}{r}
\tilde{Q}=\left(\begin{array}{cc}
\gamma_{5} & -\gamma_{5} \kappa M_{\text {even-odd }} \\
-\gamma_{5} \kappa M_{\text {odd-even }} & \gamma_{5}
\end{array}\right) \\
\rightarrow \operatorname{det} \tilde{Q}=\operatorname{det}\left(\mathbb{1}-\kappa^{2} M_{o e} M_{e o}\right)
\end{array}
$$



- determinant breakup

$$
\operatorname{det} \tilde{Q}^{2}=\left\{\left(\operatorname{det} \tilde{Q}^{2}\right)^{\frac{1}{n_{B}}}\right\}^{n_{B}}
$$

## gauge action improvement

- both terms can be optimized

$$
S=\begin{array}{ccc}
S_{g} & + & S_{f} \\
\downarrow & & \downarrow \\
& \text { DBW2 } & \\
\text { STOUT }
\end{array}
$$

- a possible gauge action is

$$
S=\beta_{11} \sum_{\text {plaq }} \operatorname{Re} \operatorname{Tr}\left(1-\frac{1}{3} U_{\text {plaq }}\right)+\beta_{12} \sum_{\text {plaq }} \operatorname{Re} \operatorname{Tr}\left(1-\frac{1}{3} U_{\text {rect }}\right)
$$



$$
\begin{array}{c|c|c|c}
\text { Wilson } & \text { TISym } & \text { Iwasaki } & \text { DBW2 } \\
\beta_{12}=0 & \beta_{12}=-1 / 12 & \beta_{12}=-0.091 & \beta_{12}=-1.4088
\end{array}
$$

## STOUT link smearing

- the $(n+1)^{t h}$ stout smeared "thick" link obtained iteratively from the $n^{\text {th }}$ level

$$
U_{\mu}^{(n+1)}(x)=\mathrm{e}^{i Q_{\mu}^{(n)}} U_{\mu}^{(n)}(x)
$$

- with

$$
Q_{\mu}(x)=\frac{i}{2}\left(\Omega_{\mu}^{\dagger}(x)-\Omega_{\mu}(x)\right)-\frac{i}{2 N} \operatorname{Tr}\left(\Omega_{\mu}^{\dagger}(x)-\Omega_{\mu}(x)\right)
$$

- and

$$
\Omega_{\mu}(x)=C_{\mu}(x) U_{\mu}^{\dagger}(x)
$$

- the staples $C_{\mu}$ are defined as

$$
\begin{aligned}
C_{\mu}(x)=\sum_{\nu \neq \mu} & \rho_{\mu \nu}\left(U_{\nu}(x) U_{\mu}(x+\hat{\nu}) U_{\nu}^{\dagger}(x+\hat{\mu})\right. \\
& \left.+U_{\nu}^{\dagger}(x-\hat{\nu}) U_{\mu}(x-\hat{\nu}) U_{\mu}(x-\hat{\nu}) U_{\nu}(x-\hat{\nu}+\hat{\mu})\right)
\end{aligned}
$$

## some data from the analysis





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## the purpose of matrix inversions

- examine the Gluino-Propagator

$$
\langle T\{\lambda(x) \bar{\lambda}(x)\}\rangle=\langle T\{\lambda(x) \lambda(x)\}\rangle \mathcal{C}=2\left[\frac{\delta^{2} \ln \mathcal{Z}[J]}{\delta J(x) \delta J(y)}\right] \mathcal{C}
$$

- with the given partition function $\mathcal{Z}$

$$
\mathcal{Z}=\int \mathcal{D}[\lambda] e^{-\frac{1}{2} \lambda C Q \lambda}
$$

- we have to solve

$$
\langle T\{\lambda(x) \bar{\lambda}(x)\}\rangle=\left\langle Q^{-1}[U]\right\rangle
$$

- $\rightarrow$ inversion of sparse matrices


## conjugate gradient algorithm I

- instead of solving $z=Q^{-1} \omega$ we solve

$$
Q z=\omega
$$

$$
\text { ( } \omega=\text { a given source, } Q=\text { the fermion matrix, } z=\text { solution vector) }
$$

- to find $z$, we use the conjugate gradient algorithm.
- the basic idea of CG is, that equivalent to solve $Q z=\omega$ is extremising

$$
E(z):=\langle\omega, z\rangle-1 / 2\langle Q z, z\rangle .
$$

- the gradient of $E$ at $z_{k}$ is

$$
g_{k}=\omega-Q z_{k}
$$

- conjugate gradient means now, to minimize $E$ in a direction $p_{k}$ instead of $g_{k}$. This direction is $Q$-conjugated, which means

$$
\left\langle Q p_{i}, p_{j}\right\rangle=0
$$

## conjugate gradient algorithm II

- the algorithm step by step
(1) take a source $\omega$ and set initially $\omega=z_{0}$
(2) calculate the residuum

$$
p_{0}=r_{0}=\omega-Q z_{0}
$$

(3) for $n=1,2, \ldots$.

$$
a_{n}=\frac{\left|r_{n}\right|^{2}}{\left\langle p_{n}, Q p_{n}\right\rangle}, \quad z_{n+1}=z_{n}+a_{n} p_{n}, \quad r_{n+1}=r_{n}-a_{n} Q p_{n}
$$

(1) if $\left|r_{n+1}\right|^{2}<\delta$ then the solution is $z_{n+1}$, else calculate

$$
b_{n}=\left|r_{n+1}\right|^{2} /\left|r_{n}\right|^{2}, \quad p_{n+1}=r_{n+1}+b_{n} p_{n}
$$

and proceed with iteration

- is valid only for positiv definite hermitian matrices, $\rightarrow$ extend to $B^{\dagger} A$ it can be used for any hermitian matrix $A$


## krylov spaces I

- consider a system of linear equations $A x=b$ and the residual vector $r \equiv b-A x_{i}$ for an approximate solution $x_{i}$
- rewriting the system as

$$
(I-(I-A)) x=b
$$

- leads to basic iteration

$$
\begin{aligned}
x_{i} & =b+(I-A) x_{i-1} \\
& =x_{i-1}+r_{i-1} \\
& =x_{i-2}+r_{i-2}+r_{i-1} \\
& \vdots \\
& =x_{0}+r_{0}+r_{1}+\ldots+r_{i-1}
\end{aligned}
$$

## krylov spaces II

- multiply $x_{i}=x_{i-1}+r_{i-1}$ with $A$ from the left

$$
A x_{i}=A x_{i-1}+A r_{i-1}
$$

- and substract from $b$

$$
\begin{aligned}
b-A x_{i} & =b-A x_{i-1}+A r_{i-1} \\
r_{i} & =r_{i-1}-A r_{i-1} \\
& =(I-A) r_{i-1}
\end{aligned}
$$

- so finally we get

$$
\begin{aligned}
x_{i} & =x_{0}+r_{0}+(I-A) r_{0}+\ldots+(I-A)^{i-1} r_{0} \\
& =x_{0}+\left[r_{0}, A r_{0}, A^{2} r_{0}, \ldots, A^{i-1} r_{0}\right]
\end{aligned}
$$

## krylov spaces III

- this linear space defines the krylov subspace

$$
\mathcal{K}_{m}(A, r)=\operatorname{span}\left\{r, A r, \ldots, A^{m-1} r\right\} .
$$

- convergence is measured by the residual $r_{n}=\left|b-A x_{n}\right|$.
- more specificially, we seek an approximate solution $x_{n}$ in $\mathcal{K}_{n}$ by imposing the petrov-galerkin condition

$$
r_{n} \equiv b-A x_{n} \perp \mathcal{L}_{n}
$$

where $\mathcal{L}_{n}$ is an $n$-dimensional subspace

- two broad choices:
- $\mathcal{L}_{n}=\mathcal{K}_{n}\left(A ; r_{0}\right) \leftrightarrow$ orthognoalisation (Arnoldi, GMRES, CG, GCR...)
- $\mathcal{L}_{n}=\mathcal{K}_{n}\left(A^{\dagger} ; r_{0}\right) \leftrightarrow$ bi-orthognoalisation (Lanczos, BCG, BiCGstab...)
on which circumstances is matrix deflation feasible?
- stochastic estimator technique

$$
\left\langle\eta_{i}^{\dagger} Z_{i}\right\rangle_{N_{\text {est }}} \stackrel{N_{\text {est }} \rightarrow \infty}{=} Q_{i i}^{-1}
$$

- collect informations about $Q$ in each CG for the next step
- feed CG with a

$$
\begin{aligned}
& \text { galerkin-projected vector } \\
& \qquad x_{0}=W\left(W^{T} A W\right)^{-1} W^{T} b .
\end{aligned}
$$

| SET |
| :---: |
| $Q z_{1}=\eta_{1 \alpha}$ |
| $\downarrow$ |
| $Q z_{2}=\eta_{2 \alpha}$ |
| $\downarrow$ |
| $Q z_{i}=\eta_{i \alpha}$ |
| $\vdots$ |
| $Q z_{N}=\eta_{N \alpha}$ |

- $\rightarrow$ convergence will raise


## deflation: the stathopoulos-orginos algorithm

- InitCG

ALGORITHM 1: BASISITERATION
iterative solution of $A y=c$
Initialisation
choose $y_{0} ;$
$s_{0}=c-A y_{0} ;$
$\omega_{0}=s_{0}$

## Iteration

for $j=0,1, \ldots$ until covergence do
$\gamma_{j}=\left(s_{j}, s_{j}\right) /\left(\omega_{j}, A \omega_{j}\right)$;
$y_{j+1}=y_{j}+\gamma_{j} \omega_{j}$;
$s_{j+1}=s_{j}-\gamma_{j} A \omega_{j}$;
$\delta_{j+1}=\left(s_{j+1}, s_{j+1}\right) /\left(s_{j}, s_{j}\right)$;
$\omega_{j+1}=s_{j+1}+\delta_{j+1} \omega_{j}$;
end do

Algorithm 2: InitcG
iterative solution of $A x=b$

## Initialisation

choose $x_{-1}$;
$r_{-1}=b-A x_{-1} ;$
$x_{0}=x_{-1}+W\left(W^{T} A W\right)^{-1} W^{T} r_{-1} ;$
$r_{0}=b-A x_{0} ;$
$p_{0}=r_{0}$;

## Iteration

for $j=0,1, \ldots$ until covergence do
$\alpha_{k}=\left(r_{k}, r_{k}\right) /\left(p_{k}, A p_{k}\right)$;
$x_{k+1}=x_{k}+\alpha_{k} p_{k}$;
$r_{k+1}=r_{k}-\alpha_{k} A p_{k}$;
$\beta_{k+1}=\left(r_{k+1}, r_{k+1}\right) /\left(r_{k}, r_{k}\right) ;$
$p_{k+1}=r_{k+1}+\beta_{k+1} p_{k} ;$
end do

## eigCG

- generate an initial $V$ with restarting-CG
- $T_{m}=\left(W^{T} A W\right)^{-1}$ is the lanczos-matrix
- in 8 . and 9 . we use raileigh ritz, to compute an orthonormal ritz basis for space $[Y, \tilde{Y}]$
- return nev ritz vectors from $V$

```
2. for \(j=0,1, \ldots\) until covergence do
        solve \(T_{m} Y=Y M\), for nev lowest eigenpairs
        solve \(T_{m-1} \tilde{Y}=\tilde{Y} \tilde{M}\), for nev lowest eigenpairs
        \([Q, R]=\operatorname{qr}([Y, \tilde{Y}, 0])\), and \(H=Q^{H} T_{m} Q\)
        solve \(H Z=Z M\) for 2 nev lowest eigenpairs
        Restart: \(V=V(Q Z)\) and \(T_{2 n e v}=M\)
        set the \(2 n e v+1\) column of \(T_{2 n e v+1}\) as \(V^{H} A r_{j}\)
    endif
    \(V=\left[V, r_{j} /\left\|r_{j}\right\|\right]\)
    end CG
```

1. $V=[]$;
2. standard CG iteration
3. update three elements of $T_{j}$
4. if $(\operatorname{size}(V, 2)==m)$
5. $\quad V=[] ;$
6. for $j=0,1, \ldots$ until covergence do
7. standard CG iteration
8. if $(\operatorname{size}(V, 2)==m)$
9. end CG

## solver convergence



Figure: convergence of the solvers. the blue ones are the 24 incremental eigCG iterations, red the last 24 init-CG iterations

## deflation: the lüscher algorithm

- at the beginning of each MD-trajectory, there will be fermion-fields $\phi_{l}(x), l=1, \ldots, N_{s}$ stochastically gernerated through a so called smoothing procedure
- then, they will be projected on non-overlapping Blocks $\Lambda$ with

$$
\phi_{l}^{\Lambda}(x)= \begin{cases}\phi_{l}(x) & \text { wenn } x \in \Lambda \\ 0 & \text { sonst }\end{cases}
$$



Figure: often used blocksize $4^{4}$

## mode projection I

- a given field $\psi$ can be projected with an orthogonal projector $P$ on the space $\mathcal{S}$, which is spanned by the orthonormalbasis $\phi_{1}(x), \ldots, \phi_{N}(x)$

$$
P \psi(x)=\sum_{k=1}^{N} \phi_{k}(x)\left(\phi_{k}, \psi\right)
$$

- the complete system is combined by the "inner" system $\mathcal{S}$ and an "outer" complementary System $\mathcal{S}^{\perp}$

$$
\psi(x)=\chi(x)+\sum_{k, l=1}^{N} \phi_{k}(x)\left(A^{-1}\right)_{k l}\left(\phi_{l}, \eta\right)
$$

- here we used the so called little Dirac-Operator

$$
A_{k l}=\left(\phi_{k}, D \phi_{l}\right), \quad k, l=1, \ldots, N
$$

## mode projection II




Figure: deviation of the smallest eigenvalues


Figure: approximation of the lowest modes by a constant

## comparison of the various methods

|  | Morgan/Wilcox | Stath./Orginos | Lüscher |
| :--- | :---: | :---: | :---: |
| Solver | GMRES / BiCGStab | CG | GCR |
| Matrix Type | non-herm. <br> (Algebraic) | herm. <br> (Algebraic) | non-herm. <br> (Lattice) |
| Simultaneous <br> solve | yes | yes | no |
| Eigenvalue <br> use for <br> multiple rhs's | every cycle (GMRES) <br> beginning (BiCGStab) | every cycle, <br> beginning $\left(s \leq s_{1}\right)$ <br> restart $\left(s>s_{1}\right)$ | every <br> outer <br> iteration |
| Algorithm <br> acceleration | mild | large | small |

Table: some points of comparison for the three algorithms considered

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