Carbon on the lattice:
From graphene to the anthropic principle

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Topics to be covered

- Hybrid Monte Carlo vs. Metropolis
- Theories with dynamical fermions
- Algorithms for global Monte Carlo updates

- Two examples of applications
  - Dirac theory of graphene
  - Carbon production in stars and the anthropic principle
I. HYBRID MONTE CARLO: DYNAMICAL FERMIONS
Monte Carlo for dynamical fermions

**Dynamical fermions:** Monte Carlo evaluation of path integrals, repeated computation of determinants ...

\[
Z = \int DA_0 \exp(-S_{\text{eff}}[A_0]) \quad S_{\text{eff}}[A_0] = -N_f \ln \det(D[A_0]) + S^g_E[A_0]
\]

Positive definite probability measure for MC calculation

\[
\sigma = \frac{1}{VZ} \int DA_0 \, \text{Tr}(D^{-1}[A_0]) \exp(-S_{\text{eff}}[A_0])
\]

\[
\langle \bar{\psi}_b \psi_b \rangle = \frac{1}{V} \langle \text{Tr} \, D^{-1}[A_0] \rangle
\]

**Metropolis algorithm:** evolution via random lattice updates, changes accepted with probability \( p \) ...

\[
p \equiv \frac{P[\theta']}{P[\theta]} = \exp(-\Delta S) \quad \Delta S = S_{\text{eff}}[\theta'] - S_{\text{eff}}[\theta]
\]

Problem: large random updates give a vanishingly small acceptance rate - only local updates possible! \( t_{\text{metropolis}} \sim V^3 \)
Global Hybrid Monte Carlo (HMC) updates

- **Step I:** Introduce random Gaussian noise:
  Physics unaffected ...

\[
H = \sum_n \frac{\pi_n^2}{2} + S_E[\theta]
\]

- **Step II:** Classical Hamiltonian dynamics:
  Global evolution of field and conjugate momentum ...

\[
(\theta_n, \pi_n) \rightarrow (\theta'_n, \pi'_n), \quad \dot{\theta}_i = \frac{\partial H[\theta, \pi]}{\partial \pi_i}, \quad \dot{\pi}_i = -\frac{\partial H[\theta, \pi]}{\partial \theta_i}
\]

- **Step III:** H should be conserved, however:
  Finite stepsize in numerical integration ...

\[
p \equiv \exp(-\Delta H), \quad \Delta H \equiv H[\theta'] - H[\theta]
\]

- **Step IV:** Refresh the random Gaussian noise
  and return to step II ...

"Hybrid" algorithm:
Correct for non-conservation of H with a Metropolis step

S. Duane et al.,
Determinantal Hybrid Monte Carlo (DHMC)

Application of HMC to problems with dynamical fermions:

\[ Z = \int D\mathbf{A}_0 \exp(-S_{\text{eff}}[\mathbf{A}_0]) \quad S_{\text{eff}}[\mathbf{A}_0] = -N_f \ln \det(D[\mathbf{A}_0]) + S_E^g[\mathbf{A}_0] \]

Fields and momenta are repeatedly evolved using the HMC equations of motion:

\[
\dot{\theta}_i = \frac{\partial H[\theta, \pi]}{\partial \pi_i}, \quad \dot{\pi}_i = -\frac{\partial H[\theta, \pi]}{\partial \theta_i}
\]

How to deal with the “fermion force term”?

Inverse (may be) extremely costly!!

\[
\frac{\partial \det(K[\lambda])}{\partial \lambda} = \det(K[\lambda]) \text{Tr} \left( K^{-1}[\lambda] \frac{\partial K}{\partial \lambda} \right)
\]

DHMC is feasible if the size of the fermion operator is small:
- Ultracold Fermi gasis
- Chiral EFT for light nuclei

typically: \( t_{\text{DHMC}} \sim V^2 \)
HMC + pseudofermions ($\phi$-algorithm)

If the inverse of the fermion operator is large (for example the size of the space-time lattice), DHMC is unworkable. Introduce pseudofermions:

$$\det(Q) \propto \int D\phi^* D\phi \exp(-S^p_E) \quad S^p_E = \sum_{n,m} \phi_n^* Q_{n,m}^{-1}[\theta] \phi_m = \sum_n \xi_n^* \xi_n$$

A “stochastic” evaluation of the fermion determinant:
- sample $\phi$ from Gaussian noise $\xi$

HMC + pseudofermions = $\phi$-algorithm:
- Lattice QCD
- QED(2+1), Thirring, graphene

$$H = \sum_n \frac{\pi_n^2}{2} + S^g_E + S^p_E$$

$t_\phi \sim \sqrt[5]{4}$

Exactness of HMC preserved by pseudofermions
2. LATTICE MONTE CARLO: GRAPHENE
Electronic band structure of graphene

Hexagonal lattice of carbon atoms

In the vicinity of a “Dirac point”: Emergent “relativistic” behavior

\[ H = -t \sum \langle i, j \rangle, \sigma = \uparrow, \downarrow \left( a_{\sigma, i}^\dagger b_{\sigma, j} + H.c. \right) \]
\[ -t' \sum \langle \langle i, j \rangle \rangle, \sigma = \uparrow, \downarrow \left( a_{\sigma, i}^\dagger a_{\sigma, j} + b_{\sigma, i}^\dagger b_{\sigma, j} + H.c. \right) \]


\[ \psi_G = \begin{pmatrix} \psi_{KA} \\ \psi_{KB} \\ \psi_{K'A} \\ \psi_{K'B} \end{pmatrix} \]

\[ E_{k_b} \simeq v k \]

\[ v \simeq c/300 \]
Dirac theory of interacting electrons in graphene

\[ S_E = -\sum_{a=1}^{N_f} \int d^2 x \, dt \, \bar{\psi}_a \, D[A_0] \, \psi_a + \frac{1}{2g^2} \int d^3 x \, dt \, (\partial_i A_0)^2 \]

\[ D[A_0] = \gamma_0 (\partial_0 + iA_0) + v\gamma_i \partial_i, \quad i = 1, 2 \]

Content of theory:
- Dynamical fermions (in 2+1 dimensions)
- Gauge field (single component in 3+1 dimensions)

\[ Z = \int DA_0 D\psi D\bar{\psi} e^{-S_E[\bar{\psi}, \psi, A_0]} = \int DA_0 e^{-S_E[A_0]} (\det[D[A_0]])^{N_f} \]

Non-perturbative region:
“graphene fine-structure constant”

\[ g^2 = \frac{e^2}{\varepsilon_0} \]

\[ \alpha_g \equiv \frac{e^2}{4\pi\varepsilon_0 \hbar v} \approx 300\alpha \sim 1 \]
Staggered fermions à la Lattice QCD

- **Gauge action:**
  \( \theta = \text{lattice gauge field, } \beta = \text{bare lattice coupling} \)
  \[
  S^g_E[\theta_0] = \frac{\beta}{2} \sum_n \left[ \sum_{i=1}^{3} (\theta_{0,n} - \theta_{0,n+\hat{e}_i})^2 \right]
  \]

- **Staggered fermion action (with bare mass term):**
  \[
  S^f_E[\bar{\chi}, \chi, U] = -\sum_{n,m} \bar{\chi}(n)D_s[U, n, m]\chi(m)
  \]
  \[
  D_s[U, n, m] = \frac{1}{2}(\delta_{n+e_0,m}U(n) - \delta_{n-e_0,m}U^+(m)) + \frac{v}{2} \sum_{i} \eta^i(n)(\delta_{n+e_i,m} - \delta_{n-e_i,m}) + m_0\delta_{n,m}
  \]

- **Gauge links, staggered phases:**
  \[
  U(n) = \exp \{i\theta(n)\}
  \]

  \[
  \eta^0(n) = 1 \\
  \eta^1(n) = (-1)^{n_0} \\
  \eta^2(n) = (-1)^{n_0+n_1}
  \]

Spatial lattice volume
Lx^3, Lt steps in time dimension

Fermion doubling problem
solved for Nf = 2

Other possibilities:
overlap fermions, hexagonal lattice ...
Calculational strategy on the Lattice

**Step I:** The bare (input) parameters are:
- the lattice coupling $\beta$
- the fermion mass $m_0$
- in principle also the number of flavors $N_f$

Phase diagram (chiral condensate / physical mass) as a function of ($\beta, m_0$)

**Step II:** Physical predictions: where in the phase diagram is physical graphene located?
- use observed $v_F$ to fix lattice $\beta$

If (for example) a gap is observed, the physical lattice spacing can be determined
- scale can be set for dimensionful quantities

**Step III:** Compute more difficult observables, such as response functions
- conductivity and viscosity of the electrons in graphene
The scenario of spontaneous gap formation

Compute the chiral condensate (and susceptibility) as a function of $\beta$ and $m_0$ ...

$$\langle \bar{\psi}_b \psi_b \rangle = \frac{1}{V} \langle \text{Tr} \left[ D^{-1} [A_0] \right] \rangle$$

$$\chi_{\bar{\psi}\psi} = \frac{1}{V} \left[ \langle \text{Tr}^2 \left[ D^{-1} \right] \rangle - \langle \text{Tr} \left[ D^{-2} \right] \rangle - \langle \text{Tr} \left[ D^{-1} \right] \rangle^2 \right]$$

Zero-temperature phase diagram:
- Critical coupling $\beta_c$
- Critical number of flavors $N_c$

Chiral condensate (Metropolis algorithm)

First results on small lattices ($L = 16$ cube)

- $N_f = 2$
  - Possible transition below
  - $\beta \sim 0.10$

- $N_f = 4$
  - Possible transition below
  - $\beta \sim 0.05$

- $N_f = 6$
  - No transition observed
  - $4 < N_{\text{crit}} < 6$
Chiral condensate (HMC algorithm)

\[ \beta_c \sim 0.073 \pm 0.002 \]

Best estimate so far, appears robust, however:
critical exponents difficult

Analysis: “Equation of State” (EOS)

Finite size effects need to be better understood
Phenomenology of electron-electron interactions

Coulomb coupling:
Likely to be larger in suspended graphene ...

On a SiO$_2$ substrate
\[ \alpha_g \sim 0.80 \]

Suspended graphene
\[ \alpha_g \sim 2.16 \]

Experiment:
So far no gap observed, but strong interaction-induced velocity renormalization ...

D. C. Elias et al.,
Nature Phys. 7, 701 (2011)
Fermi velocity from Lattice propagator

Staggered fermion propagator
- Fermion mass and velocity in an interacting system
- Interactions renormalize the bare parameters

\[ C_f(x, y, t) \equiv \langle \chi(x, y, t) \bar{\chi}(x_0, y_0, t_0) \rangle \]

Lattice correlators
- Both “timeslice” and “spaceslice” correlators are considered
- Analysis of \( v_F \) requires correlators for non-zero momenta

\[
C_{ft}(p_1, p_2, t) \equiv \sum_{x,y} \exp(-ip \cdot x) C_f(x, y, t) \quad \quad p_0 = \frac{2\pi(n - 1/2)}{N_t}, \quad n = 0, \ldots, N_t/4
\]
\[
C_{fx}(p_0, p_2, t) \equiv \sum_{t,y} \exp(-ip \cdot x) C_f(x, y, t) \quad \quad p_1 = \frac{2\pi n}{N_x}, \quad p_2 = \frac{2\pi n}{N_x}, \quad n = 0, \ldots, N_x/4
\]

Consistent results are found by measuring \( v_F \) in both the temporal and spatial directions.
Fixing the lattice (inverse) coupling

Results for vFR/vF at strong coupling (preliminary)

Experiment
- \( \frac{v_{FR}}{v_F} \approx 2 - 2.5 \)

The experimental vFR/vF is reached at \( \beta \approx 0.10 \) ...

Coulomb coupling not (yet?) strong enough to generate a gap

To be published
3. NUCLEAR LATTICE SIMULATIONS

Figure produced by Jülich Supercomputing Center (JSC)
Carbon production in red giant stars
The triple alpha process

---> Reaction rate given by:

\[
r_{3\alpha} = 3^3 \left( \frac{2\pi \hbar^2}{M_\alpha k_B T} \right)^3 \frac{\Gamma_\gamma}{\hbar} \exp \left( -\frac{\Delta E_{h+b}}{k_B T} \right)
\]

\[
\Delta E_{h+b} \equiv \Delta E_h + \Delta E_b = E_{12}^* - 3E_4
\]

\[
\Delta E_h \equiv E_{12}^* - E_8 - E_4
\]

\[
\Delta E_b \equiv E_8 - 2E_4
\]

Anthropic arguments
What happens if the fundamental constants (esp. quark masses) shift slightly?

Experiment: 
\[
379.47 \pm 0.18 \text{ keV}
\]
Hamiltonian
Chiral Effective Field Theory

\[ H_{\text{LO}} = H_{\text{free}} + V_{\text{LO}} \]

\[ H_{\text{free}} = \frac{1}{2m} \sum_{i,j=0,1} \int \, d^3\vec{r} \, \vec{\nabla} a_{i,j}^\dagger (\vec{r}) \cdot \vec{\nabla} a_{i,j} (\vec{r}) \]

Interaction (LO)
OPEP + 2 contact terms ...

\[ V_{\text{LO}} = V + V_{I2} + V_{\text{OPEP}} \]

\[ \sim c_{11} \quad \sim c_{i;i} \times \tau_A \cdot \tau_B \]

\[ V = \frac{C}{2} \int d^3\vec{r} : \left[ \rho_{a,\dagger}^{a,\dagger} (\vec{r}) \right]^2 : \]

\[ V_{I2} = \frac{C_I^2}{2} \sum_{l=1,2,3} \int d^3\vec{r} : \left[ \rho_l^{a,\dagger} (\vec{r}) \right]^2 \]

\[ V_{\text{OPEP}} = \sum_{S_1, S_2, l=1,2,3} \int d^3\vec{r}_1 d^3\vec{r}_2 G_{S_1 S_2} (\vec{r}_1 - \vec{r}_2) : \rho_{S_1,l}^{a,\dagger} (\vec{r}_1) \rho_{S_2,l}^{a,\dagger} (\vec{r}_2) : \]

\[ G_{S_1 S_2} (\vec{r}_1 - \vec{r}_2) = - \left( \frac{g_A}{2f_\pi} \right)^2 \int \frac{d^3q}{(2\pi)^3} \frac{q_{S_1} q_{S_2} e^{i\vec{q} \cdot (\vec{r}_1 - \vec{r}_2)}}{q^2 + m^2_\pi} \]
Shifts in the light quark masses
Equivalent to shifts in the pion masses

\[ m_{\pi\pm}^2 \sim (m_u + m_d) \]

Energies of 4He and the Hoyle state
Pion mass dependence at LO in Chiral Effective Field Theory

\[ E_i = E_i^{\text{OPE}}(m_\pi, m_N(m_\pi), \tilde{g}_{\pi N}(m_\pi), c_{11}(m_\pi), c_{ii}(m_\pi)) \]

\[ \tilde{g}_{\pi N} \equiv g_A/(2f_\pi) \]

Pion mass dependence
Small perturbations around the physical point ...

\[ \left. \frac{\partial E_i}{\partial m_\pi} \right|_{m_\pi^{\text{phys}}}^{\text{phys}} = \left. \frac{\partial E_i}{\partial m_\pi^{\text{OPE}}} \right|_{m_\pi^{\text{phys}}}^{\text{phys}} + x_1 \left. \frac{\partial E_i}{\partial m_N} \right|_{m_N^{\text{phys}}}^{\text{phys}} + x_2 \left. \frac{\partial E_i}{\partial \tilde{g}_{N}} \right|_{\tilde{g}_{N}^{\text{phys}}}^{\text{phys}} + x_3 \left. \frac{\partial E_i}{\partial c_{11}} \right|_{c_{11}^{\text{phys}}}^{\text{phys}} + x_4 \left. \frac{\partial E_i}{\partial c_{ii}} \right|_{c_{ii}^{\text{phys}}}^{\text{phys}} \]

\[ x_1 \equiv \left. \frac{\partial m_N}{\partial m_\pi} \right|_{m_\pi^{\text{phys}}}^{\text{phys}}, \quad x_2 \equiv \left. \frac{\partial \tilde{g}_{N}}{\partial m_\pi} \right|_{m_\pi^{\text{phys}}}^{\text{phys}} \]

\[ x_3 \equiv \left. \frac{\partial c_{11}}{\partial m_\pi} \right|_{m_\pi^{\text{phys}}}^{\text{phys}}, \quad x_4 \equiv \left. \frac{\partial c_{ii}}{\partial m_\pi} \right|_{m_\pi^{\text{phys}}}^{\text{phys}} \]

Lattice QCD and CHPT

Two-nucleon problem
Lattice formulation
Auxiliary Field Quantum Monte Carlo (AFQMC)

--- Discretized space-time:

\[ V = L_s^3 \times L_t \]

Our Lattices:
\[ N_x = 6 \]
\[ L_s = 11.8 \text{ fm} \]
\[ a = 1.97 \text{ fm} = 100 \text{ MeV}^{-1} \]

Discretized chiral potential
Pion exchange + contact interactions

--- Auxiliary fields introduced for contact interactions
Hubbard-Stratonovich transformation

\[ \exp(\rho^2/2) \propto \int_{-\infty}^{\infty} ds \exp(-s^2/2 - s\rho), \quad \rho \sim a^\dagger a \]

Global Lattice updates
Hybrid Monte Carlo (pion + auxiliary fields)
Energies via Projection Monte Carlo

--- Euclidean time derivative of the correlator

\[ Z_A(t) = \langle \psi_A | \exp(-tH) | \psi_A \rangle \]

Lattice Hamiltonian with
Auxiliary Field

Slater determinant
for A free nucleons

--- Define “transient” energy \( E(t) \):

\[ E_A(t) = - \frac{d}{dt} \ln Z_A(t) \]

\[ E_A^0 = \lim_{t \to \infty} E_A(t) \]

Ground state energy
filtered out at large times

Operator expectation values

--- Projection Monte Carlo calculation of the derivatives ...

\[ Z_A^O(t) = \langle \psi_A | \exp(-tH/2)O \exp(-tH/2) | \psi_A \rangle \]

\[ \lim_{t \to \infty} \frac{Z_A^O(t)}{Z_A(t)} = \langle \psi_A | O | \psi_A \rangle \]

--- Extrapolation (exponential) to large Euclidean time!

For a thorough review:
D. Lee,
Extrapolation validated against the deuteron
(exact solution of Schrödinger equation in a periodic box)
Determination of LECs

---> Two-nucleon scattering analysis

B. Boraso\textit{y et al.},

Predictions can be made
for heavier nuclei

Derivatives of LECs w.r.t. the pion mass

---> Lüscher's finite volume formula ...

\[ p \cot \delta = \frac{1}{\pi L} S(\eta) \approx -\frac{1}{a}, \quad \eta \equiv m_N E \left( \frac{L}{2\pi} \right)^2 \]

Two-nucleon energy levels
in a periodic cube related
to S-wave phase shifts

Replace derivatives w.r.t. LECs

---> derivatives w.r.t. \( a^{-1} \) ...

\[ x_3 \equiv \left. \frac{\partial c_{11}}{\partial m_\pi} \right|_{m_\pi^{\text{phys}}} \]

\[ x_4 \equiv \left. \frac{\partial c_{ii}}{\partial m_\pi} \right|_{m_\pi^{\text{phys}}} \]

\[ \bar{A}_s \equiv \left. \frac{\partial a_s^{-1}}{\partial m_\pi} \right|_{m_\pi^{\text{phys}}} \]

\[ \bar{A}_t \equiv \left. \frac{\partial a_t^{-1}}{\partial m_\pi} \right|_{m_\pi^{\text{phys}}} \]
Shifts of the $^4$He and Hoyle states

--> Input needed from CHPT and LQCD ...

\[ x_1 \equiv \frac{\partial m_N}{\partial m_\pi} \bigg|_{m_\pi}^{\text{phys}} \]
\[ x_2 \equiv \frac{\partial g_{\pi N}}{\partial m_\pi} \bigg|_{m_\pi}^{\text{phys}} = \frac{1}{2f_\pi} \frac{\partial g_A}{\partial m_\pi} \bigg|_{m_\pi}^{\text{phys}} - \frac{g_A}{2f_\pi^2} \frac{\partial f_\pi}{\partial m_\pi} \bigg|_{m_\pi}^{\text{phys}} \]

--> Use conservative error estimates for $x_1$ and $x_2$ (effects shown in red):

\[ x_1 = 0.73 (0.57 \ldots 0.97) \quad x_2 = -0.024 (-0.058 \ldots 0.008) \text{ l.u.} \]

\[ \frac{\partial E_4}{\partial m_\pi} \bigg|_{m_\pi}^{\text{phys}} = -0.339(5) \frac{\partial a_s^{-1}}{\partial m_\pi} \bigg|_{m_\pi}^{\text{phys}} - 0.697(4) \frac{\partial a_t^{-1}}{\partial m_\pi} \bigg|_{m_\pi}^{\text{phys}} + 0.0380(14) + 0.008 - 0.006 \]

\[ \frac{\partial E_{12}^*}{\partial m_\pi} \bigg|_{m_\pi}^{\text{phys}} = -1.588(11) \frac{\partial a_s^{-1}}{\partial m_\pi} \bigg|_{m_\pi}^{\text{phys}} - 3.025(8) \frac{\partial a_t^{-1}}{\partial m_\pi} \bigg|_{m_\pi}^{\text{phys}} + 0.178(4) + 0.026 - 0.021 \]
Small changes in the fundamental parameters

--> Light quark masses + EM fine structure constant ...

\[ \delta(\Delta E_{h+b}) \approx \left( \frac{\partial \Delta E_{h+b}}{\partial m_\pi} \right)_{m_\pi^{\text{phys}}} \times \delta m_\pi + \left( \frac{\partial \Delta E_{h+b}}{\partial \alpha_{\text{em}}} \right)_{\alpha_{\text{em}}^{\text{phys}}} \times \delta \alpha_{\text{em}} \]

\[ = \left( \frac{\partial \Delta E_{h+b}}{\partial m_\pi} \right)_{m_\pi^{\text{phys}}} \times K^q_m \pi \left( \frac{\delta m_q}{m_q} \right) + Q(\Delta E_{h+b}) \left( \frac{\delta \alpha_{\text{em}}}{\alpha_{\text{em}}} \right) \]

\[ \left( \frac{\partial \Delta E_{h+b}}{\partial m_\pi} \right)_{m_\pi^{\text{phys}}} = -0.572(19) \left( \frac{\partial a^-_s}{\partial m_\pi} \right)_{m_\pi^{\text{phys}}} - 0.933(15) \left( \frac{\partial a^-_t}{\partial m_\pi} \right)_{m_\pi^{\text{phys}}} + 0.064(6)^{+0.010}_{-0.009} \]

Models of stellar evolution

--> Produce $^{12}\text{C}$, do not convert it all to $^{16}\text{O}$ ...

\[ |\delta(\Delta E_{h+b})| < 100 \text{ keV} \]

H. Oberhummer, A. Csótó, H. Schlattl, Science 289, 88 (2000) ...

--> Feasibility of carbon-based life:

\[ \left[ 0.572(19) \bar{A}_s + 0.933(15) \bar{A}_t - 0.064(6) \right] \times \left( \frac{\delta m_q}{m_q} \right) < 0.15\% \]
How well are the remaining parameters known?

--- Information from Chiral EFT and Lattice QCD ...

\[
-
\frac{\partial a_s^{-1}}{\partial m_\pi} \equiv \frac{A_s}{a_s m_\pi}, \quad A_s \equiv \frac{K_{a_s}^q}{K_{\pi}^q}, \quad -\frac{\partial a_t^{-1}}{\partial m_\pi} \equiv \frac{A_t}{a_t m_\pi}, \quad A_t \equiv \frac{K_{a_t}^q}{K_{\pi}^q}
\]

Quark mass variation in Chiral EFT:
E. Epelbaum et al., to be published ...

\[
K_{a_s}^q = 2.3_{-1.8}^{+1.9}, \quad K_{a_t}^q = 0.32_{-0.18}^{+0.17}
\]

Relatively large uncertainty
Will be improved dramatically by Lattice QCD
(note: preliminary!)
How does our Universe compare with the predictions?
--> The END OF THE WORLD plot :) 

How about EM effects (variation of fine structure constant)?
--> Carbon-based possible within 2% variation (preliminary AFQMC results)