

Carbon on the lattice: From graphene to the anthropic principle

Timo A. Lähde

Institute for Advanced Simulation and Institut für Kernphysik Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany

Light Nuclei from First Principles (Program INT 12-3) University of Washington, Seattle, Tuesday Nov. 13, 2012 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

HYBRID MONTE CARLO: DYNAMICAL FERMIONS

1.

Monte Carlo for dynamical fermions

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

$$
\mathcal{Z} = \int \mathcal{D}A_0 \underbrace{\exp(-S_{\text{eff}}[A_0])}_{\text{Positive definite probability measure}}
$$
\n
$$
S_{\text{eff}}[A_0] = -N_f \ln \det(D[A_0]) + S_E^g[A_0]
$$
\n
$$
\sigma = \frac{1}{V\mathcal{Z}} \int \mathcal{D}A_0 \operatorname{Tr}(D^{-1}[A_0]) \exp(-S_{\text{eff}}[A_0])
$$
\n
$$
\langle \bar{\psi}_b \psi_b \rangle = \frac{1}{V} \langle \operatorname{Tr} [D^{-1}[A_0]] \rangle
$$

Metropolis algorithm: evolution via random lattice updates, changes accepted with probability p ...

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

Problem: large random updates give a vanishingly small $t_{\text{metropolis}} \sim V^3$ acceptance rate - only **local** updates possible!

Global Hybrid Monte Carlo (HMC) updates

Step I: Introduce random Gaussian noise:

Determinantal Hybrid Monte Carlo (DHMC)

Application of HMC to problems with dynamical fermions:

$$
\mathcal{Z} = \int \mathcal{D}A_0 \, \exp(-S_{\text{eff}}[A_0]) \qquad S_{\text{eff}}[A_0] = -N_f \ln \det(D[A_0]) + S_E^g[A_0]
$$

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

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

How to deal with the "fermion force term"?

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

DHMC is feasible if the

size of the fermion operator is small:

- Ultracold Fermi gasis
- Chiral EFT for light nuclei

typically: t DHMC \sim V^2

HMC + pseudofermions (φ-algorithm)

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

$$
\det(Q) \propto \int {\cal D}\phi^\dagger {\cal D}\phi \, \exp(-S_E^p) \qquad S_E^p = \sum_{{\bf n},{\bf m}} \phi_{\bf n}^\dagger \, Q_{\bf n,m}^{-1}[\theta] \, \phi_{\bf m} = \sum_{\bf n} \xi_{\bf n}^\dagger \xi_{\bf n}
$$

A "stochastic" evaluation of the fermion determinant:

- sample \phi from Gaussian noise \xi

HMC + pseudofermions = **ϕ-algorithm:**

- Lattice QCD
- QED(2+1), Thirring, graphene

$$
\dot{\theta}_{\mathbf{n}} = \frac{\delta H}{\delta \pi_{\mathbf{n}}} = \pi_{\mathbf{n}},
$$
\n
$$
\dot{\pi}_{\mathbf{n}} = -\frac{\delta H}{\delta \theta_{\mathbf{n}}} \equiv F_{\mathbf{n}}^{g} + F_{\mathbf{n}}^{p}
$$

$$
H=\sum_{\bf n}\frac{\pi_{\bf n}^2}{2}+S_E^g+S_E^p
$$

$$
t_{\varphi} \sim V^{5/4}
$$

Exactness of HMC preserved by pseudofermions

LATTICE MONTE CARLO: GRAPHENE

Electronic band structure of graphene

Hexagonal lattice of carbon atoms

a² δⁱ i = 1, 2, 3 **In the vicinity of a "Dirac point":** Emergent "relativistic" behavior

$$
E_k
$$

!(q) = q2/(2m) m

$$
\psi_G = \left(\begin{array}{c} \psi_{KA} \\ \psi_{KB} \\ \psi_{K'A} \\ \psi_{K'B} \end{array} \right)
$$

$$
E_k \simeq v k
$$

! = 0.2t

$$
v \simeq c/300
$$

0. L. Diut, D. T. OON,
Dhuc Dov R 77 075115 (2008) G. Semenoff, Phys. Rev. Lett. **54**, 2449 (1984) J. E. Drut, D. T. Son, Phys. Rev. B **77**, 075115 (2008)

\$

Dirac theory of interacting electrons in graphene

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

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

Content of theory:

- Dynamical fermions (in 2+1 dimensions)
- Gauge field (single component in 3+1 dimensions)

$$
\mathcal{Z}=\int\mathcal{D}A_0\mathcal{D}\psi\mathcal{D}\bar{\psi}e^{-S_E[\bar{\psi}_a,\psi_a,A_0]}=\int\mathcal{D}A_0e^{-S_E^g[A_0]}(\text{det}[D[A_0]])^{N_f}
$$

Non-perturbative region: "graphene fine-structure constant"

$$
g^2 = e^2/\epsilon_0
$$

$$
\alpha_g \equiv \frac{e^2}{4\pi\epsilon_0 \hbar v} \simeq 300\alpha \sim 1
$$

Staggered fermions à la Lattice QCD

Gauge action:

(θ = lattice gauge field, β = bare lattice coupling)

$$
S_E^g[\theta_0] = \frac{\beta}{2} \sum_n \left[\sum_{i=1}^3 \left(\theta_{0,n} - \theta_{0,n+\hat{e}_i} \right)^2 \right]
$$

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

Staggered fermion action (with bare mass term):

$$
S_E^f[\bar{\chi}, \chi, U] = -\sum_{\mathbf{n}, \mathbf{m}} \bar{\chi}(\mathbf{n}) D_s[U, \mathbf{n}, \mathbf{m}] \chi(\mathbf{m})
$$

$$
D_s[U, \mathbf{n}, \mathbf{m}] = \frac{1}{2} (\delta_{\mathbf{n}+\mathbf{e}_0, \mathbf{m}} U(\mathbf{n}) - \delta_{\mathbf{n}-\mathbf{e}_0, \mathbf{m}} U^{\dagger}(\mathbf{m})) + \frac{v}{2} \sum_i \eta^i(\mathbf{n}) (\delta_{\mathbf{n}+\mathbf{e}_i, \mathbf{m}} - \delta_{\mathbf{n}-\mathbf{e}_i, \mathbf{m}}) + m_0 \delta_{\mathbf{n}, \mathbf{m}}
$$

Gauge links, staggered phases:

 $U(\mathbf{n}) = \exp\{i\theta(\mathbf{n})\}$

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

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 m0
	- in principle also the number of flavors Nf

Phase diagram (chiral condensate / physical mass) as a function of (\beta, m0)

- **Step II:** Physical predictions: where in the phase diagram is physical graphene located?
	- use observed vF 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 m0 ...

$$
\begin{aligned}\n\langle \bar{\psi}_b \psi_b \rangle &= \frac{1}{V} \langle \text{Tr} \left[D^{-1} [A_0] \right] \rangle \\
\chi_{\bar{\psi}\psi} &= \frac{1}{V} \left[\langle \text{Tr}^2 \left[D^{-1} \right] \rangle - \langle \text{Tr} \left[D^{-2} \right] \rangle - \langle \text{Tr} \left[D^{-1} \right] \rangle^2 \right]\n\end{aligned}
$$

Zero-temperature phase diagram:

- Critical coupling \beta_c
- Critical number of flavors N_c

Chiral condensate (Metropolis algorithm)

J. E. Drut, T. A. Lähde, Phys. Rev. Lett. **102**, (2009) 026802

Chiral condensate (HMC algorithm)

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

Phenomenology of electron-electron interactions

Coulomb coupling:

Likely to be larger in suspended graphene ...

On a SiO2 substrate $\alpha_{\rm g}$ ~ 0.80

 $\alpha_{\rm g}$ ~ 2.16 Suspended graphene

Experiment:

So far no gap observed, but strong interactioninduced 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

 $C_f(x, y, t) \equiv \langle \chi(x, y, t) \overline{\chi}(x_0, y_0, t_0) \rangle$

Lattice correlators

- Both "timeslice" and "spaceslice" correlators are considered
- Analysis of vF requires correlators for non-zero momenta

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

$$
C_{fx}(p_0, p_2, t) \equiv \sum_{t,y} \exp(-ip \cdot x) C_f(x, y, t) \qquad p_1 = \frac{2\pi n}{N_x}, \quad p_2 = \frac{2\pi n}{N_x}, \quad n = 0, \dots, N_x/4
$$

Consistent results are found by measuring vF in both the temporal and spatial directions

Fixing the lattice (inverse) coupling

Results for vFR/vF at strong coupling (preliminary)

The experimental vFR/vF is reached at \beta ≈ 0.10 ...

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

Figure produced by
Jülich Supercomputing Cent Jülich Supercomputing Center (JSC)

NUCLEAR LATTICE SIMULATIONS

Carbon production in red giant stars

The triple alpha process

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 ...

$$
V_{\rm LO} = V + V_{I^2} + V^{\rm OPEP}
$$

$$
\sim c_{11}
$$

$$
\sim c_{ii} \times \tau_A \cdot \tau_B
$$

$$
\rho^{a^{\dagger},a}(\vec{r}) = \sum_{i,j=0,1} a^{\dagger}_{i,j}(\vec{r}) a_{i,j}(\vec{r})
$$

$$
V = \frac{C}{2} \int d^3 \vec{r} : \left[\rho^{a^{\dagger},a}(\vec{r}) \right]^2 : \qquad V^{\text{OPEP}} = \sum_{S_1,S_2, I=1,2,3} \int d^3 \vec{r}_1 d^3 \vec{r}_2 G_{S_1S_2}(\vec{r}_1 - \vec{r}_2) : \rho^{a^{\dagger},a}_{S_1,I}(\vec{r}_1) \rho^{a^{\dagger},a}_{S_2,I}(\vec{r}_2) : \\ V_{I^2} = \frac{C_{I^2}}{2} \sum_{I=1,2,3} \int d^3 \vec{r} : \left[\rho^{a^{\dagger},a}_{I}(\vec{r}) \right]^2 \qquad G_{S_1S_2}(\vec{r}_1 - \vec{r}_2) = -\left(\frac{g_A}{2f_\pi} \right)^2 \int \frac{d^3 \vec{q}}{(2\pi)^3} \frac{q_{S_1}q_{S_2}e^{i\vec{q} \cdot (\vec{r}_1 - \vec{r}_2)}}{q^2 + m_\pi^2}
$$

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

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

\n
$$
V
$$
\n
$$
V
$$
\n
$$
V_{I^2}
$$
\n
$$
\tilde{g}_{\pi N} \equiv g_A/(2f_\pi)
$$

Pion mass dependence

Small perturbations around the physical point ...

Lattice formulation

Auxiliary Field Quantum Monte Carlo (AFQMC)

--> Discretized space-time:

$$
V = L_s^3 \times L_t
$$

Our Lattices:
\n
$$
N_x = 6
$$

\n $L_s = 11.8$ fm
\n $a = 1.97$ fm = 100 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)

D $\mathbf n$ D O. n \sim 2 fm

Borasoy, Krebs, Lee, Meißner, Nucl. Phys. **A768** (2006) 179; Eur. Phys. J. **A31** (2007) 105 ...

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): $\quad E_A(t) = -\frac{d}{dt} \ln Z_A(t)$

$$
E_A^0 = \lim_{t \to \infty} E_A(t) \quad \text{if}
$$

Ground state energy filtered out at large times

Operator expectation values

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

$$
Z_A^{\mathcal{O}}(t) = \langle \psi_A | \exp(-tH/2) \mathcal{O} \exp(-tH/2) | \psi_A \rangle
$$

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

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

For a thorough review: D. Lee, Prog. Part. Nucl. Phys. **63**, (2009)

Summary of Monte Carlo results

Substantial investment of supercomputing resources (JUQUEEN, RWTH Aachen) ...

Extrapolation validated against the deuteron (exact solution of Schrödinger equation in a periodic box)

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

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

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

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

Replace derivatives w.r.t. LECs \rightarrow derivatives w.r.t. a^{-1} ...

$$
x_3 \equiv \frac{\partial c_{11}}{\partial m_{\pi}}\Big|_{m_{\pi}^{\text{phys}}}\qquad \qquad \bar{A}_s \equiv \frac{\partial a_s^{-1}}{\partial m_{\pi}}\Big|_{m_{\pi}^{\text{phys}}}
$$

$$
x_4 \equiv \frac{\partial c_{ii}}{\partial m_{\pi}}\Big|_{m_{\pi}^{\text{phys}}}\qquad \qquad \bar{A}_t \equiv \frac{\partial a_t^{-1}}{\partial m_{\pi}}\Big|_{m_{\pi}^{\text{phys}}}
$$

for x_1 and x_2 (effects shown in red):

$$
x_1 = 0.73 (0.57...0.97) \qquad x_2 = -0.024 (-0.058...0.008) \text{ l.u.}
$$

$$
\frac{\partial E_4}{\partial m_\pi}\bigg|_{m_\pi^{\rm phys}}=-0.339(5)\left.\frac{\partial a_s^{-1}}{\partial m_\pi}\right|_{m_\pi^{\rm phys}}-0.697(4)\left.\frac{\partial a_t^{-1}}{\partial m_\pi}\right|_{m_\pi^{\rm phys}}+0.0380(14)_{-0.006}^{+0.008}
$$

$$
\frac{\partial E^{\star}_{12}}{\partial m_{\pi}}\bigg|_{m_{\pi}^{\rm phys}}=-1.588(11)\left.\frac{\partial a_{s}^{-1}}{\partial m_{\pi}}\right|_{m_{\pi}^{\rm phys}}-3.025(8)\left.\frac{\partial a_{t}^{-1}}{\partial m_{\pi}}\right|_{m_{\pi}^{\rm phys}}+0.178(4)^{+0.026}_{-0.021}
$$

Small changes in the fundamental parameters

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

$$
\delta(\Delta E_{h+b}) \approx \frac{\partial \Delta E_{h+b}}{\partial m_{\pi}} \bigg|_{m_{\pi}^{\text{phys}}} \times \delta m_{\pi} + \frac{\partial \Delta E_{h+b}}{\partial \alpha_{em}} \bigg|_{\alpha_{em}^{\text{phys}}} \times \delta \alpha_{em}
$$

$$
= \frac{\partial \Delta E_{h+b}}{\partial m_{\pi}} \bigg|_{m_{\pi}^{\text{phys}}} \times K_{\pi}^q m_{\pi} \left(\frac{\delta m_q}{m_q} \right) + Q(\Delta E_{h+b}) \left(\frac{\delta \alpha_{em}}{\alpha_{em}} \right)
$$

$$
\frac{\partial \Delta E_{h+b}}{\partial m_{\pi}} \bigg|_{m_{\pi}^{\text{phys}}} = -0.572(19) \frac{\partial a_s^{-1}}{\partial m_{\pi}} \bigg|_{m_{\pi}^{\text{phys}}} - 0.933(15) \frac{\partial a_t^{-1}}{\partial m_{\pi}} \bigg|_{m_{\pi}^{\text{phys}}} + 0.064(6)^{+0.010}_{-0.009}
$$

Models of stellar evolution

 \rightarrow Produce ¹²C, do not convert it all to ¹⁶O ...

$$
|\delta (\Delta E_{h+b})| < 100 \ \mathrm{keV}
$$

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

--> Feasibility of carbon-based life:

$$
\left| \left[0.572(19) \bar{A}_s + 0.933(15) \bar{A}_t - 0.064(6) \right] \times \left(\frac{\delta m_q}{m_q} \right) \right| < 0.15\%
$$

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)