Simulation of graphene on the graphene lattice

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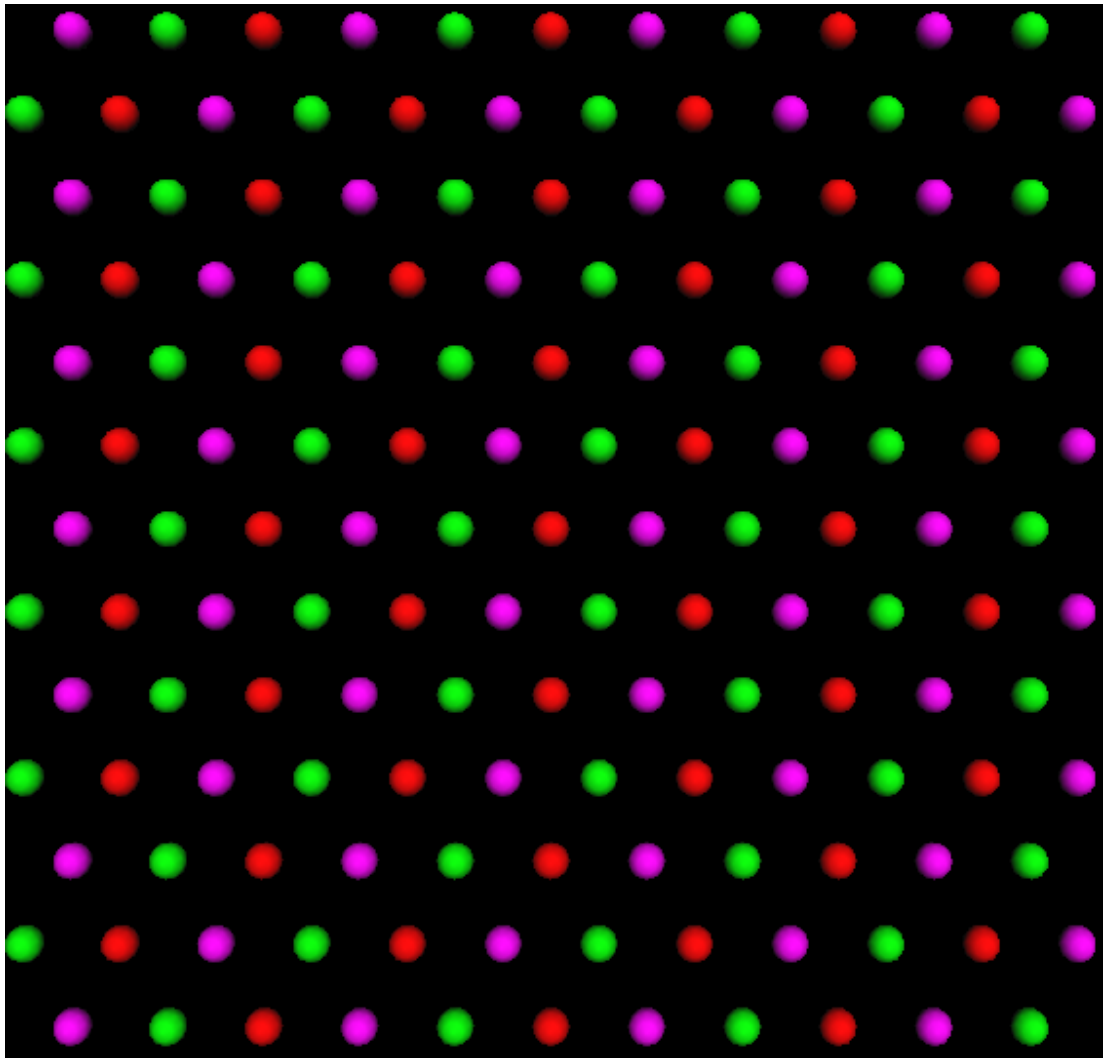
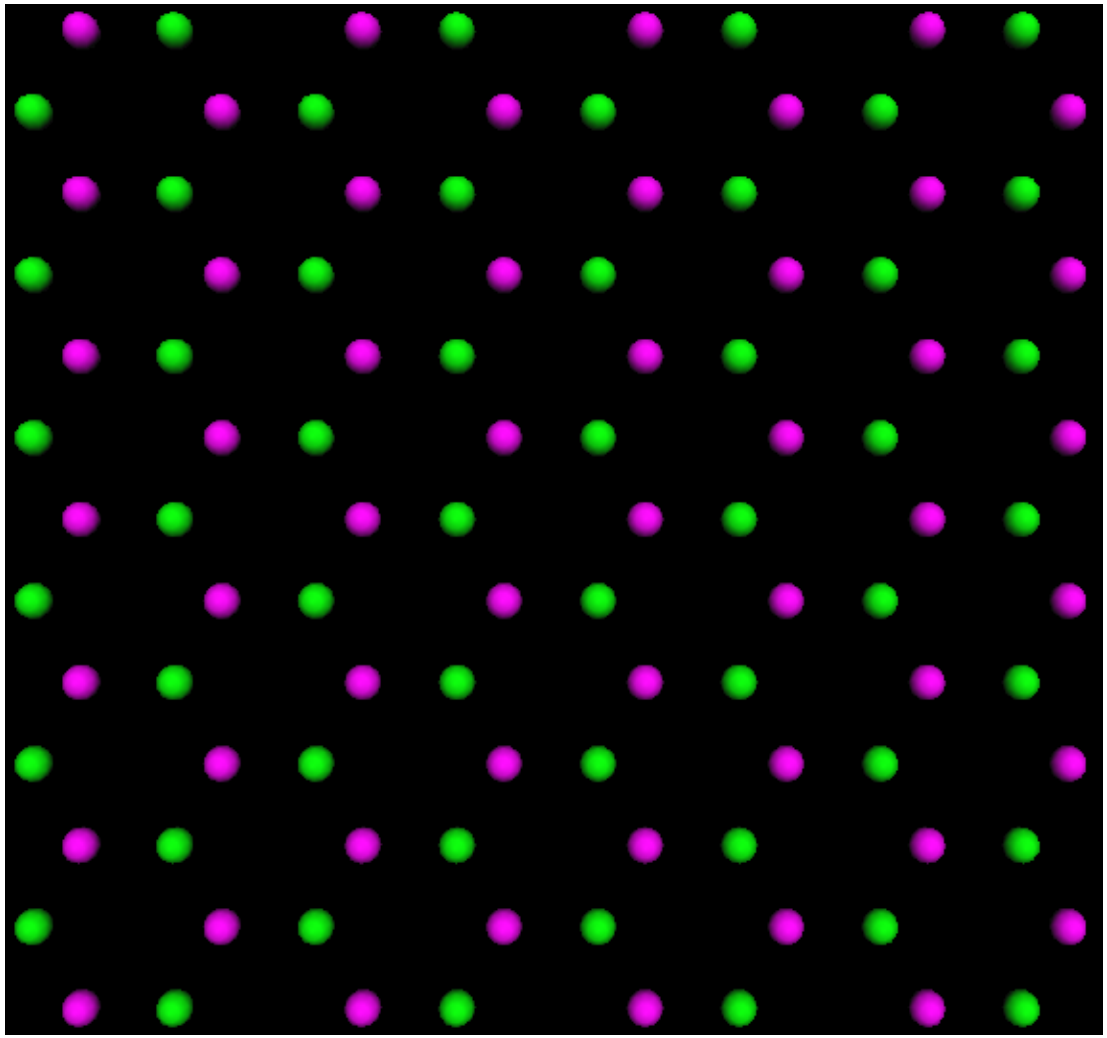
The underlying lattice



The A and B sublattices



The dynamical system

We label the lattice sites by a single index x and the sublattice index A, B. We impose periodic boundary conditions with period L.

To each lattice site we associate creation and annihilation operators for electrons of spin $s = \uparrow, \downarrow$:

$$a_{x,s}, \qquad a^{\dagger}_{x,s}$$

The Hamiltonian

$$H = \sum_{\langle x,y\rangle,s} \kappa(a^\dagger_{x,A,s}a_{y,B,s} + a^\dagger_{x,B,s}a_{y,A,s}) + e^2 \sum_{x,y} V_{x,y}q(x)q(y)$$

where $\langle x, y\rangle$ stands for nearest neighbors, the sublattice indices have been omitted in the Coulomb term, and

$$q(x) = a^\dagger_{x,\uparrow}a_{x,\uparrow} + a^\dagger_{x,\downarrow}a_{x,\downarrow} - 1$$

The -1 stands for the charge of the nucleus and insures neutrality at half filling. We demand that V be positive definite. (Both will be important for the MC formulation.) We will set $\kappa = 1$.

The quadratic Hamiltonian

$$H_2 = \sum_{\langle x,y\rangle,s} (a^\dagger_{x,A,s} a_{y,B,s} + a^\dagger_{x,B,s} a_{y,A,s})$$

can be diagonalized by Fourier transform. It is diagonal in Fourier space, but couples the A and B sublattices.

The Observables

We wish to calculate

$$Z = \mathrm{Tr}\, e^{-\beta H}$$

and Green functions of the type

$$G(t) = \mathrm{Tr}\, \mathrm{T}[a(t)a^\dagger(0)e^{-\beta H}]$$

where the time ordering (T) stands for

$$G(t) = \mathrm{Tr}\, [e^{-H(\beta-t)}ae^{-Ht}a^\dagger]$$

Path integral formulation

We formulate the path integral by introducing coherent states (see Negele and Orland, Quantum Many-Particle Systems)

$$|\alpha\rangle = e^{-\sum_x \alpha_x a_x^\dagger}|0\rangle$$

Completeness reads

$$I = \int \prod d\alpha^* d\alpha \, e^{\sum -\alpha^* \alpha} \, |\alpha\rangle\langle\alpha^*|$$

Path integral formulation, cont'd

We split the evolution by Euclidean time β into the product of N_t evolutions by $\delta = \beta/N_t$ and use completeness:

$$\operatorname{Tr} e^{-\beta H} = \int \prod_{i=0}^{N_t-1} d\alpha_i^* d\alpha_i \prod_{i=0}^{N_t-1} e^{-\alpha_i^* \alpha_{i+1}} \langle \alpha_i^* | e^{-H\,\delta} | \alpha_i \rangle$$

(We shifted a dummy index, $\alpha_i \to \alpha_{i+1}$, to conform to the discretization in Q.F.T.)

Path integral formulation, cont'd

We finally use

$$\langle \alpha_i^* | F(a^\dagger, a) | \alpha_i \rangle = F(\alpha_i^*, \alpha_i)\, e^{\alpha_i^* \alpha_i}$$

valid for any normal ordered operator function $F(a^\dagger, a)$

$e^{-H\,\delta}$ is not normal ordered, but differs from its normal ordered expression by $O(\delta^2)$

Path integral formulation

In conclusion we get

$$\mathrm{Tr}\, e^{-\beta H} = \int \prod_{i=0}^{N_t-1} d\alpha_i^* d\alpha_i \prod_{i=0}^{N_t-1} e^{-\alpha_i^*(\alpha_{i+1}-\alpha_i)} e^{-H(\alpha_i,\alpha_i)\,\delta}$$

$$= \int \prod_{i=0}^{N_t-1} d\alpha_i^* d\alpha_i \, e^{-S(\alpha^*,\alpha)}$$

The Coulomb interaction

The Hamiltonian consists of two terms (dropping the sublattice indices): $H = H_2 + H_c$

$$H_2 = \sum_{x,y,s} a^\dagger_{x,s} K_{x,y} a_{y,s} + \text{h.c.} \equiv a^\dagger K a + \text{h.c.}$$

and

$$H_C = \sum_{x,y} e^2 V_{x,y} : q_x q_y :$$

with

$$q_x = a^\dagger_{x,\uparrow} a_{x,\uparrow} + a^\dagger_{x,\downarrow} a_{x,\downarrow} - 1$$

Looking ahead to a positive definite measure

We rewrite q_x as

$$q_x = a^\dagger_{x,\uparrow} a_{x,\uparrow} - a_{x,\downarrow} a^\dagger_{x,\downarrow}$$

and define

$$b^\dagger_x = a_{x,\downarrow} \qquad b_x = a^\dagger_{x,\downarrow}$$

This gives (we drop the index $\uparrow$)

$$q_x = a^\dagger_x a_x - b^\dagger_x b_x$$

while H_2 can be cast in the form

$$H_2 = \sum_{x,y} [a^\dagger_x K_{x,y} a_y + b^\dagger_x K_{x,y} b_y + \mathrm{h.c.}]$$

by changing the sign of the $b, b^\dagger$ operators on one of the sublattices.

The path integral

We now can write

$$Z = \lim_{N_t \to \infty} \int \prod_{m=0}^{N_t-1} d\psi_m^* d\psi_m \prod_{m=0}^{N_t-1} d\eta_m^* d\eta_m$$

$$e^{-\sum_{m,n}(\psi_m^* M_{m,n} \psi_n + \eta_m^* M_{m,n} \eta_n)} e^{-\sum_{i,x,y} e^2 q_{i,x} q_{i,y} V_{x,y} \delta}$$

with

$$q_{i,x} = \psi_{i,x}^* \psi_{i,x} - \eta_{i,x}^* \eta_{i,x}$$

The final ingredient is a Hubbard-Stratonovich transformation

$$e^{-\sum_{i,x,y} e^2 q_{i,x} q_{i,y} V_{x,y} \delta} = \int \prod_{i,x} d\phi_{i,x} e^{-\sum_{i,x,y} \phi_{i,x} \phi_{i,y} V^{-1}_{x,y} \delta/4}$$

$$e^{-\sum_{i,x} \imath e \phi_{i,x} (\psi^*_{i,x} \psi_{i,x} - \eta^*_{i,x} \eta_{i,x}) \delta}$$

which gives

$$Z = \lim_{N_t \to \infty} \int \prod_{i,x} d\psi^*_{i,x} d\psi_{i,x} \prod_{i,x} d\eta^*_{i,x} d\eta_{i,x} \prod_{i,x} d\phi_{i,x}$$

$$e^{-\sum_{i,x,y} \phi_{i,x} \phi_{i,y} V^{-1}_{x,y} \delta/4} e^{-\sum_{i,x,j,y} (\psi^*_{i,x} M_{i,x;j,y} \psi_{j,y} + \eta^*_{i,x} M_{i,x;j,y} \eta_{j,y})}$$

$$e^{-\sum_{i,x} \imath e \phi_{i,x} (\psi^*_{i,x} \psi_{i,x} - \eta^*_{i,x} \eta_{i,x}) \delta}$$

The path integral, cont'd

Introducing Φ, diagonal with diag. entries

$$\Phi_{i,x} = \phi_{i,x}\delta$$

the partition function can be written very compactly

$$Z = \lim_{N_t \to \infty} \int d\phi e^{-\phi V^{-1} \phi \delta/4} \int d\psi^* d\psi d\eta^* d\eta$$

$$e^{-\psi^*(M+\imath e\Phi)\psi - \eta^*(M-\imath e\Phi)\eta}$$

or, integrating over the fermions

$$Z = \int d\phi e^{-\phi V^{-1} \phi \delta/4} \det(M + \imath e\Phi) \det(M - \imath e\Phi)$$

which lends itself to Hybrid Monte Carlo integration.

Hybrid Monte Carlo

$$Z = \int d\phi e^{-\phi V^{-1}\phi\delta/4} \det(M + \imath e\Phi)\det(M - \imath e\Phi)$$

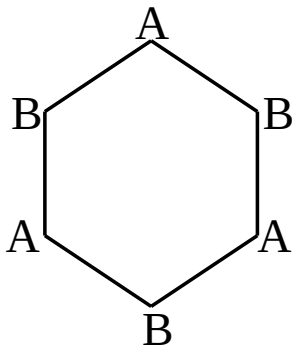
$$= \int d\phi dp d\psi^* d\psi e^{-\phi V^{-1}\phi\delta/4 - p^2/2} e^{-\psi^*(M-\imath e\Phi)^{-1\dagger}(M-\imath e\Phi)^{-1}\psi}$$

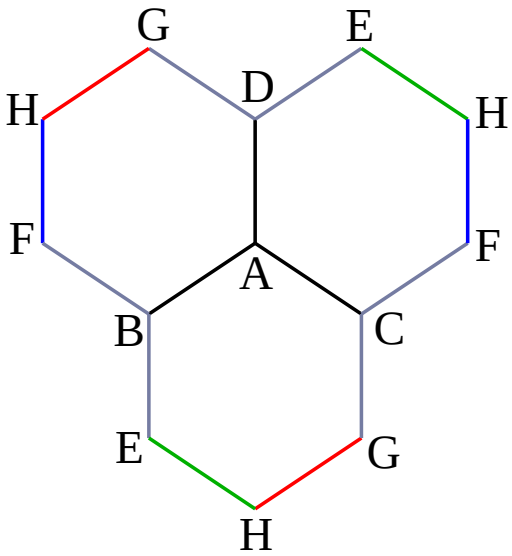
Then one explores phase space by extracting the now bosonic fields p, ψ, ψ^* with their Gaussian measure, evolving ϕ, p with

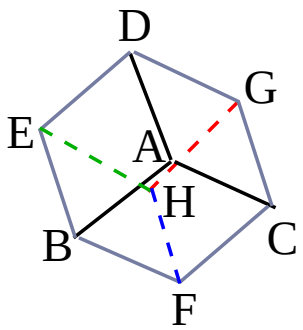
$$H = \phi V^{-1}\phi\delta/4 + p^2/2 + \psi^*(M - \imath e\Phi)^{-1\dagger}(M - \imath e\Phi)^{-1}\psi$$

and correcting for the errors in the discretized evolution with a global MC accept-reject step.

HMC vs. exact for small systems

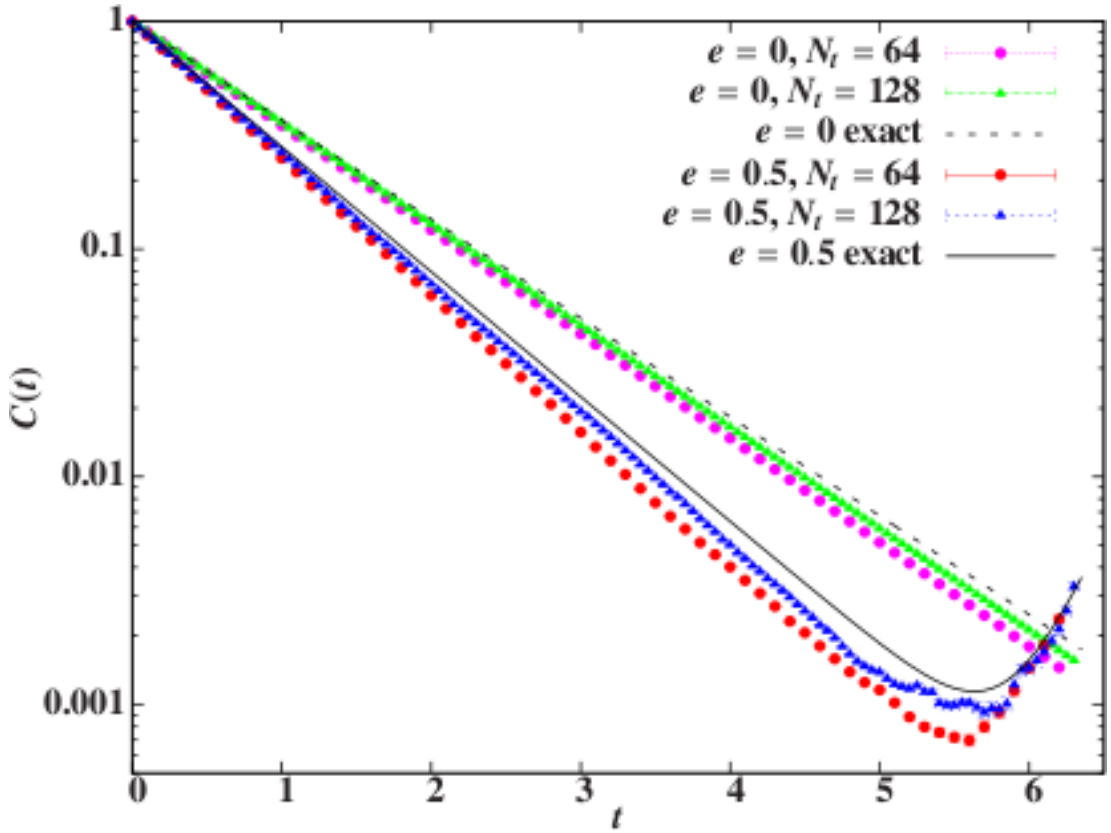






Graphene lattices with period one and two.

Two-sites system - HMC vs. exact



$$C_a(t) = \langle (a_0 - a_1)(t)\,(a_0^\dagger - a_1^\dagger)(0)\rangle/2$$

for $\beta = 6.4$, $N_t = 64$ and 128, $e = 0$ and $e = 0.5$

Numerical diagonalization of the eight-site system

Dimensionality of basis: 65,536 !!!

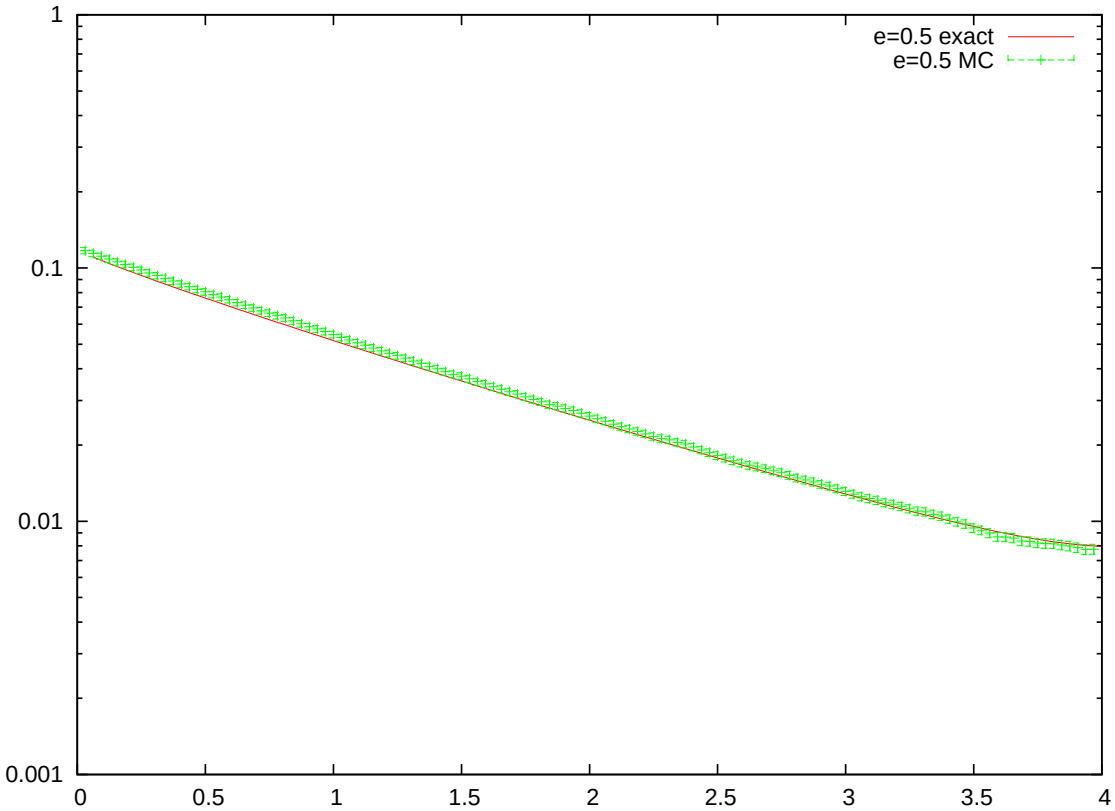
Convenient numerical representation:

$$b_5^\dagger b_2^\dagger a_7^\dagger a_4^\dagger a_3^\dagger a_0^\dagger |\rangle \leftrightarrow |0010010010011001\rangle = |9369\rangle$$

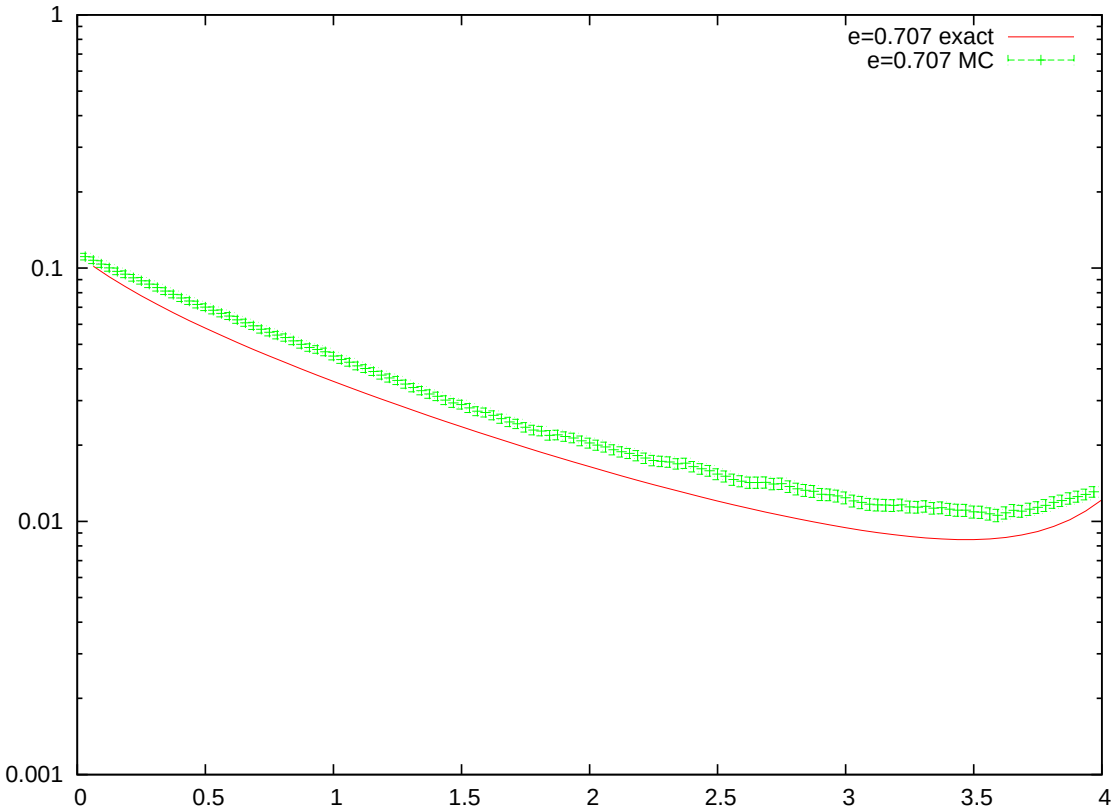
Use conservation laws with suitable ordering of basis states to make the Hamiltonian block diagonal. Calculate numerically eigenvalues and eigenvectors block by block. Calculate the correlators

$$C(t) = \langle \psi(t)\, \psi^\dagger(0) \rangle$$

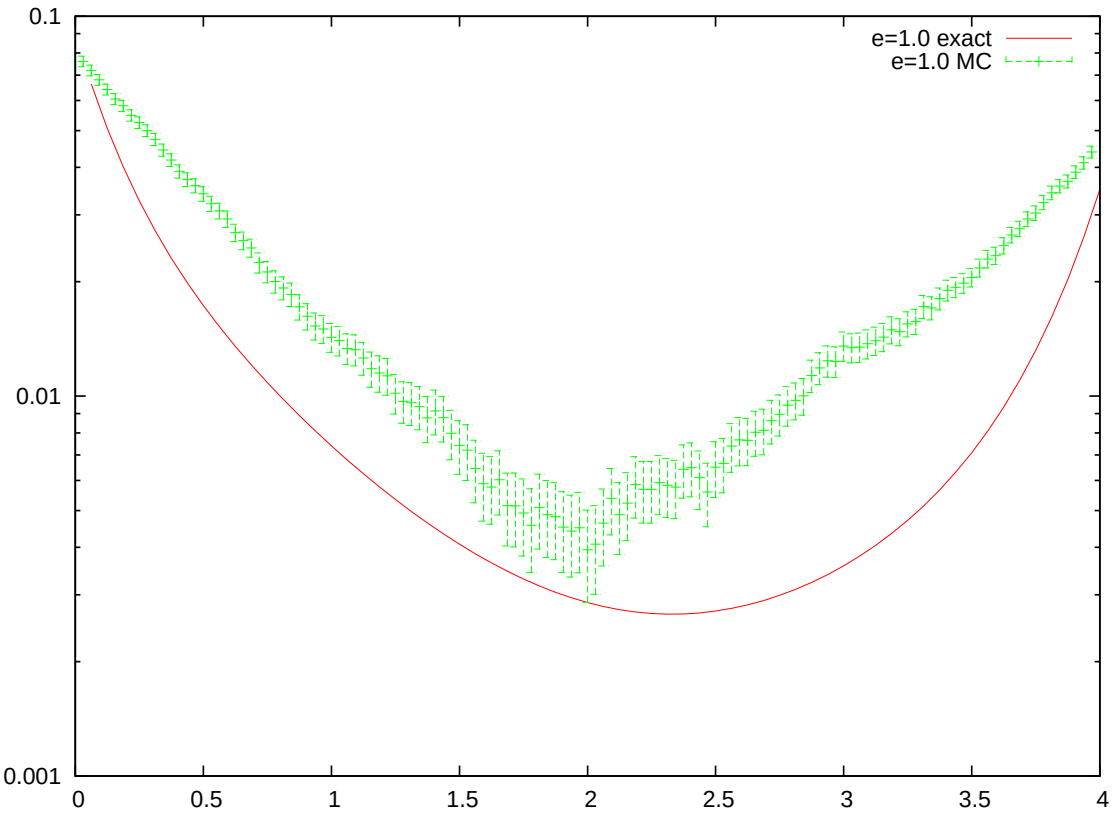
Eight-sites system - HMC vs. exact: $e = 0.5, N_t = 128$



Eight-sites system - HMC vs. exact: $e = \sqrt{2}/2, N_t = 128$



Eight-sites system - HMC vs. exact: $e = 1.0, N_t = 128$



The trend is correct, but the agreement is not fully satisfactory. The disagreement could be due to an error in the programs (checking), lack of convergence, critical behavior... (?)

Conclusions

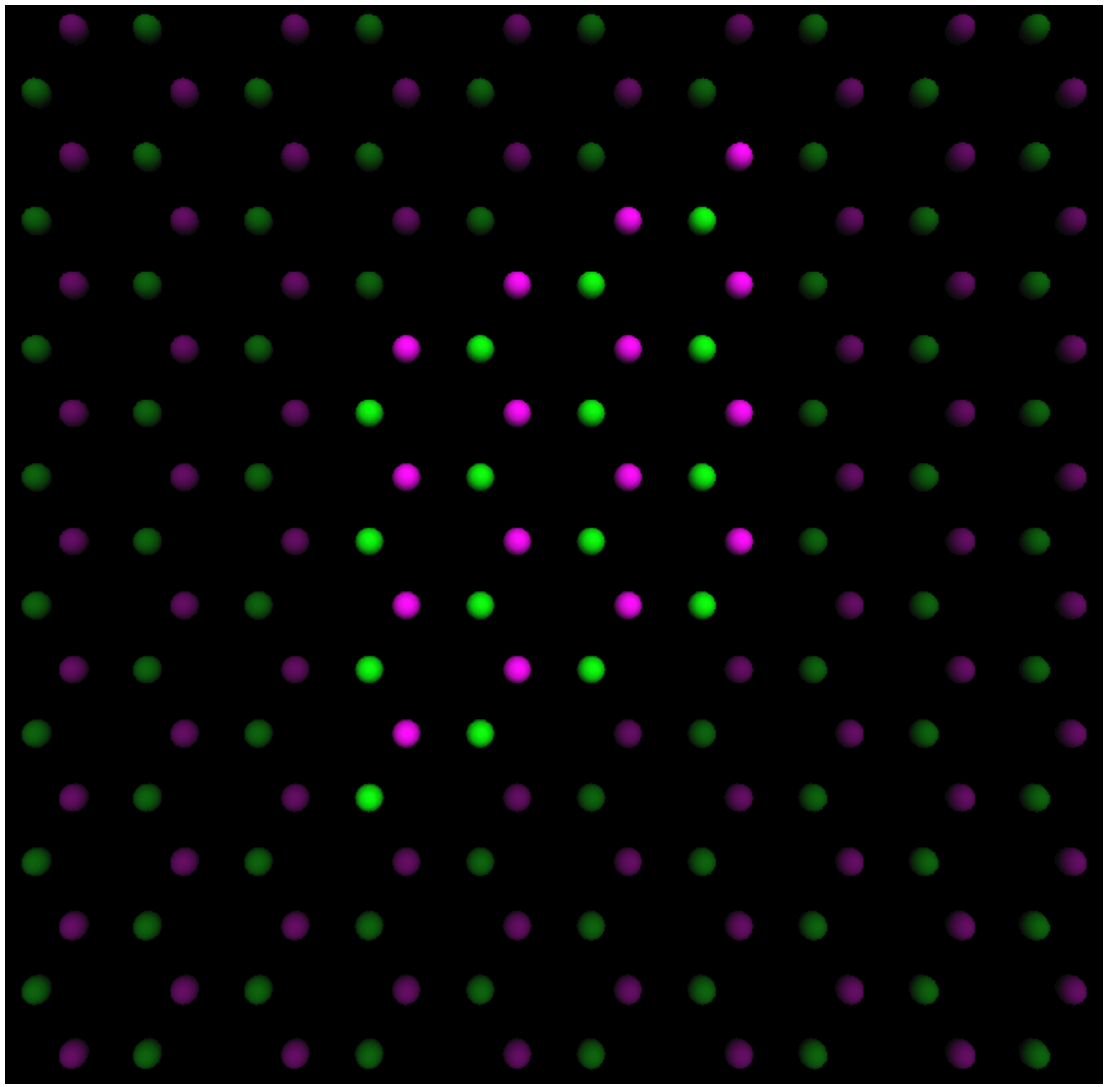
It appears possible to use the hybrid Monte Carlo method to simulate graphene directly on the graphene lattice.

Variants of the method (e.g. the use of central difference approximation and staggering in time to represent both spins) are being investigated. Simulations on large lattices are in progress to study the emergence of a gap.

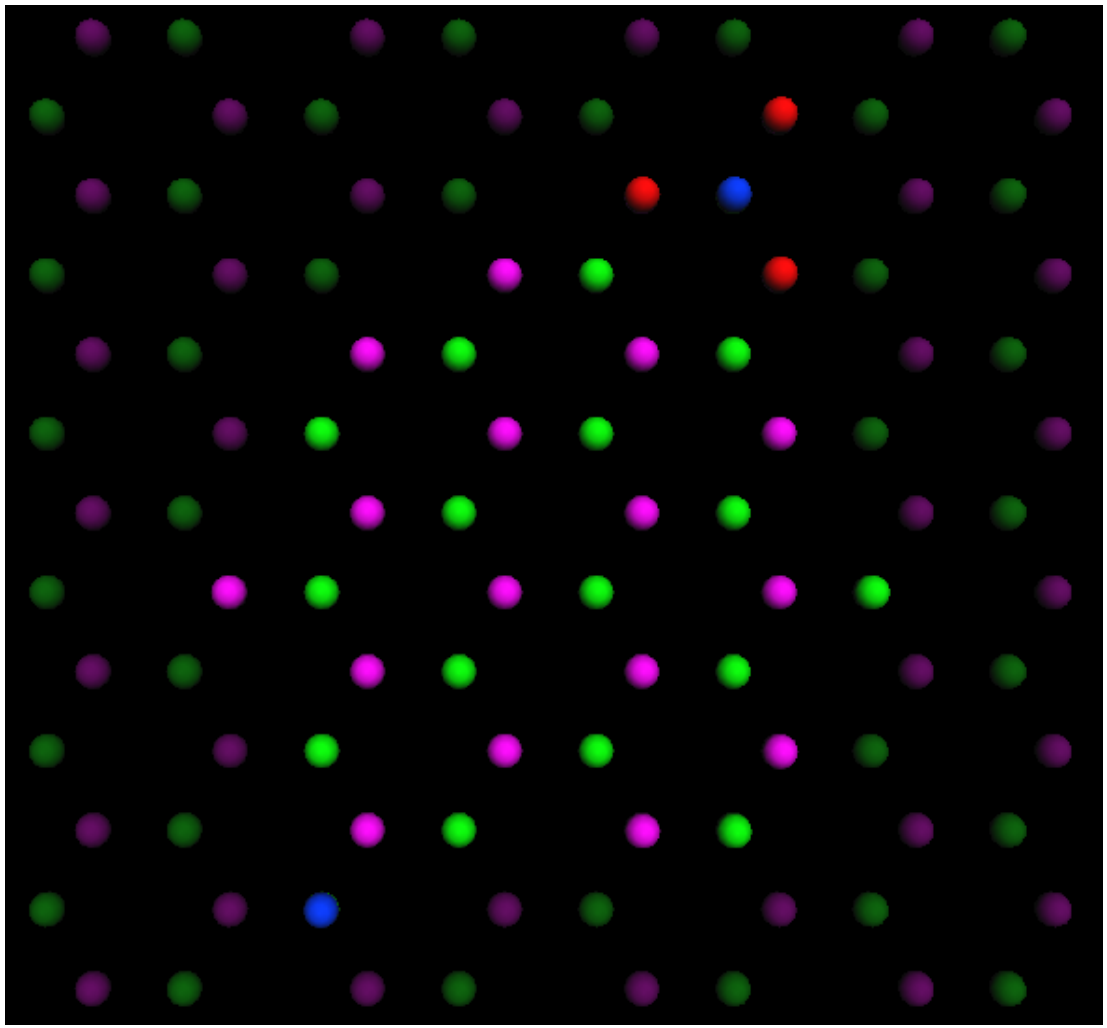
It the method is fully validated, it has potential applications to a wide range of problems (lattice distortions, external magnetic fields, etc.)

Additional slides

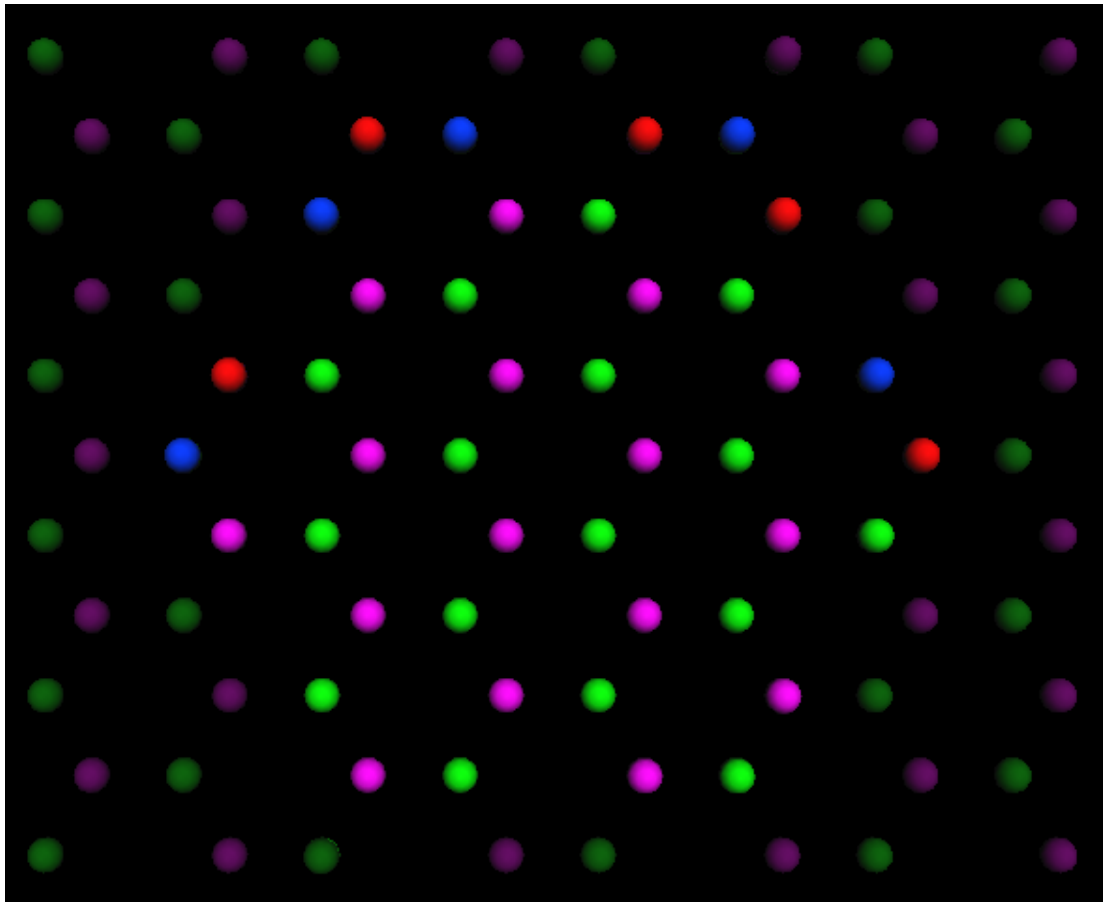
Periodicity



Periodicity, rearranged



Hexagonal symmetry



The coupling matrix:

$$\begin{pmatrix} 0 & 1 + e^{2\pi\imath k_1/L} + e^{2\pi\imath k_2/L} \\ 1 + e^{-2\pi\imath k_1/L} + e^{-2\pi\imath k_2/L} & 0 \end{pmatrix}$$

$$\equiv \begin{pmatrix} 0 & e[k_1, k_2]e^{\imath\phi[k_1,k]_2} \\ e[k_1, k_2]e^{-\imath\phi[k_1,k_2]} & 0 \end{pmatrix}$$

where ϕ, e are the phase and magnitude of

$$1 + e^{2\pi\imath k_1/L} + e^{2\pi\imath k_2/L}$$

The zero modes

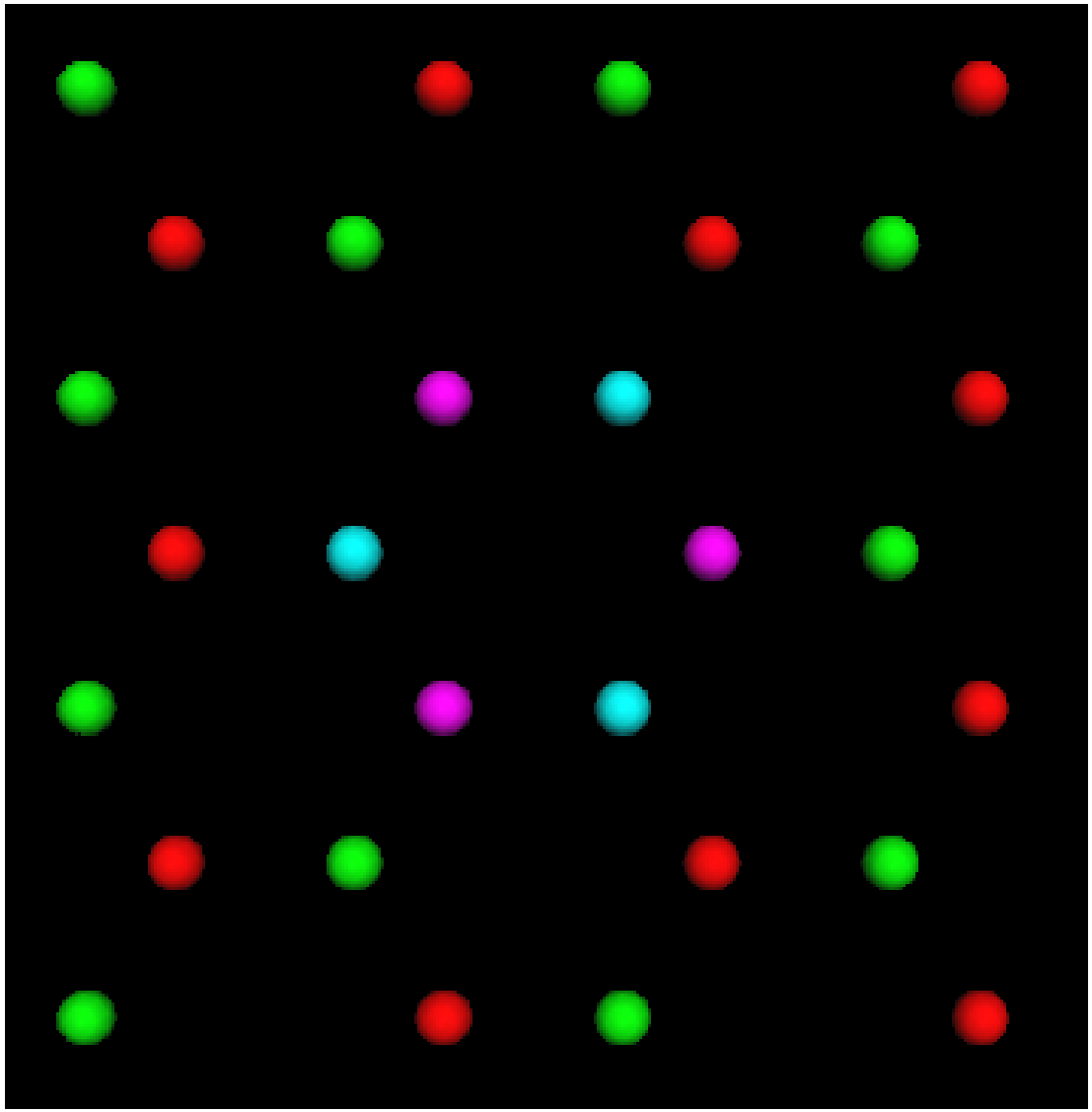
$$1 + e^{2\pi\imath k_1/L} + e^{2\pi\imath k_2/L}$$

vanishes for

$$2\pi\imath k_1/L = -2\pi\imath k_2/L = \pm 2\pi/3$$

On an infinite lattice, and also on finite lattices where periodicity is up to a factor of 3, the quadratic Hamiltonian has two zero modes at two different points in momentum space and, with an infinite system, the dispersion relation similar to the one of massless Dirac fermions in the neighborhood of the zeroes.

Simulation of a two sites system



Simulation of a two sites system

We label the sites $x = 0, 1$. With $\kappa = 1/3$. H_2 and H_C are now

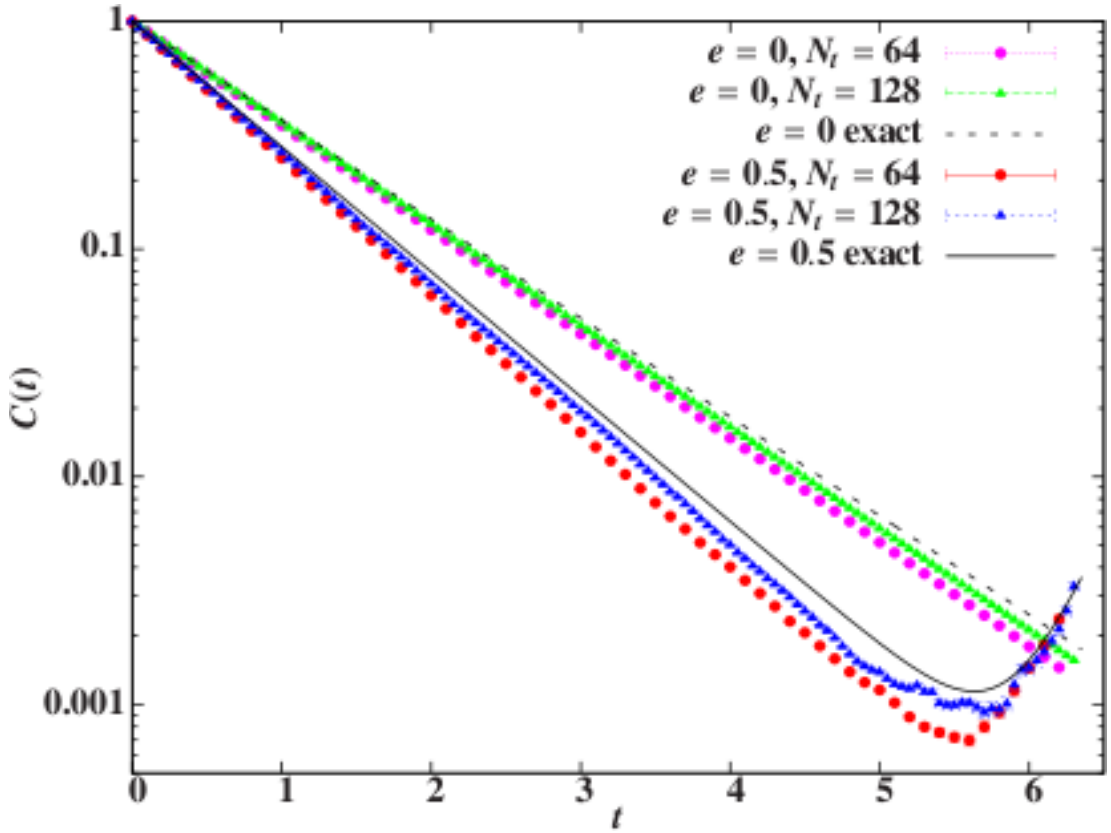
$$H_2 = (a_1^\dagger a_0 + a_0^\dagger a_1 + b_1^\dagger b_0 + b_0^\dagger b_1)$$

$$H_C = 2e^2(a_0^\dagger a_0 - b_0^\dagger b_0)(a_1^\dagger a_1 - b_1^\dagger b_1) + (2e^2/r_0)a_x^\dagger b_x^\dagger a_x b_x$$

$$+(e^2/r_0)(a_x^\dagger a_x + b_x^\dagger b_x)$$

The spectrum can be calculated exactly and compared with HMC simulations.

Two sites system - HMC vs. exact



$$C_a(t) = \langle (a_0 - a_1)(t)\,(a_0^\dagger - a_1^\dagger)(0)\rangle/2$$

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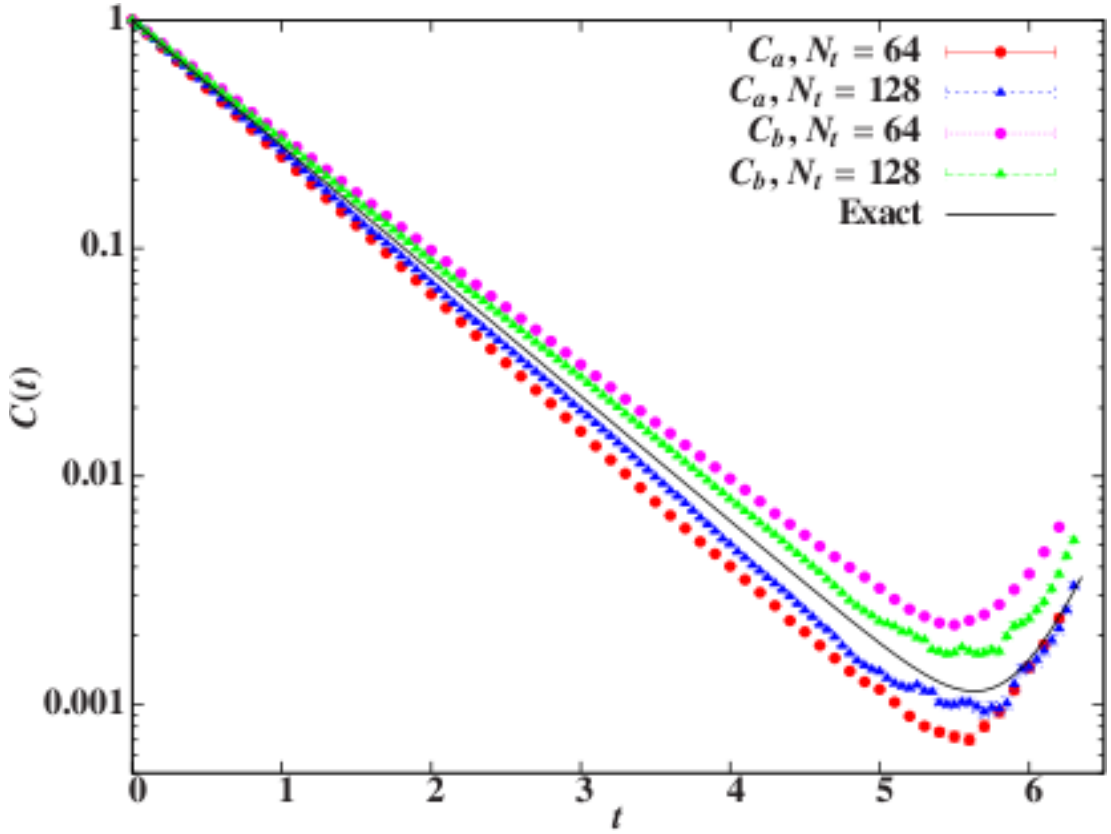
Two sites system - HMC vs. exact



$C_a(t) = \langle (a_0 - a_1)(t)\,(a_0^\dagger - a_1^\dagger)(0)\rangle/2 \quad C_b(t) = \langle (b_0^\dagger + b_1^\dagger)(t)\,(b_0 + b_1)(0)\rangle/2$

for $\beta = 6.4$, $N_t = 64$ and 128, $e = 0.5$