Constrained Molecular Dynamics (CoMD) for Fermions

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- Introduction
- Molecular Dynamics with constraints for Pauli/Heisenberg principle.
- Infinite systems of ud quarks at zero temperature and finite baryon densities, results at high T
- Ground states of Atoms. S-factor calculations with electrons
- Muon catalyzed fusion
- The case of D,T, Li plasma. How does the free fusion cross section change in medium?
- Nuclear ground states and heavy ion collisions
- Conclusions and outlook
**Virtual tour**

- First radioactive $^8$Li beam extracted at the EXCYT facility
- 80 AMeV reached at the Superconducting Cyclotron
- 100 W beam power successfully extracted from the Superconducting Cyclotron
- CHIMERA is complete and started its physics operations
- MAGNEX spectrometer is currently under commissioning
- NEMO a project for a 1km$^3$ underwater neutrino telescope
The exact one body classical distribution function satisfies the equation:

\[ \partial_t f(r,p,t) + \frac{P}{E} \cdot \nabla_r f(r,p,t) - \nabla U \cdot \nabla_p f(r,p,t) = 0 \]

where: \( E = \sqrt{p^2 + m_q^2} \) is the energy, \( m_q \) is the (e,ion) mass

\[ U = \sum_j V(r_{ij}) \]

is the exact potential

with \( V(r_{ij}) \) is the Coulomb potential.

Numerically the exact equation is solved by writing the one body distribution function as:

\[ f(r,p,t) = \sum_i \delta(r-r_i(t)) \delta(p-p_i(t)) \]

\( Q = q + \overline{q} \) is the total number of ions and electrons, zero net charge.

Inserting this expression we get the Hamilton equations of motion for our system (CMD).
The Balescu Lennard Vlasov equation

Define average (over ensembles) distribution function and mean field.

\[ f_1 = \bar{f}_1 + \delta f_1 \quad U = \bar{U} + \delta U \]

Inserting into the exact equation gives:

\[
\partial_t \bar{f}_1 + \frac{p}{E} \nabla_r f_1 - \nabla_r \bar{U} \nabla_p f_1 = \left\langle \nabla_r \delta U \nabla_p \delta f_1 \right\rangle
\]

Where we recognize the Vlasov equation on the LHS and The BL collision term on the RHS.

Numerically we solve CMD and average over ensembles to get the Mean field and fluctuations. Important to have particles fusion and Creations of new particles.
The exact one body classical distribution function satisfies the equation:

\[ \partial_t f(\mathbf{r}, \mathbf{p}, t) + \frac{\mathbf{p}}{E} \cdot \nabla f(\mathbf{r}, \mathbf{p}, t) - \nabla U \cdot \nabla f(\mathbf{r}, \mathbf{p}, t) = 0 \]

where: \( E = \sqrt{\mathbf{p}^2 + m_q^2} \) is the energy, \( m_q \) is the (u,d) quark mass

\[ U = \sum_{ij} V(r_{ij}) \]

is the exact potential

with \( V(r_{ij}) \) Richardson’s potential:

\[
V(r_{ij}) = 3 \sum_{a=1}^{8} \frac{\lambda^a_i \lambda^a_j}{2} \left[ \frac{8\pi}{33 - 2n_f} \Lambda \left( \Lambda r_{ij} - \frac{f(\Lambda r_{ij})}{\Lambda r_{ij}} \right) + \frac{8\pi}{9} \alpha_s \frac{\langle \sigma_{ai} \sigma_{aj} \rangle}{m_q m_q} \delta(r_{ij}) \right]
\]

and

\[
f(t) = 1 - 4 \int_{q}^{e} dq \left[ \frac{e^{-qt}}{\ln (q^2 - 1) + \pi^2} \right]
\]

\( n_f \) (number of flavours) = 2

\( \Lambda = 0.250 \text{ Gev} \)

\( \lambda^a_i \) (Gell-Mann matrices)

Initially we distribute randomly the quarks in a box of side $L$ in coordinate space and in a sphere of radius $P_f$ in momentum space.

For a Fermi gas model:

$$p_f^3 = \frac{6\pi^2 \rho_q}{g_q}$$

$$g_q = n_c \cdot n_f \cdot n_s \quad (Degeneracy\ Number)$$

- We impose periodic boundary conditions
- We consider many events and we impose that $\bar{f}_i(r,p,t) \leq 1 \quad \forall i$
**Constraint:**

At each time step we control the value of \( f_i(r,p,t) \) and consequently we change the momenta of the particles:

\[ \dot{p}_i = \dot{p}_i \cdot \text{det} \]

- **If** \( f(r,p,t) > 1 \)
  \[ \text{det} > 1 \]

- **If** \( f(r,p,t) < 1 \)
  \[ \text{det} < 1 \]
We define an *Order Parameter* as:

\[
M_c = \frac{1}{N} \sum_{i=1}^{N} \sum_{a=3,8} (\lambda^a_j \lambda^a_k + \lambda^a_i \lambda^a_j + \lambda^a_i \lambda^a_k)
\]

\[
= M_{cr} + \frac{1}{N} \sum_{a=3,8} (\lambda^a_j \lambda^a_k + \lambda^a_i \lambda^a_k)
\]

j and k are the two quarks closest to quark i

\[M_{cr} = \text{Reduced order parameter.}\]

We normalize the order parameter:

\[
\bar{M}_c = \frac{2}{9} [M_c + 3]
\]

\[
\bar{M}_{cr} = \frac{2}{3} [M_{cr} + 1]
\]

- if the three closest quarks have different colours \(\bar{M}_c = 1\); \(\bar{M}_{cr} = 1\) *Isolated white nucleon*
- if the three closest quarks have two different colors \(\bar{M}_c = \frac{2}{3}\); \(\bar{M}_{cr} = \frac{2}{3}\) *Quark Gluon Plasma*
- if the three closest quarks have the same colour \(\bar{M}_c = 0\); \(\bar{M}_{cr} = 0\) *Exotic colour clustering*
Test for atomic ground states where masses and forces (Coulomb) are exactly known

Constrained Molecular Dynamics (CoMD)

Lagrange multiplier method for constraints

\[ \mathcal{L} = \sum_i \frac{p_i^2}{2m_i} - \sum_{i \neq j} U(r_{ij}) + \sum_{i \neq j} \lambda_i \left( \frac{r_{ij}p_{ij}}{\xi \hbar} - 1 \right) \]

\[ r_{ij} = |r_i - r_j|; \quad p_{ij} = |p_i - p_j| \]

\[ \xi = 1 \text{ (for Heisenberg principle)} \]

Variational calculus leads Hamilton Equation with Constraint:

\[ \frac{dr_i}{dt} = \frac{p_i}{m_i} + \lambda_i \frac{r_{ij} p_{ij}}{\xi \hbar} \frac{\partial p_{ij}}{\partial r_i} \]

\[ \frac{dp_i}{dt} = -\nabla_r U(r_i) \frac{\lambda_i r_{ij} p_{ij}}{\xi \hbar} \frac{\partial r_{ij}}{\partial r_i} \]
Convergence of Atomic G.S.

**Constraint** changes
Phase Space Occupation
\[ f(r,p,t) \leq 1 \]

Binding energies of Atoms (in eV)

<table>
<thead>
<tr>
<th>Element</th>
<th>CoMD</th>
<th>exper.</th>
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<tbody>
<tr>
<td>H</td>
<td>−13.56</td>
<td>−13.61</td>
</tr>
<tr>
<td>He</td>
<td>−77.70</td>
<td>−78.88</td>
</tr>
<tr>
<td>Li</td>
<td>−203.78</td>
<td>−203.43</td>
</tr>
<tr>
<td>Be</td>
<td>−404.91</td>
<td>−399.03</td>
</tr>
<tr>
<td>F</td>
<td>−2644.4</td>
<td>−2713.45</td>
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</table>
S-factor calculations at astrophysical energies

\[ f_e = \frac{\sigma(E)}{\sigma_0(E)} = \frac{\sigma_0(E + U_e)}{\sigma_0(E)} \]

\[ \sim \exp\left\{ \pi \eta(E) \frac{U_e}{E} \right\} \]

\[ U_e \sim \frac{E}{\pi \eta(E)} \log f \]

\( U_e \) : Screening Energy
Large Enhancement

$^3\text{He}(d,p)^4\text{He}$


Energy loss, electron screening and the astrophysical $^3\text{He}(d,p)^4\text{He}$ cross section
### Screening potential

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<tbody>
<tr>
<td>( \text{D(d,p)T} )</td>
<td>8.7(Quadratic)</td>
<td>20</td>
<td>7.3(Cubic)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( ^3\text{He(d,p)}^4\text{He} )</td>
<td>34(Quadratic)</td>
<td>119</td>
<td>180\pm40</td>
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<td></td>
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<tr>
<td></td>
<td>60(( R )-matrix)</td>
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<td>200(( R )-matrix)</td>
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<tr>
<td>( ^6\text{Li(d,\alpha)}^4\text{He} )</td>
<td>259(Cubic)</td>
<td>175</td>
<td>320\pm50</td>
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<td>( ^7\text{Li(p,\alpha)}^4\text{He} )</td>
<td>134(Cubic)</td>
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<td>204(Cubic)</td>
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<td>242(( R )-matrix)</td>
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**Problem has not been settled yet**
Tunneling process

\[ \frac{dr_i}{dt} = \frac{p_i}{m_i}, \quad \frac{dp_i}{dt} = -\nabla_r U(r_i) \]

Collective coordinates and momenta

\( R^{coll} \equiv r_P - r_T; \quad P^{coll} \equiv p_P - p_T; \quad F^{coll}_P \equiv \dot{P}^{coll} \)

\[ \frac{dr^{\text{coll}}_T(P)}{d\tau} = \frac{p^{\text{coll}}_T(P)}{m_T(P)}, \quad \frac{dp^{\text{coll}}_T(P)}{d\tau} = -\nabla_r U(r^{\text{coll}}_T(P)) - 2F^{coll}_T(P) \]

Tunneling penetrability: \( \Pi(E) = (1 + \exp(2A(E)/\hbar))^{-1} \)

\( A(E) = \int_{r_b}^{r_a} P^{coll} dR^{coll} \)

without electron \( \Rightarrow \Pi_0(E) \)

Enhancement factor: \( f_e = \frac{\Pi(E)}{\Pi_0(E)} \)
Dissipative Limit
Bound electron emission
Electronic Motion

Inter-nuclear motion

S. Kimura, and A. Bonasera

Oscillational motion of Electron around the target

Sensitive Initial Phase
Space Configuration Dependence $\Rightarrow$ Chaos
Enhancement factor with Polarized target
S. Kimura, and A. Bonasera
Nucl. Phys. A in press
nucl-th/0504005
Muon catalyzed fusion

- Effective sticking: \( \#s = (1-R)\#s_0 \)
- Reactivation 3.5 MeV
- Neutron R ~ 0.35
- Initial sticking X-rays
- Thermalized K

\[ \lambda_n = \frac{Y_n}{Y_n} \]

\[ W = (1-R_0)Y_n \]

\[ \omega_S = W - W_{dd} - W_{tt} \ldots \]
Muon Catalyzed Fusion

d  t

\[ \text{d} \quad \text{t} \]
Muon Catalyzed Fusion

\[ \mu^- : 200 \times \text{heavier than } e^- \]
Muon Catalyzed Fusion

Catalyze fusion

\[
\text{µ} \rightarrow \text{fusion}
\]
Muon Catalyzed Fusion
release and ... more than 100 fusion reactions/$\tau_\mu$
Muon Catalyzed Fusion
Muon Catalyzed Fusion

\[ \mu - \alpha \text{ Sticking} \]
FIG. 1: Enhancement factor by the bound muon (top panel) and $\Delta f_\mu^2/f_\mu$ (bottom panel) as functions of the incident center-of-mass energy. The arrows in the figure indicate the point where total energy is zero.

S. Kimura and A.B.
FIG. 2: Surface of section for 2 events, one has small $f_\mu$ (top panels) and the other has large $f_\mu$ (bottom panels), on the $x$-$p_x$ (left panels) and the $z$-$p_z$ (right panels) planes at the incident c.o.m energy 0.18keV, in the atomic unit.
FIG. 3: Incident energy dependence of the sticking probability of the muon on the α particle. The statistical error is shown by error bars, otherwise it is within the size of the points in the figure. (top panel) Distance between the muon and the alpha particle as a function of the inter-nuclear separation (bottom panel)
μ⁻ Stripping

Stripping

\[ \begin{align*}
 4.5 & \quad 4.4 & \quad 4.3 & \quad 4.2 & \quad 4.1 & \quad 4 & \quad 10^{-4} & \quad 10^{-3} & \quad 10^{-2} & \quad 10^{-1} & \quad 10^0 \\
p \times 10^4 \text{[a.u.]} & \quad \text{r[a.u.]} & \quad \text{no coupling} & \quad \gamma = 2\gamma_\mu \\
\end{align*} \]
Simulate fusion in plasmas: Mean free path approach.

At each time step we search the closest particle \( l \) to each ion \( k \) and calculate the local density \( \rho \) and the relative velocity \( v_{kl} \), from this we obtain the fusion cross section (parametrized from data) \( \sigma \).

Define the local mean free path for particles \( k \) and \( l \) at time \( t \):

\[
\Pi = \frac{v_{kl} dt}{\lambda} = \rho \sigma(r_k)v_{kl} dt
\]

In a Montecarlo way it is decided if the two ions fuse and the reaction is performed according to the \( Q \)-value.

Tokamak case: JET & ITER

D+T (squares), D(circles) and D+Li (triangles) at $9.8 \times 10^{19} \text{m}^{-3}$ density. D+T (dashed line) and JET result (cross) at $10^{19} \text{m}^{-3}$.
Tokamak + ion beam

- D plasma + T(full lines) or Li (dashed lines) beams at T=1KeV (squares) and T=20 KeV (triangles). The plasma density is $4.1 \times 10^{21} \text{m}^{-3}$ and the beam is 400 times smaller.
Laser induced fusion

- Initial density $10^{28} \text{m}^{-3}$ (top) and zero $T$. 
  Density $4 \times 10^{31} \text{m}^{-3}$ 
  $T=0.8$ KeV (center) and 
  $T=1$eV (bottom). $D+T$ (full), $D+Li$ (dashed) 
  and $D$ (dashed-dotted). 
  Triangles $D+Li$ with linear radial energy 
  (center). Triangles (top) 
  $D+T$ without Coulomb force.

- Note that number of 
  particles finite ($<10^4$).
Pellet with ‘periodic’ boundary conditions. I.e. insert a particle which is escaping the outer surface.
- D+T \( E_i = 50, 5 \text{ KeV} \)
- D \( E_i = 50, 5 \text{ KeV} \)
CoMD for Heavy Ion Collisions

**Constraint for Fermionic nature**

\[
\bar{f}_i < 1 \quad \text{(for all } i),
\]

\[
\bar{f}_i = \sum_j \delta_{s_j, s_i} \delta_{\tau_j, \tau_i} \int_{V_i(h)} f_j(r, p) \, dr \, dp,
\]

where \( s_i \) and \( \tau_i \) are the spin and isospin coordinate of the nucleon \( i \).

\( V_i(h) \) is the phase-space around \( (R_i, J_i) \) with volume \( h^3 \).

**Numerical method for constraint**

At every timestep, we check \( \bar{f}_i \) of each particle.

If \( \bar{f}_i > 1 \) then we force multiple "elastic scatterings" among neighbors of the particle \( i \). We accept the final state if \( \bar{f}_i \) reduces.
Effect of the constraint

Time evolution of $f_i$

$f_i$ remain below 1 for CoML. QMD calculation breaks this condition.

REDUCED VELOCITY PLOTS:

Note: BNV model accounts only for the "prompt" component of IMF's

 Collision of heavy systems

\[ ^{197}\text{Au} + ^{197}\text{Au} \quad E_{\text{lab}} = 5 \sim 20 \text{ MeV/\text{n}}. \]

\[ E_{\text{lab}} = 10 \text{ MeV \text{b} \sim 6 \text{ fm} } \]

Almost complete fusion occurs and then evaporation of nucleons proceeds. Then a fission takes place.

Conclusions

✓ Studied EOS for quarks with colours and Pauli principle, $T=0$ and $\rho g_B \neq 0$ within a microscopic dynamical simulation.

✓ Found exotic quark clustering at high densities and small quark masses.
   First order phase transition.

✓ Larger quark masses no exotic clustering. QGP at high densities and may be Second order phase transition.

At high densities we note always a residual coupling of quarks of different colors due to the competing effect of residual attraction and Fermi motion.

$J/\psi$ plays a role similar to order parameter. Study other signals of criticality such as intermittency.

Extend approach to RHIC including qq creation and annihilation
✓ Found good ground state energies for light atoms
✓ S-factor calculations with electron screening show occurrence of chaos.
✓ Found good agreement with JET-tokamak result.
✓ Good ‘performance’ for tokamak + beam of Li. Avoid handling T.

At high densities and excitation energies as in laser induced reactions, found a modest energy gain even for D+T plasma for small pellet sizes. Increasing the size energy gain even for D+D.

Extend approach to calculate EOS for materials (H, D, Li etc..) also including quantum effects for zero T and high densities cases.

Promising for heavy ion collisions. Needs parameters fitting and lots of simulations (and somebody to do it!).