



SOM 2024

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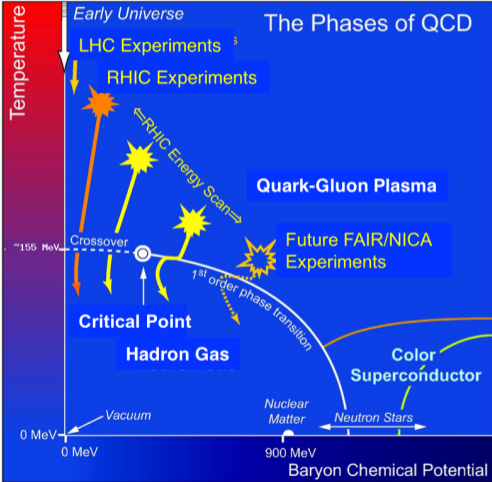
Spinodal decomposition in a rapidly expanding fluid

Mayank Singh

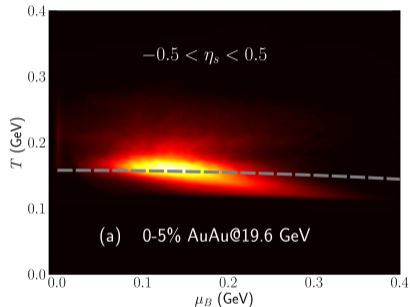


In Collaboration with Joe Kapusta

QCD phase diagram



Trajectories of heavy-ion collisions



- Realistic heavy-ion collisions do not follow a clean trajectory on the phase diagram
- The phase space volume passing near the critical point may not be large
- It makes sense to look for signatures of the first order phase transition as a larger system volume could pass through that

Chun Shen, Quark Matter 2018

Spinodal separation

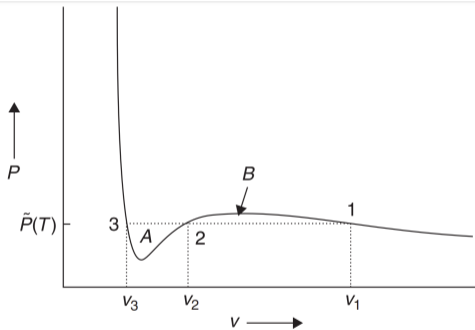


Figure from Pathria and Beale, *Statistical Mechanics*

- The region between A and B is unstable (spinodal region). It is energetically favorable for phases to separate
- The region from 3 to A and B to 1 is metastable. This is where nucleation dominates
- If nucleation rate is small, spinodal separation is the dominant mechanism of phase transition

Cahn-Hilliard model

- Consider the Helmholtz free energy functional at temperature T

$$\begin{aligned} F\{n(\mathbf{x}, t)\} &= \int d^3x \left[\frac{1}{2}K(\vec{\nabla}n)^2 + f(T, n) \right] \\ &= \int d^3x \tilde{f}(T, n) \end{aligned}$$

- For small changes in density

$$\begin{aligned} F\{n + \delta n\} - F\{n\} &= \int d^3x \left[K\vec{\nabla}\delta n \cdot \vec{\nabla}n + \frac{\partial f}{\partial n}\delta n \right] \\ &= \int d^3x \left[K\vec{\nabla} \cdot (\delta n \vec{\nabla}n) - K\delta n \nabla^2 n + \frac{\partial f}{\partial n}\delta n \right] \end{aligned}$$

Cahn-Hilliard model

- The chemical potential is

$$\tilde{\mu} = \frac{\delta F}{\delta n} = \frac{\partial f}{\partial n} - K\nabla^2 n = \mu - K\nabla^2 n$$

- The isotropic pressure is

$$\begin{aligned}\tilde{P} &= n\mu - [f + \frac{1}{2}K(\vec{\nabla}n)^2] \\ &= n\frac{\partial f}{\partial n} - f - Kn\nabla^2 n - \frac{1}{2}K(\vec{\nabla}n)^2 \\ &= P - Kn\nabla^2 n - \frac{1}{2}K(\vec{\nabla}n)^2\end{aligned}$$

- Assuming negligible dependence of K on temperature the entropy density is as usual

$$s = -\frac{\partial f}{\partial T}$$

Cahn-Hilliard model

- Local energy density

$$\tilde{\epsilon} = f - T \frac{\partial f}{\partial T} + \frac{1}{2} K (\vec{\nabla} n)^2 = \epsilon + \frac{1}{2} K (\vec{\nabla} n)^2$$

- The local enthalpy is

$$\begin{aligned} \tilde{w} &= \tilde{\epsilon} + \tilde{P} = n \frac{\partial f}{\partial n} - T \frac{\partial f}{\partial T} - Kn \nabla^2 n \\ &= \tilde{\mu} n + Ts = w - Kn \nabla^2 n \end{aligned}$$

Cahn-Hilliard model

- Keeping the baryon number fixed, let's minimize the Helmholtz free energy

$$I = \int d^3x \left[\tilde{f}(T, n) - \lambda n \right]$$

- The resulting Euler-Lagrange equation is

$$\partial_i \frac{\partial(\tilde{f} - \lambda n)}{\partial(\partial_i n)} - \frac{\partial(\tilde{f} - \lambda n)}{\partial n} = 0$$

- The Lagrange multiplier is

$$\lambda = \mu - K \nabla^2 n = \tilde{\mu} = \text{constant}$$

- If $n(x)$ solves the above equation, then the equilibrium surface free energy is

$$\sigma = K \int_{-\infty}^{\infty} dx \left(\frac{dn}{dx} \right)^2$$

Metastable and unstable states

- For $T < T_c$ and $n_G \leq n \leq n_L$ we parameterize the pressure in terms of the density as

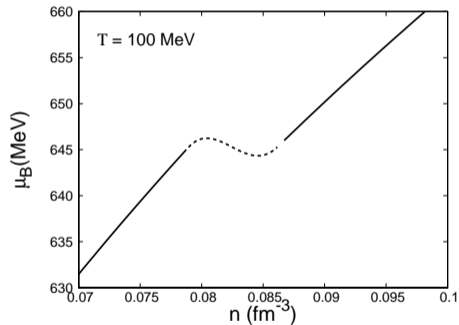
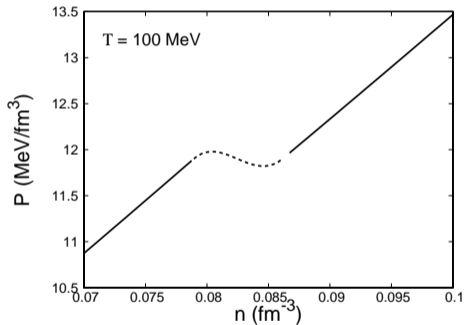
$$P_{in}(n) = P_X(T) + \sum_{i=1}^4 c_i (n - n_G)^i$$

- The chemical potential is

$$\mu_{in}(n) = \mu_X(T) + d_0 \ln(n/n_G) + \sum_{i=1}^3 d_i (n - n_G)^i$$

- We get constraints from $P_{in}(n_L) = P_X(T)$ and the continuity of first derivatives of P at n_L and n_G
- Further constraints are obtained by thermodynamics relations between P , n and μ and by $\mu_{in}(n_L) = \mu_X(T)$

Metastable and unstable states



Correlation length and surface energy

- Near critical density n_c , we can reasonably assume $n_L - n_c = n_c - n_G = \Delta n/2$. For $\delta n = n - n_c$ with $-\Delta n/2 \leq \delta n \leq \Delta n/2$. Then

$$\mu - \mu_X \approx d_3(\delta n + \Delta n/2)(\delta n + \Delta n/2)\delta n$$

- The planar surface equation is

$$K \frac{\partial^2 \delta n}{\partial x^2} = \mu - \mu_X$$

with solution

$$\delta n = \frac{\Delta n}{2} \tanh(x/2\zeta)$$

Correlation length and surface energy

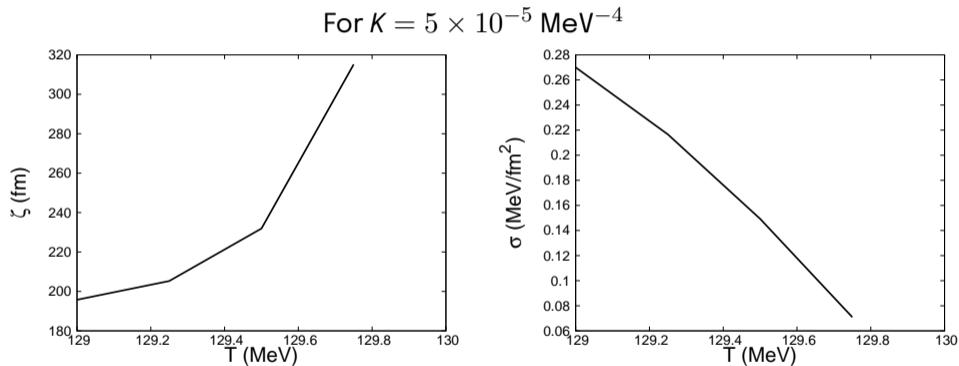
- The correlation length ζ is

$$\zeta^2 = \frac{2K}{\alpha\Delta n^2}$$

- The surface free energy is

$$\sigma = K \int_{-\infty}^{\infty} dx \left(\frac{dn}{dx} \right)^2 = \frac{K\Delta n^2}{6\zeta}$$

Correlation length and surface energy



Equation of state

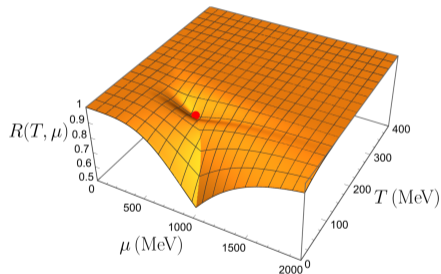
- Background EOS is obtained by matching pQCD EOS in QGP phase to HRG EOS using a smooth function. It is matched to Lattice calculations at $\mu_B = 0$

[M. Albright, J. Kapusta and C. Young, *Phys. Rev. C* 90, (2014)]

- The critical point is embedded on it at

$T_c = 130$ MeV and $\mu_c = 450$ MeV

J. Kapusta, T. Welle and C. Plumberg, *Phys. Rev. C* 106, (2022)



Hydrodynamics

- The relativistic energy momentum tensor is

$$T^{\mu\nu} = \tilde{P}(u^\mu u^\nu - g^{\mu\nu}) + \tilde{\epsilon}u^\mu u^\nu + K(D^\mu n)(D^\nu n)$$

where the gradient is orthogonal to velocity

$$D^\mu n \equiv \partial^\mu n - u^\mu u^\alpha \partial_\alpha n$$

- The local thermodynamic quantities are

$$\tilde{\mu} = \mu + KD^2 n$$

$$\tilde{P} = P + KnD^2 n + \frac{1}{2}K(D^\mu n)(D_\mu n)$$

$$\tilde{\epsilon} = \epsilon - \frac{1}{2}K(D^\mu n)(D_\mu n)$$

$$\tilde{w} = \tilde{P} + \tilde{\epsilon} = Ts + \tilde{\mu}n = w + KnD^2 n$$

1+1 D flow

We use a simple model of 1 + 1 D inviscid fluid with baryon dimension in Bjorken coordinates. In Landau frame, to 1st order

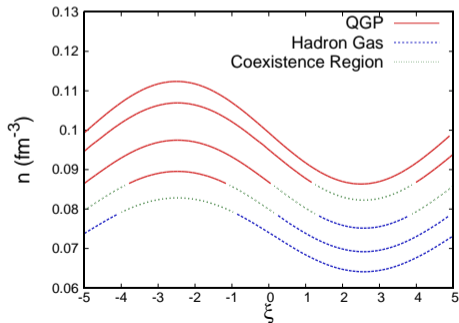
$$J^\mu = nu^\mu + \sigma_B T D^\mu \left(\frac{\tilde{\mu}}{T} \right)$$

The equations to solve are

$$\begin{aligned} \frac{\partial \epsilon(n, T)}{\partial \tau} + \frac{w(n, T)}{\tau} + \frac{K}{\tau^2} \frac{\partial n}{\partial \xi} \frac{\partial^2 n}{\partial \tau \partial \xi} - \frac{K}{\tau^3} n \frac{\partial^2 n}{\partial \xi^2} &= 0 \\ \frac{\partial}{\partial \tau} (\tau n) - \frac{\sigma_B T}{\tau} \frac{\partial^2}{\partial \xi^2} \left(\frac{\tilde{\mu}}{T} \right) - \frac{1}{\tau} \frac{\partial}{\partial \xi} (\sigma_B T) \frac{\partial}{\partial \xi} \left(\frac{\tilde{\mu}}{T} \right) &= 0 \\ \tilde{\mu} = \mu(n, T) - \frac{K}{\tau^2} \frac{\partial^2 n}{\partial \xi^2} \end{aligned}$$

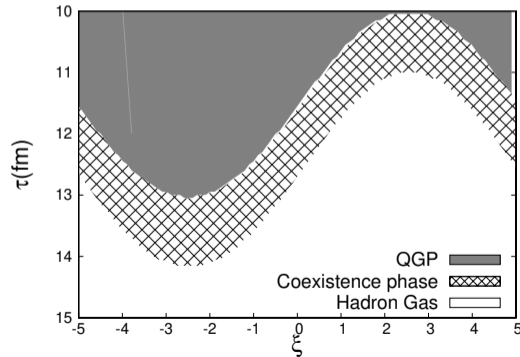
Setting up the system

- Due to fourth order derivatives, it is difficult to do this numerically with any level of generality with finite difference methods
- Dedicated finite element routines exist for many systems at equilibrium
- Here, we set up boost invariant energy density and a sinusoidal baryon density such that the lowest point touches the phase transition curve from above

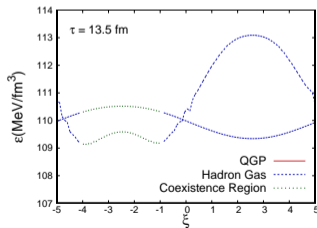
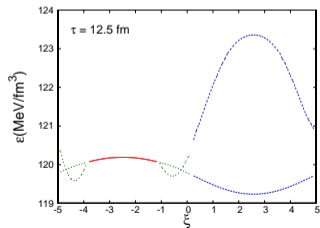
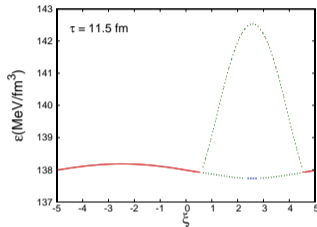
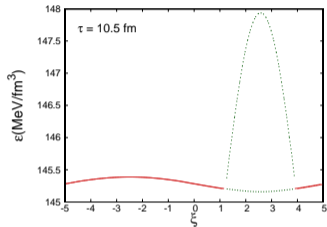


Evolution across the phase boundary

- We chose a relatively small K so that the change in n is negligible and the gradients in n are determined by the initial sinusoidal distribution
- We get the phase separation, but eventually all QCD matter is in hadronic phase

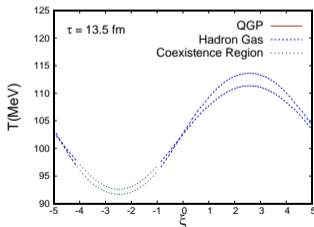
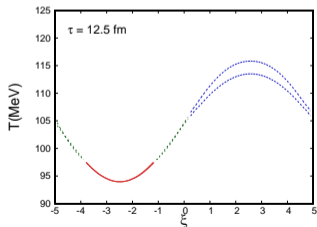
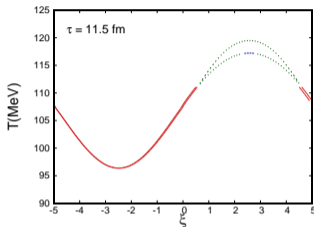
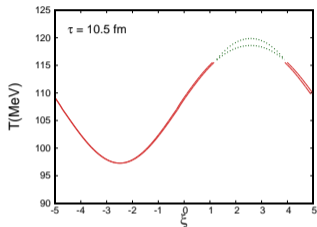


Energy density



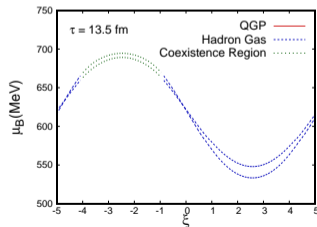
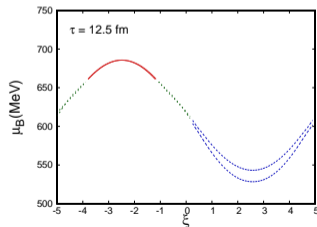
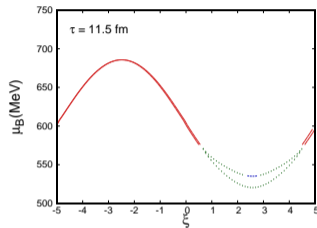
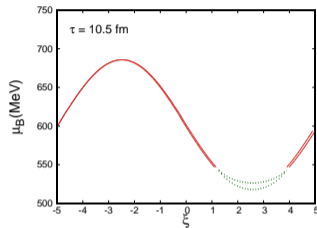
- The two different curves correspond to $K = 0$ and $K = 5 \times 10^{-5} \text{ MeV}^{-4}$. The energy density increases or decreases in the coexistence phase for different K
- This energy change will be balanced by energy flow in the hadronic phase

Temperature



- Temperature evolution for different K
- The QGP temperature is lower than the hadron gas temperature as μ_B has opposite sign

Baryon chemical potential



- Specifics of temperature and chemical potential changes are sensitive to the exact choice of the EOS

Summary

- It has been postulated that the QCD phase diagram has a first order phase transition curve at high baryon chemical potential
- If such a curve exists, it is very likely that a large volume of QCD matter at some collision energy will undergo phase transition via spinodal decomposition
- We present the equations of relativistic hydrodynamics with the phase transition and solve it for a simple system
- Realistically simulating phase transitions for a rapidly expanding fluid in HIC is challenging and will likely require generalizations of finite element techniques used to study chemical and condensed matter systems