

**How Good is “Avrami’s Law”?
Application to a kinetic Ising model in two
dimensions**

P.A. Rikvold
Physics, MARTECH, SCRI
Florida State University

R.A. Ramos
University of Puerto Rico at Mayaguez

S.W. Sides and M.A. Novotny
Florida State University

Supported by NSF, DOE, and FSU

http://www.scri.fsu.edu/~rikvold/matsci_html/matsci-mag.html

Why interesting?

The Kolmogorov-Johnson-Mehl-Avrami (KJMA) approximation, or “Avrami’s Law,” for the decay of the volume fraction of a metastable phase

- is an **extremely simple approximation** proposed almost sixty years ago
- is **widely used** to analyse metastable decay in fields ranging from metallurgy to food science
- appears to give **reasonable results**, even when its restrictive assumptions are not well satisfied
- was **recently extended to correlation functions**

We present a detailed test of KJMA predictions, both at the single-point (volume-fraction) and two-point (correlation-function) levels for a 2D kinetic Ising model.

The simple idea:

A system is equilibrated, and the control parameter (“the field”) is changed suddenly through a first-order phase transition to a value corresponding to a different equilibrium phase.

KJMA theory describes the decay as follows.

- Negligibly small “droplets” of the stable phase nucleate from the metastable background [homogeneous or heterogeneous nucleation].
- The droplets subsequently grow independently without substantial deformation.
- The stable phase is pictured as randomly placed, freely overlapping, growing spheres.

The **total** volume of stable phase, *not* correcting for overlaps, is

$$Ct^\alpha$$

The random overlaps reduce the **net** volume fraction:

$$\varphi_s(t) = 1 - \exp(-Ct^\alpha)$$

giving the remaining volume fraction of *metastable* phase:

$$\varphi_{ms}(t) = \exp(-Ct^\alpha)$$

C and $\alpha \geq d$ depend on dimensionality d and details of the nucleation and growth processes.

Here we concentrate on *homogeneous nucleation*, which gives $\alpha = d + 1$.

Model

Ising Hamiltonian:

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} s_i s_j - H \sum_i s_i$$

Order parameter is magnetization:

$$m = N^{-1} \sum_i s_i$$

The temperature T is below T_c , so m for $H=0$ takes one of two equilibrium values:

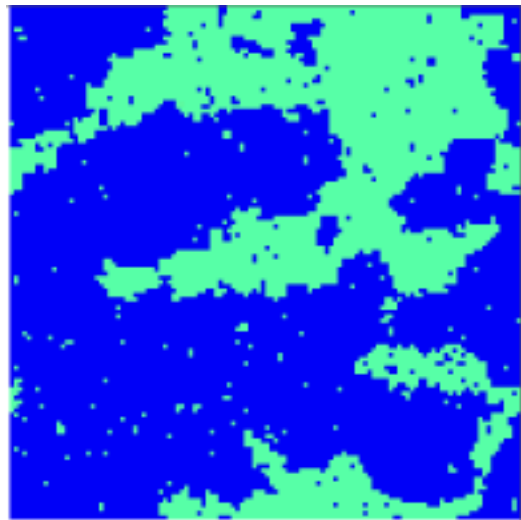
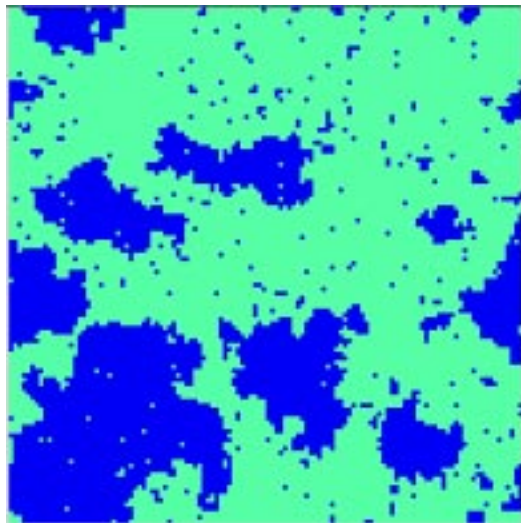
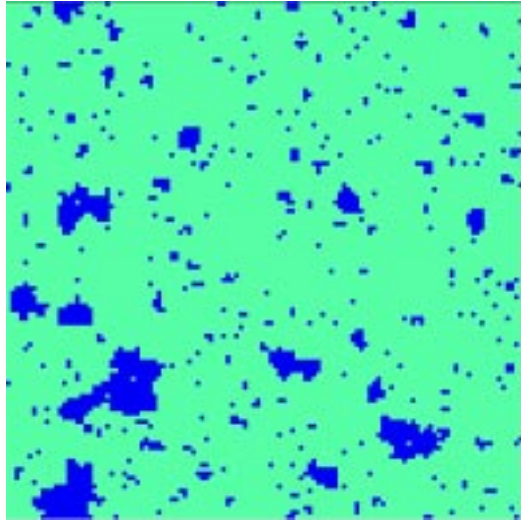
$$m(T < T_c, H=0) = \pm m_s(T)$$

Dynamic

Glauber (nonconserved) dynamic with transition probability

$$W(s_i \rightarrow -s_i) = \frac{\exp(-\beta \Delta E_i)}{1 + \exp(-\beta \Delta E_i)}$$

where ΔE_i is the proposed energy change.



Nucleation theory of metastable decay

Relevant fluctuations are **compact droplets** of radius R and volume $\Omega_d R^d$ with free energy

$$F(R) \approx d\Omega_d\sigma(T)R^{d-1} - |H|2m_s(T)\Omega_d R^d$$

$\sigma(T)$: Droplet surface tension.

$m_s(T)$: Spontaneous magnetization.

$F(R)$ is maximum for the **critical radius**

$$R_c \approx \frac{(d-1)\sigma(T)}{2m_s(T)|H|}$$

Nucleation rate:

$$I(T, H) = B(T)|H|^K \exp \left[-\frac{\beta\Xi(T)}{|H|^{d-1}} \right]$$

$\Xi(T)$ and $K = 3$ exactly known for 2D Ising model.

Nucleation and growth

KJMA (Avrami) approximation.

Large supercritical droplets grow at **constant velocity, v** (Lifshitz-Allen-Cahn approximation):

$$\begin{aligned} v &= (d-1)\nu (R_c^{-1} - R^{-1}) \\ &\xrightarrow{R \rightarrow \infty} (d-1)\nu R_c^{-1} \equiv v \propto |H| \end{aligned}$$

Volume fraction of stable phase

(randomly placed, freely overlapping droplets):

$$\begin{aligned} \varphi_s(t) &\approx 1 - \exp \left[-I \int_0^t \Omega_d (vs)^d ds \right] \\ &= 1 - \exp \left[-\frac{\Omega_d}{d+1} \left(\frac{t}{t_0} \right)^{d+1} \right] \end{aligned}$$

where $t_0 = (v^d I)^{-1/(d+1)}$ is the **average time of free growth.**

With t_0 is associated the
characteristic distance of free growth:

$$R_0 \propto vt_0 = v / (Iv^d)^{\frac{1}{d+1}} = (v/I)^{\frac{1}{d+1}}$$

Recall nucleation rate:

$$I(T, H) \propto |H|^K \exp \left[-\frac{\beta \Xi(T)}{|H|^{d-1}} \right]$$

Using this, we have:

$$t_0(T, H) \propto \exp \left[\frac{1}{d+1} \frac{\beta \Xi(T)}{|H|^{d-1}} \right]$$

and

$$R_0(T, H) \propto \exp \left[\frac{1}{d+1} \frac{\beta \Xi(T)}{|H|^{d-1}} \right]$$

Range of validity of KJMA theory:

$$\text{lattice constant} \ll R_c \ll R_0 \ll L$$

where L is the *linear system size*.

Relaxation Function

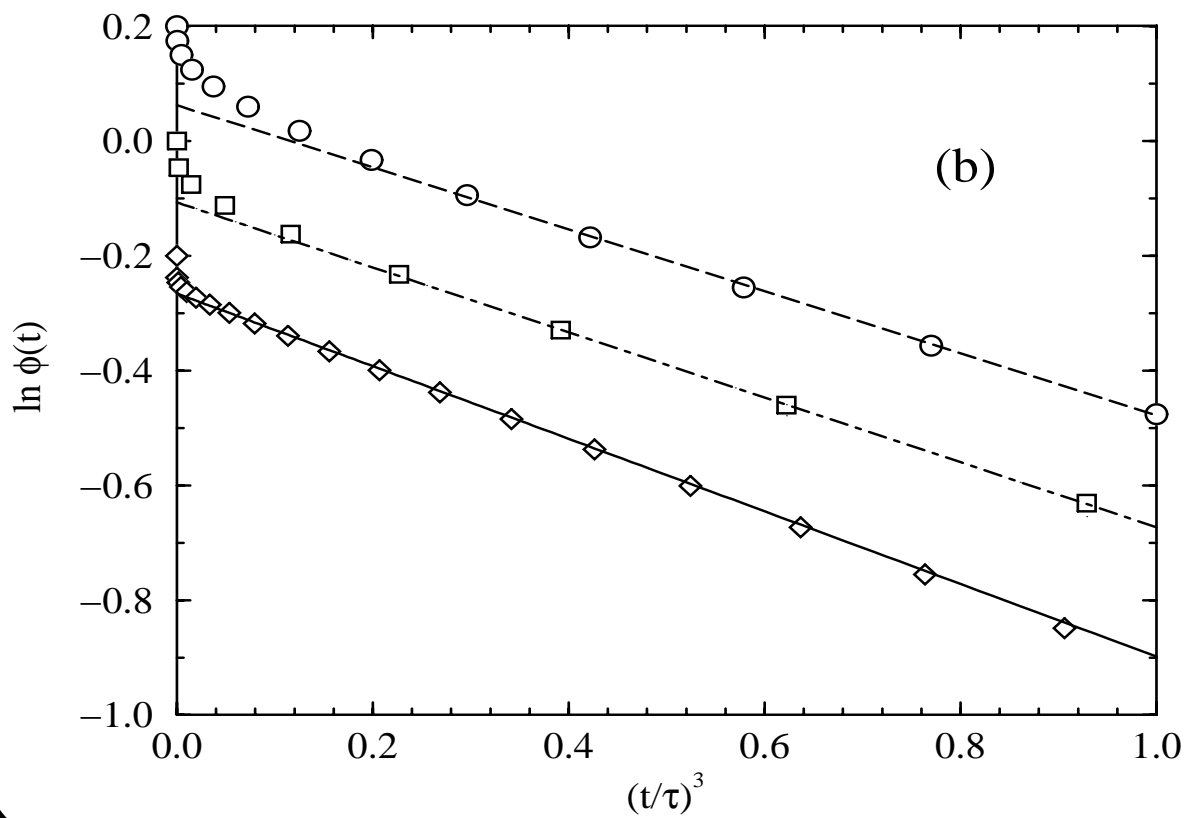
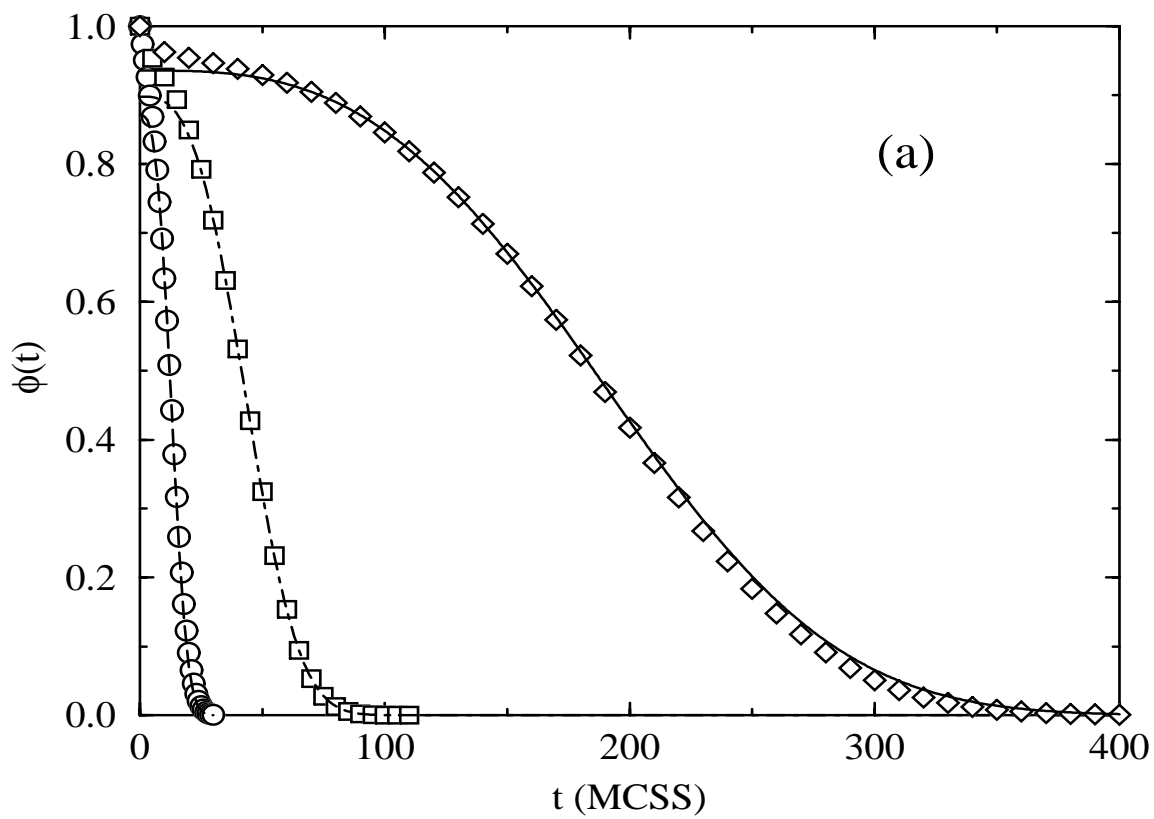
Metastable decay usually analysed in terms of the **relaxation function**:

$$\begin{aligned}\phi(t) &= \frac{m(t) - m(\infty)}{m(0) - m(\infty)} \approx \frac{m_{\text{ms}} - m(\infty)}{m(0) - m(\infty)} \varphi_{\text{ms}}(t) \\ &= \frac{m_{\text{ms}} - m(\infty)}{m(0) - m(\infty)} \exp \left[-\frac{\Omega_d I v^d t^{d+1}}{d+1} \right]\end{aligned}$$

The *metastable magnetization* m_{ms} and the combination Iv^d can be estimated by plotting $\ln \phi(t)$ versus t^{d+1} .

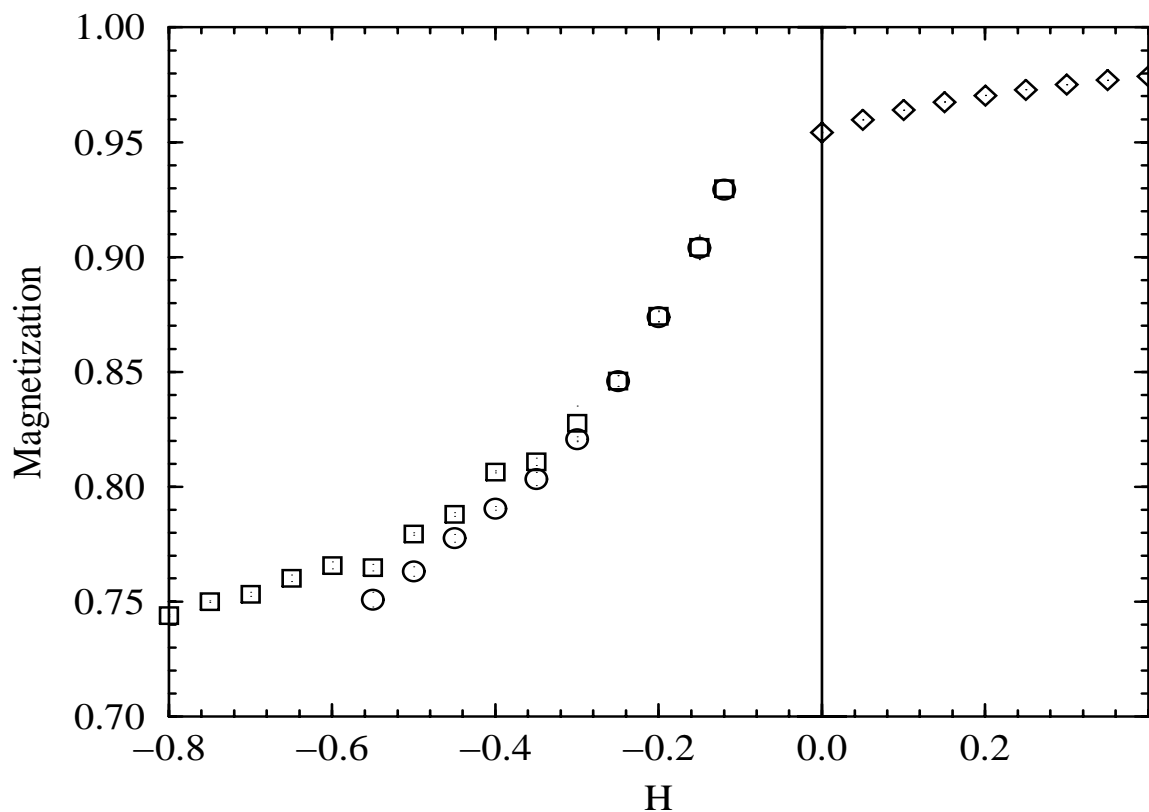
Define the *metastable lifetime*, $\tau(H)$, by

$$\langle m(\tau(H)) \rangle = 0$$



Metastable magnetization vs H

From the fits of $\ln \phi(t)$ versus t^{d+1} for different values of H we find $m_{\text{ms}}(H)$.



Information from correlation functions

Without further information we cannot resolve the product Iv^d of the nucleation rate and the growth velocity.

Within the KJMA framework, Sekimoto, and Ohta, Ohta, and Kawasaki have derived the two-point correlation function:

$$\begin{aligned}\Gamma(\vec{r}, t) &\equiv \langle u(\vec{x}, t)u(\vec{x} + \vec{r}, t) \rangle - \langle u(\vec{x}, t) \rangle^2 \\ &= \begin{cases} \langle u(t) \rangle^2 \left\{ \exp \left[Iv^d t^{d+1} \Psi_d(r/2vt) \right] - 1 \right\}, & r < 2vt \\ 0, & r > 2vt \end{cases}\end{aligned}$$

where $r=|\vec{r}|$ and

$$\begin{aligned}\Psi_2(y) &= \frac{2}{3} \left[\arccos y - 2y \sqrt{1-y^2} + y^3 \ln \left(\frac{1 + \sqrt{1-y^2}}{y} \right) \right] \\ \Psi_3(y) &= \frac{\pi}{3} (1-y)^3 (1+y)\end{aligned}$$

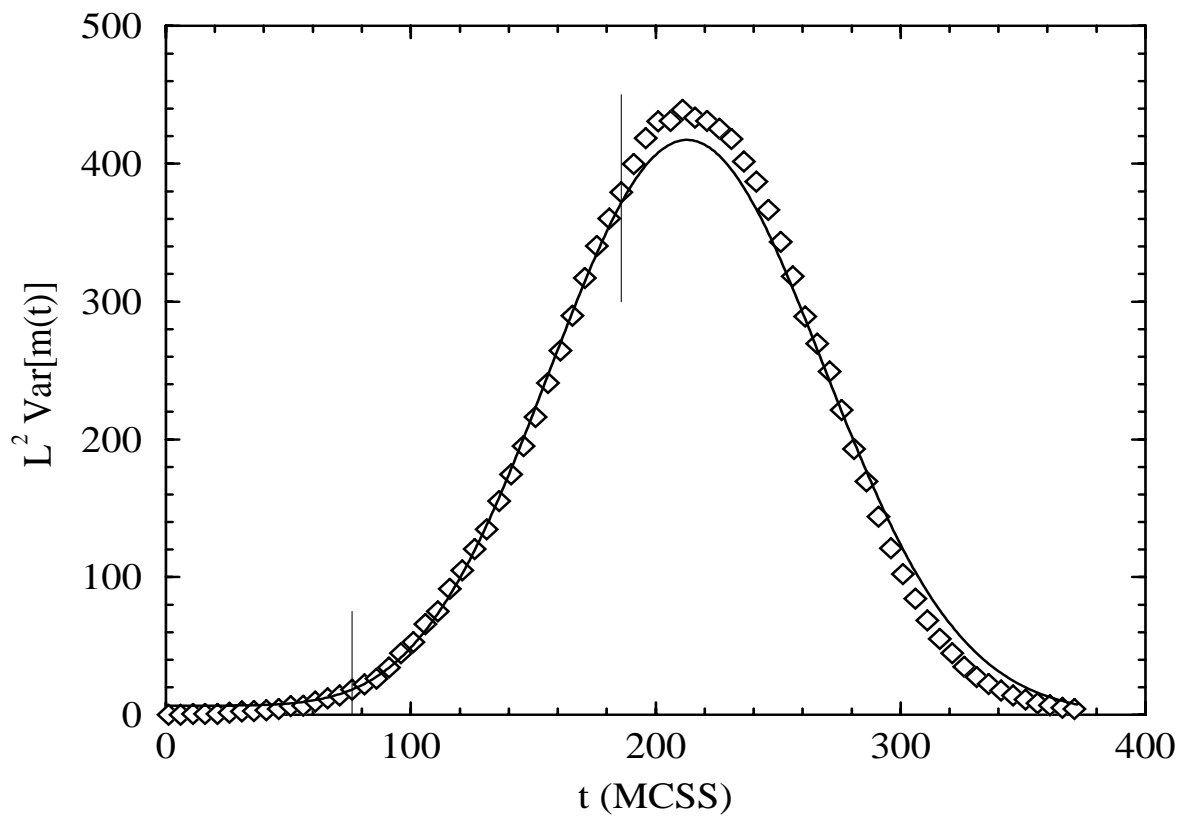
These results can be used to obtain the *variance of the magnetization*, $\text{Var}[m(t)]$, as

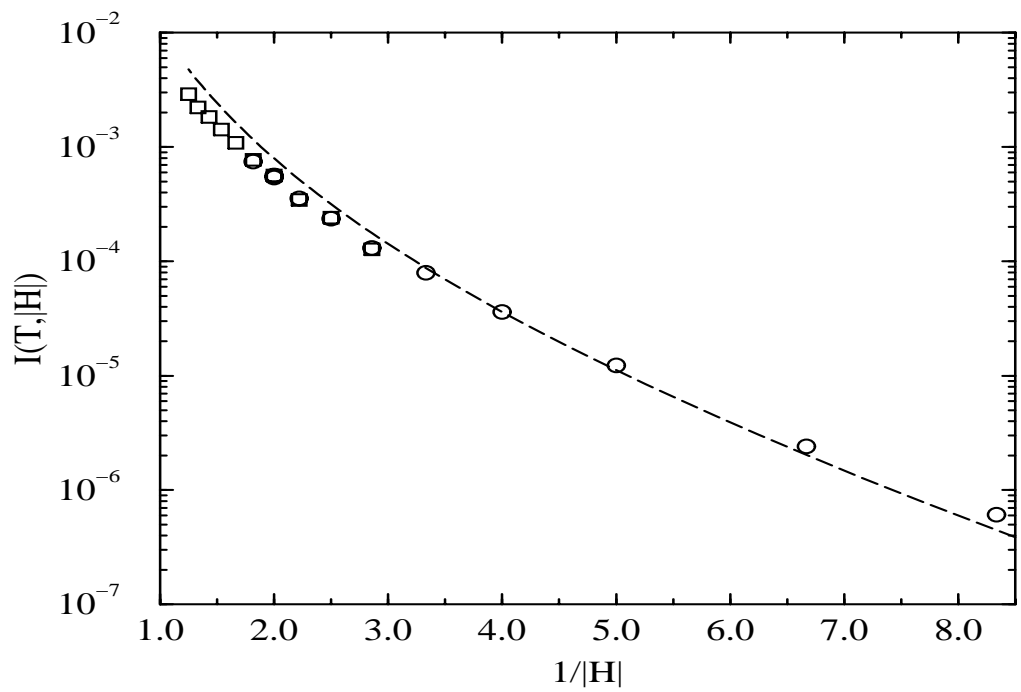
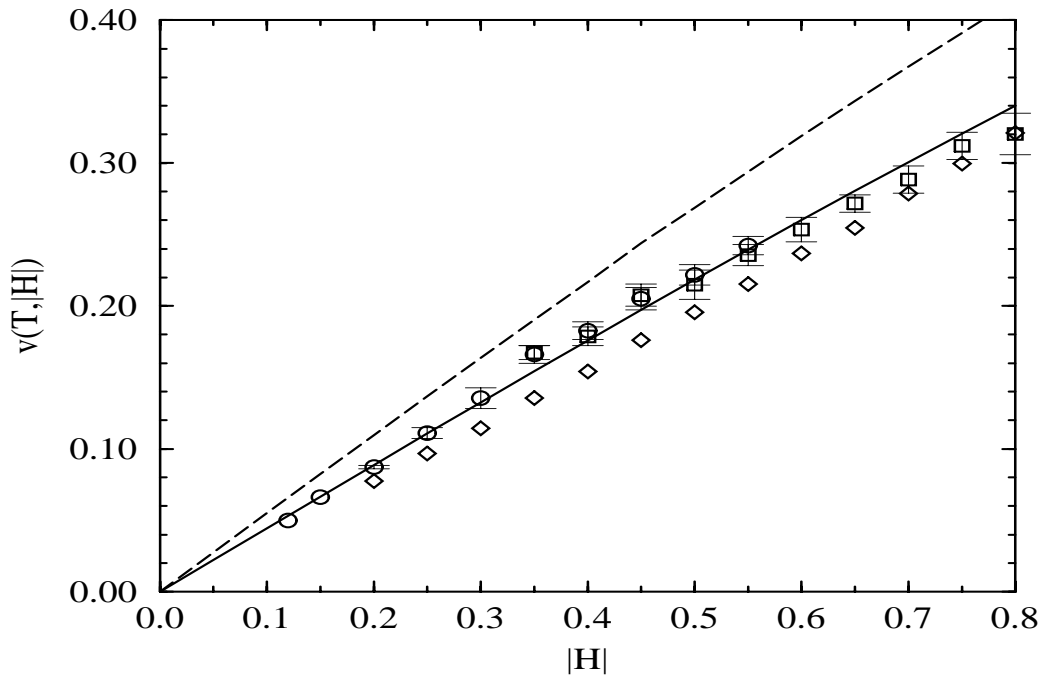
$$L^d \text{Var}[m(t)] \approx [m_{\text{ms}} - m(\infty)]^2 d\Omega_d \varphi_{\text{ms}}^2(t) \left[\Theta_d(Iv^d t^{d+1}) - \frac{1}{d} \right] (2t)^d v^d$$

where

$$\Theta_d(Iv^d t^{d+1}) = \int_0^1 y^{d-1} \exp \left[Iv^d t^{d+1} \Psi_d(y) \right] dy$$

This allows us to estimate v^d from $\text{Var}[m(t)]$.

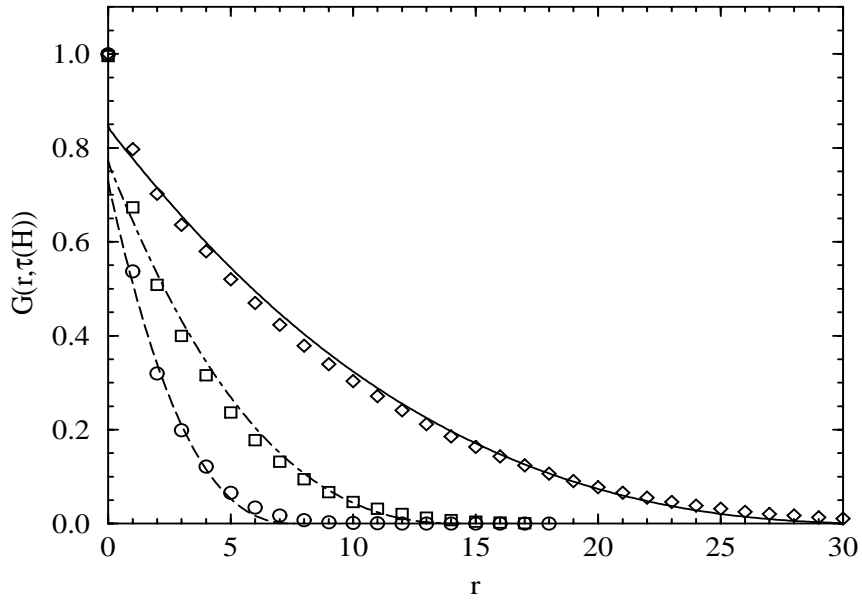




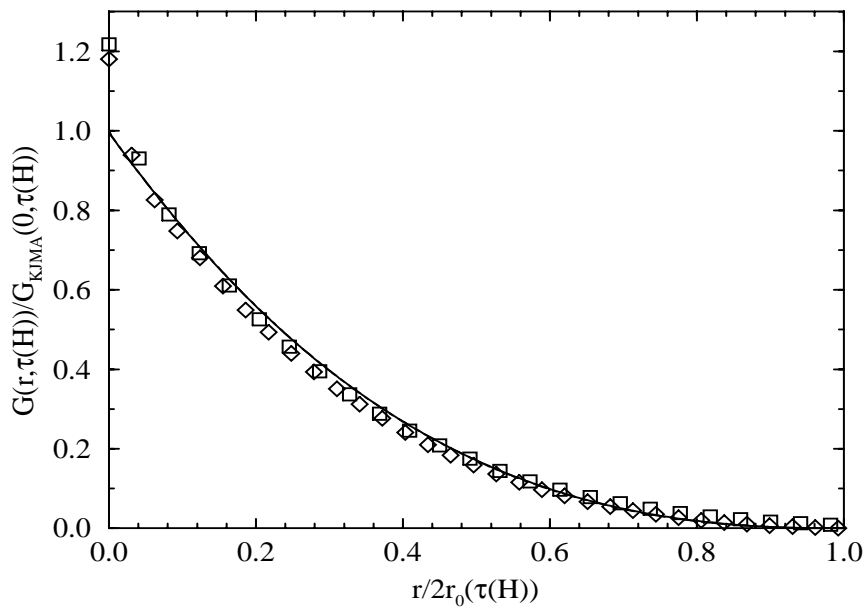
Correlation functions

$$\Gamma(\vec{r}, t) \equiv \langle u(\vec{x}, t)u(\vec{x} + \vec{r}, t) \rangle - \langle u(\vec{x}, t) \rangle^2$$

$$= \begin{cases} \langle u(t) \rangle^2 \left\{ \exp \left[I v^2 t^3 \Psi_2(r/2vt) \right] - 1 \right\}, & r < 2vt \\ 0, & r > 2vt \end{cases}$$

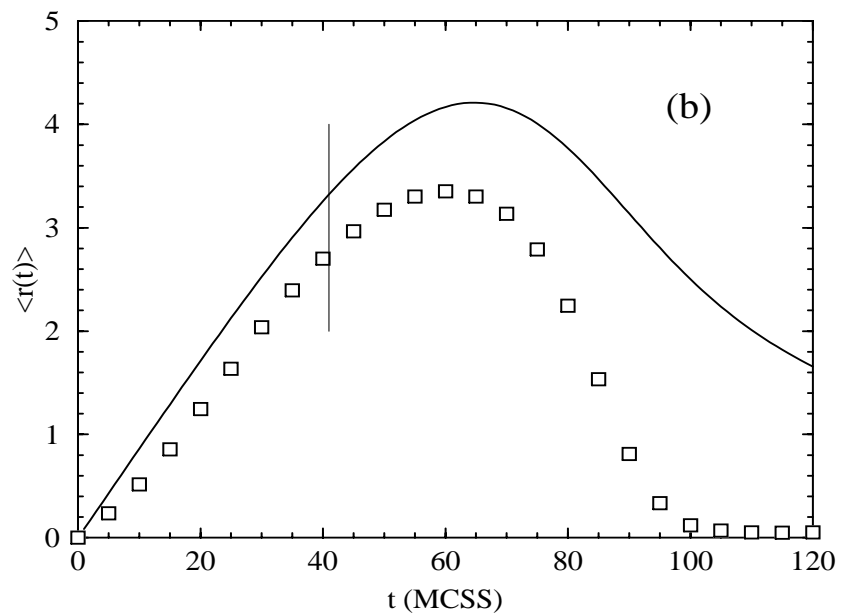
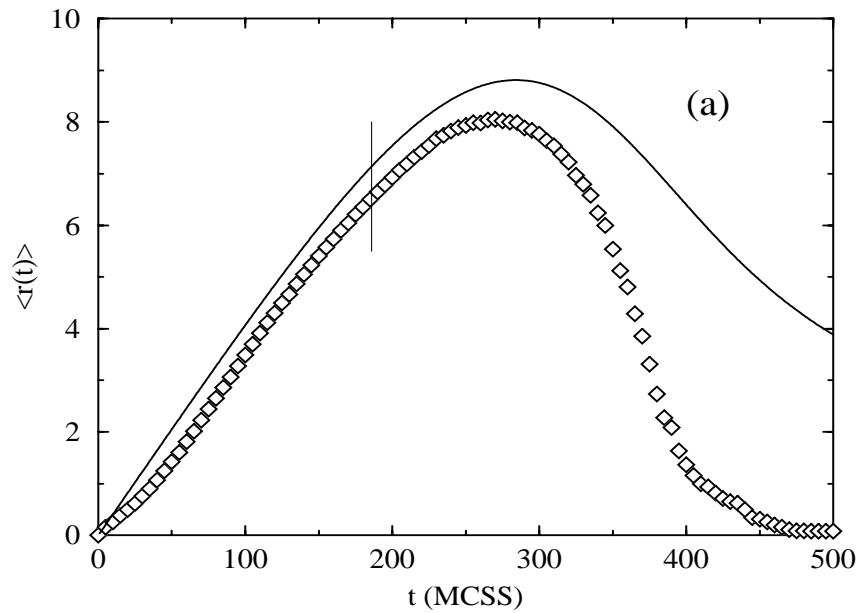


Two-parameter scaling in r/r_0 and r_0/R_0 , where $r_0(t) = vt$.



Time-dependent Correlation Length

$$\langle r(t) \rangle = \int r \Gamma(r, t) dr / \int \Gamma(r, t) dr$$



CONCLUSIONS

- Despite the irregular shapes of the growing stable-phase droplets, the KJMA approximation as extended to the level of two-point correlation functions allows reasonable and consistent measurement of
 - A “metastable magnetization,” m_{ms} , which serves as an order parameter for the metastable phase.
 - The average velocity, $v(H)$, of the field-driven interfaces.
 - The nucleation rate, $I(T, H)$, for critical droplets of the stable phase.
- The approximation works well considerably past the lifetime, $\tau(H)$, when half the volume is converted to the stable phase.
- For later times, surface-tension effects accelerate the decay and the KJMA approximation breaks down.