INTERNATIONAL ATOMIC ENERGY AGENCY
UNITED NATIONS EDUCATIONAL, SCIENTIFIC AND CULTURAL ORGANIZATION
INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS
I.C.T.P., P.O. BOX 586, 34100 TRIESTE, ITALY, CABLE: CENTRATOM TRIESTE

SMR. 758 - 17

SPRING COLLEGE IN CONDENSED MATTER
ON QUANTUM PHASES
(3 May - 10 June 1994)

MAGNETIC PHASE TRANSITIONS AT LOW TEMPERATURES

PART II

MPTI Description in Terms of Stochastic Exchange Fields

G.G. LONZARICH
Department of Physics
Cavendish Laboratory
University of Cambridge
Madingley Road
Cambridge, CB3 OHE, U.K.

MPTII Description in Terms of Stochastic Exchange Fields

- Introduction
- The classical Ginzburg-Landau Model
- Quantum m^4 Field Description
- Temperature dependence of the Susceptibility; The Curie Temperature and its Pressure Dependence
- The Quantum Ginzburg Criterion; Temperature Dependence of the Mode Coupling Parameter

1. Introduction

- Models for low energy description ($E < E_c$)

  Fermions with initial spectrum ε_p (and density of states $g(\varepsilon)$) interact with each other via a two body potential (I)

  = Non-interacting Fermions with ε_p interact with harmonic stochastic fields* (II)

- In quantum electrodynamics the potential in (I) is the retarded charge and current interactions, while the fields in (II) are the electromagnetic potentials.

- In the Hubbard model the potential in (I) is

  $$U\sum_i n_{i\uparrow}n_{i\downarrow}\ , \tag{1.1}$$

  while the fields in (II) (obtained via the Hubbard-Stratonovich transformation) are related to the particle and spin densities. We focus on the latter, i.e. on the exchange field $\lambda m(\rho)$.

- In MPTI we considered scattering of fermions from $\lambda m(\rho)$ near the Fermi surface. The Born approximation may be applicable because (i) high energy ($E > E_c$) contributions have been 'integrated out' so that the effective interaction of the fermions with the field is 'screened', (ii) the full unconstrained statistics of $m(\rho)$ enters and (iii) the Pauli principle severely restricts the scattering. The Landau Theory of a Fermi liquid is approached as E_c and T tend to zero.

---

* Generalisation of molecular field theory.

- The fermions coupled to the fields may be described in a Langevin model of degrees of freedom interacting with a bath. The field seen by the fermions will have a stochastic component plus a part which depends on the state of the fermions themselves. This can be viewed in terms of a fermion self-interaction that leads to a shift in spectrum from ε_p to $E = E_p$ satisfying

$$E = \varepsilon_p + \Sigma_E , \tag{1.2}$$

where Σ_E is the memory function or self-energy (which depends explicitly on both p and E, in general).

- Σ_E'' yields the relaxation rate τ_E^{-1} (evaluated in MPTI for $E > 0$)

$$\Sigma_E'' = -\hbar / 2\tau_E , \tag{1.3}$$

and Σ_E', which follows from Σ_E'' (generalised to describe both particles $E > 0$ and holes $E < 0$) via the Kramers-Krönig relation, gives the effective mass in the form

$$m_E^* = m(1 - \partial\Sigma_E' / \partial E) , \tag{1.4}$$

if the p dependence of Σ_E can be ignored.

- This approach may be used to describe the entropy and (with greater difficulty) the magnetic susceptibility. In the critical limit $\chi^{-1} \to 0$, $n = 1$ and $z = 3$ (MPTI) we find, for example

$$m_E^* \propto ln(E^* / E), \tag{1.5}$$

and

$$S / T \propto ln(T^* / T), \tag{1.6}$$

$$\chi^{-1} \propto T^{4/3}. \tag{1.7}$$

- The procedure is, however, difficult to implement and to generalise to real anisotropic multiband systems.

- Here we adopt an alternative description based on the idea that effects of interactions of the fermions with the fields may be inferred from the unconstrained behaviour of the fields themselves. By integrating out the fermions in (II) we arrive at a third description based on

anharmonic stochastic fields (III)

- This leads us to consider a quantum generalisation of the Ginzburg Landau Model.

2. *The Classical Ginzburg-Landau Model*

- Classical availability for an isotropic system in terms of a scalar m(r) with Fourier components $m_q(t)$
  $q < q_c$ and $\hbar\Gamma_q << k_B T$

$$F[m] = \int d^d r\left(\frac{a}{2}m^2 + \frac{b}{4}m^4 + \frac{c}{2}|\nabla m|^2 + \ldots\right), \tag{2.1}$$

$$Z = Z_o \sum_{[m]} e^{-\beta F[m]} . \tag{2.2}$$

- Parameters a, b and c from (II) after integrating out the fermions (and plus density fluctuations and components of the local magnetisation for q outside of the sphere of radius q_c).

- Evaluation of parameters from a more microscopic model and of Z from F[m] are treated separately.

- Fourier representation for $q < q_c$

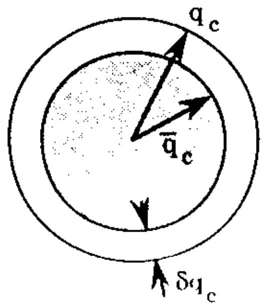
$$F[m] = \sum \frac{a_q}{2}|m_q|^2 + \frac{b}{4\upsilon_o}\sum^{*} m_1 \ldots m_4 , \tag{2.3}$$

where $a_q = a + cq^2$

and * denotes the condition $q_1 + q_2 + q_3 + q_4 = 0$.

(The variables to be summed are unambiguous and will be dropped hence forth in writing Σ.)

- Shift in a and b due to integration of q's in shell.



$$\delta F[m] = \tilde{\Sigma}\frac{a_q}{2}|m_q|^2 + \frac{3b}{2\upsilon_o}\bar{\Sigma}|m_{q'}|^2 \tilde{\Sigma}|m_q|^2 + \ldots$$

$$= \tilde{\Sigma}\frac{\tilde{a}_q}{2}|m_q|^2 \tag{2.4}$$

$$\tilde{a}_q = a_q + \frac{3b}{\upsilon_o}\bar{\Sigma}|m_{q'}|^2 + \ldots$$

$\bar{\Sigma}$ and $\tilde{\Sigma}$ represent sums in shaded region and shell, respectively.

For each pair (q,-q) in shell

$$\int dm_q dm_{-q}\, e^{-\frac{\beta}{2}\tilde{a}_q|m_q|^2} = \frac{2\pi}{\beta\tilde{a}_q} = \frac{2\pi}{\beta}e^{-ln\,\tilde{a}_q},$$

$$ln\,\tilde{a}_q = ln\,a_q + \frac{3b}{a_q\upsilon_o}\bar{\Sigma}|m_{q'}|^2 - \frac{9b^2}{2a_q^2\upsilon_o^2}\left(\bar{\Sigma}|m_{q'}|^2\right)^2 + \ldots \tag{2.5}$$

- Thus,

$$\delta a = \frac{3b}{\beta\upsilon_o}\tilde{\Sigma}a_q^{-1} , \tag{2.6}$$

$$\delta b = -\frac{9b^2}{\beta\upsilon_o}\tilde{\Sigma}a_q^{-2} . \tag{2.7}$$

- Perturbation series for total shift of a and b as $\overline{q}_c \to 0$ (in paramagnetic phase)

$$\Delta a = \frac{3b}{\beta}\hat{\Sigma}\,\chi_q \quad +\ldots \quad = \tag{2.8}$$

$+ \ldots$

$$\Delta b = \frac{-9b^2}{\beta}\hat{\Sigma}\,\chi_q^2 \quad +\ldots \quad = \tag{2.9}$$

$+ \ldots$

- $$\Delta F = \frac{1}{2\beta}\,\Sigma\, ln\ \chi_q^{-1} - \frac{3}{4}\,\upsilon_o\,\overline{\overline{m^2}}^{2} + \ldots \tag{2.10}$$

$$\overline{m^2} = \hat{\Sigma}\,\overline{|m_q|^2}\,, \quad \overline{|m_q|^2} = \frac{\chi_q}{\beta}\,. \tag{2.11}$$

$\hat{\Sigma}$ represents sum ($\times\ 1/\upsilon_o$) over all $q < q_c$.

- The self consistent Hartree approximation

$$m^4 \to 3m^2\,\overline{m^2} + 3\,\overline{m^2}\,m^2 - 3\,\overline{m^2}^{2}\,, \tag{2.12}$$

$$\chi_q^{-1} = a_q + 3b\,\overline{m^2}\,, \tag{2.13}$$

(i.e. each mode m_q is coupled to average contribution of all others).

- Range of validity of mean field description may be inferred by a Ginzburg criterion (e.g. $|\Delta b/b| \sim 1$, i.e. the coupling parameter is substantially screened from its bare value b).

- For an N component field in the paramagnetic state $3 \to 2 + N$ in (2.8), $9 \to 8 + N$ in (2.9) and ΔF in (2.10) is enhanced by N.

3. *Quantum m^4 Model*

- Quantisation of the field must be consistent with Nyquist's theorem in which statistics depend on the dynamical behaviour of the field, e.g.

$$\overline{|m_q|^2} = \frac{\chi_q}{\beta} \to \frac{\hbar}{\pi}\int_{-\infty}^{\infty} d\omega\left(\frac{1}{2} + n_\omega\right)\chi_k'' = \frac{1}{\beta}\,\Sigma\,\chi_k$$

$$= \text{'zero point' component} + \upsilon_q\,. \tag{3.1}$$

$$k = (q, i\nu)\,, \quad \nu = \frac{2\pi|n|}{\tau_o}\,, \quad \tau_o = \hbar\beta\,, \quad n = 0,\ \pm 1,\ \pm 2, \ldots$$

- The arguments in the appendix suggest the generalisation of the Ginzburg Landau Model is of the form

$$\beta F[m] \to A[m]/\hbar\,, \tag{3.2}$$

$$A[m] = \Sigma\,\frac{a_k}{2}\,|m_k|^2 + \frac{b}{4u_o}\,\Sigma^*\,m_1\ldots m_4 + O[m^3] \tag{3.3}$$

where $u_o = \upsilon_o\tau_o$ and in a one pole model

$$a_k = a_q + \frac{|\nu|}{\gamma_q}\,. \tag{3.4}$$

- An analysis analogous to that in §2, then yields (2.8-2.10 in paramagnetic phase) with $\chi_q \to \chi_k$ (and sums over k instead of q alone)

$$\Delta a = \frac{3b}{\beta\upsilon_o} \sum \chi_k + \ldots = 3b\,\overline{m^2} + \ldots \tag{3.5}$$

$$\Delta b = \frac{-9b^2}{\beta\upsilon_o} \sum \chi_k^2 + \ldots \tag{3.6}$$

$$\Delta F = \frac{1}{2\beta} \sum \ln \chi_k^{-1} - \frac{3}{4}\,\upsilon_o\,\overline{m^2}^2 + \ldots \tag{3.7}$$

$$\chi_k^{-1} = a_k + \Delta a\,. \tag{3.8}$$

4. *Temperature Dependence of $\chi(T)$ in Low T Limit*

- Redefining a to include the 'zero point' part of Δa, then

$$\chi^{-1} = a + 3b\,\overline{m_T^2}\,, \quad \text{where } \overline{m_T^2} = \hat{\sum} \upsilon_q\,. \tag{4.1}$$

- For a 1-pole model for χ_k (MPTI)

$$\overline{m_T^2} = \frac{\eta_d \hbar}{\pi^3} \int q^{d-1}\,dq\,d\omega\, \frac{\omega n_\omega\, \gamma q^n}{\omega^2 + \left(\zeta q^z\right)^2}\,, \tag{4.2}$$

where $\eta_d = 1, \pi, 2\pi$ for $d = 3, 2, 1$, respectively.

- When $d + n > 2z$

$$\overline{m_T^2} \propto T^2\,, \tag{4.3}$$

as expected for a Fermi liquid.

- For $d + z \le 2z$, the low q regime dominates and

$$\overline{m_T^2} \propto T^{\frac{d+n}{z}}\,. \tag{4.4}$$

- More generally, $\overline{m_T^2} = \hat{\sum} \upsilon_q\,, \qquad \upsilon_q = \overline{|m_q|_T^2}\,,$

$$\upsilon_q = \frac{\chi_q}{\beta}\, g\left(\frac{\hbar\beta\Gamma_q}{2\pi}\right), \tag{4.5}$$

$$g(x) = 2x\left[\ln x - \frac{1}{2x} - \psi(x)\right] \tag{4.6}$$

$$\simeq \frac{1}{1 + 6x}\,. \tag{4.7}$$

where $\psi(x)$ is the digamma function (Gradshteyn and Ryzhik). (4.7) differs from (4.5) by at most a few % for all x and is identical to (4.5) in leading order in x and 1/x.

5. *The Curie Temperature* (a < 0)

- The condition $\chi^{-1}(T_c) = 0$ yields

$$a + b\,\frac{3\eta_d}{2\pi^2\beta_c c} \int q^{d-1} dq\, \frac{g(x)}{q^2} = 0\,, \qquad x = \frac{\hbar\beta_c \gamma c q^z}{2\pi}\,, \quad z = n + 2. \tag{5.1}$$

- For $d \leq 2$, $T_c \rightarrow 0$ (as for classical case).
- For $d = 3$

$$a + \eta b (k_B T_c)^{1+\frac{1}{z}} = 0, \tag{5.2}$$

$$\eta = \frac{3\Gamma\left(1 + \frac{1}{z}\right)\zeta\left(1 + \frac{1}{z}\right)}{2\pi^2 z \cos\left(\frac{\pi}{2z}\right) c(\hbar\gamma c)^{\frac{1}{z}}} . \tag{5.3}$$

- For N components, the factor $3 \rightarrow 2 + N$ in (5.3).
- If temperature dependence of a and b can be neglected $-a/b \rightarrow M_0^2$. Then for a pure isotropic metallic ferromagnet in 3 dimensions with weakly spin polarised ground state

$$k_B T_c = 2.39 \, c M_0^{3/2} (\hbar\gamma)^{1/4} . \tag{5.4}$$

Model consistent with observed T_c and measured M_0, c, and γ for the low T ferromagnets $ZrZn_2$, Ni_3Al, YNi_3, and MnSi.

Table 1. Properties of the magnetic equation of state for Ni_3Al: $a = a(T = 0) = -1.15 \times 10^{3}$[a], $b = 0.53\ G^{-2}$[a], $c = 1.5 \times 10^5$ Å^2[b], $\hbar\gamma = 3.3$ μeV Å[b]; also $q_{sw} = q_{sw}(T = 0) = 0.1$ Å^{-1} and $T_0 \simeq 300\ \mathrm{K} \gg T_c$[c]. The quantities α, p_0 and p_{eff} in the table are defined respectively through the equations $\alpha = \langle \partial M(T)/M_0 \partial T^2 \rangle$, $M_0 = (-a/b)^{1/2} = N_a \mu_B p_0 / V$ and $\langle \partial \chi^{-1}/\partial T \rangle = 3k_B V / N_a \mu_B^2 p_{eff}^2$, where $\langle\ \rangle$ designates an average over the temperature ranges given in the table, in the zero-field limit. $p \simeq 0.075$/Ni atom[a].

Property	Experiment	Present model
$M(T, 0)$	Quadratic[d]	Quadratic[d]
$T \leq 0.7\ T_c$		
$\chi^{-1}(T)$	Linear[d]	Linear[d]
$2T_c \leq T \leq 10\ T_c$		
$\alpha(10^{-4}\ \mathrm{K}^{-2})$	3.7–4.0	3.4–3.7
T_c(K)	41.0(5)	39
p_{eff}/p_0[e]	16(2)	22

[a] De Boer *et al* (1969).
[b] Bernhoeft *et al* (1982, 1983, 1985).
[c] Sigfusson *et al* (1984).
[d] Approximate temperature dependence in the temperature range given.
[e] Assuming N_a in the equations defining p_0 and p_{eff} to be the number of Ni atoms. Corresponding values given by Lonzarich (1984) are for N_a equal to the total number of atoms (Ni and Al).

Table 2. Properties of the magnetic equation of state for MnSi above T_c: $a = a(T = 0) = -3.5 \times 10^{3}$[a], $b = 0.15\ G^{-2}$[a], $c = 2.1 \times 10^4$ Å^2[b], $\hbar\gamma = 2.6$ μeV Å[b]. Below T_c, MnSi is ferromagnetic at high magnetic fields and orders in a long-wavelength helical structure below about 6 kG[a]. $p_0 = 0.4$/Mn atom.[a]

Property	Experiment	Present model
$\chi^{-1}(T)$	Linear[c]	Linear[c,d]
$2T_c \leq T \leq 10\ T_c$		
T_c(K)	29.5(5)	31
p_{eff}/p_0[e]	5.5(4)	4.7

[a] Levinson *et al* (1973), and Bloch *et al* (1975). Values were estimated from $p_0 = 0.4$/Mn atom and the high-field slope of M^2 versus B/M at 4.2 K.
[b] Values deduced from neutron scattering data of Ishikawa *et al* (1982) above T_c.
[c] *Approximate* temperature dependence in the temperature range given.
[d] Preliminary numerical calculations were carried out by De Souza (1984).
[e] Assuming N_a to be the number of Mn atoms.

6. *Pressure Dependence of T_c*

- If a mean field model is applicable ($d_{eff} = d + z > 4$, §7), then expect that a(p) can be expanded in a power series about the critical pressure $a(p_c) = 0$ so that for $T \geq T_c$

$$\chi^{-1} \simeq a'(p_c)\,(p - p_c) + (2 + N)b\,\overline{m_T^2} . \qquad (6.1)$$

- Then $\chi^{-1}(T_c) = 0$ yields

$$T_c^{1+\frac{1}{z}} \propto p . \qquad (6.2)$$

- For a pure metallic ferromagnet $z = 3$, so that (if $d_{eff} > 4$)

$$T_c^{4/3} \propto p , \qquad (6.3)$$

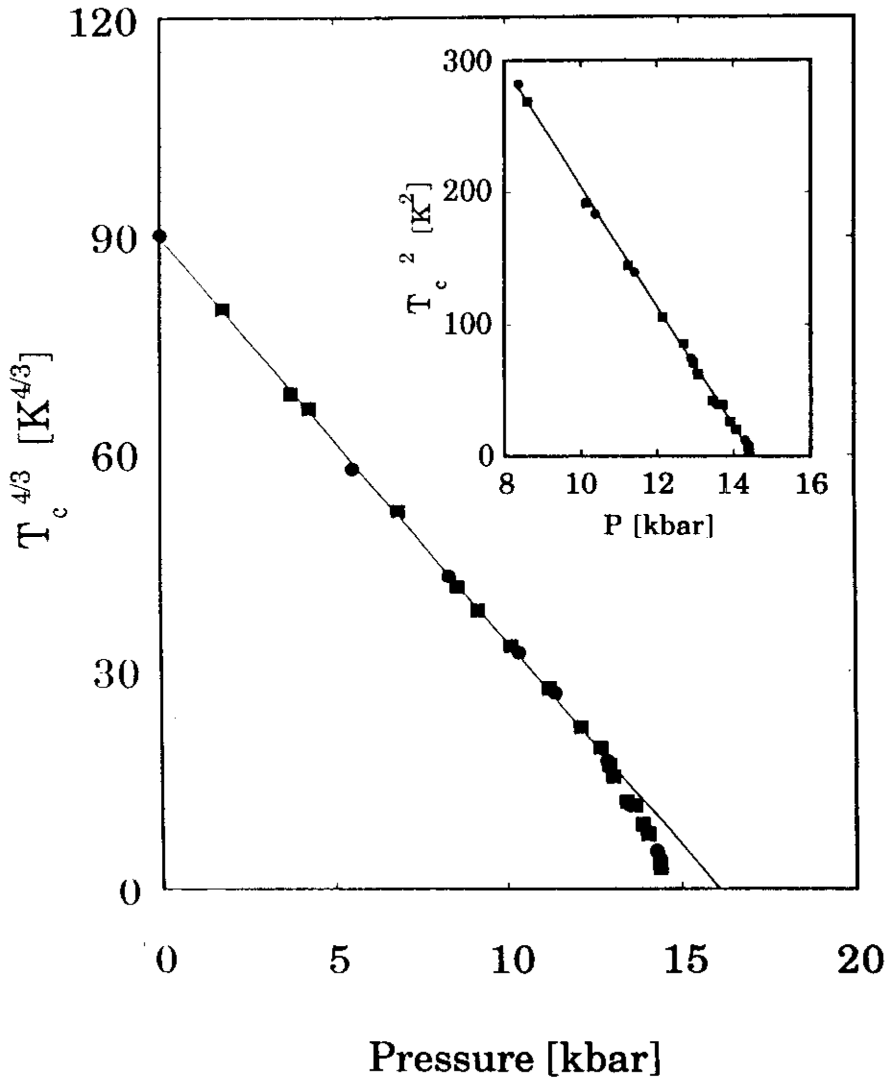
consistent with measurements in MnSi and $ZrZn_2$, except close to p_c (see MPTIII).

- For an antiferromagnet $z = 2$, so that (if $d_{eff} > 4$)

$$T_c^{3/2} \propto p \qquad (6.4)$$

(measurements in progress).

Pressure Dependence of the Transition Temperature



7. *The Quantum 'Ginzburg Criterion'*

- In the limit $T \to 0$ the sum for Δb (3.6) can be replaced by an integral

$$\frac{1}{\tau_o}\sum \to 2\int_0^\infty \frac{d\nu}{2\pi}, \tag{7.1}$$

where $\tau_o = \hbar\beta$.

- For the 1-pole model, (3.6) then yields for $T \to 0$

$$\frac{\Delta b}{b} \simeq \frac{-(8+N)\eta_d \hbar b}{2\pi^3} \underbrace{\int_0^\infty d\nu \int_0^{q_c} \frac{q^{d-1}dq}{\left(\chi_q^{-1} + \nu/\gamma q^n\right)^2}}_{J}. \tag{7.2}$$

- $$J = \gamma \int_0^{q_c} \frac{q^{d+n-1}dq}{\chi^{-1} + cq^2}. \tag{7.3}$$

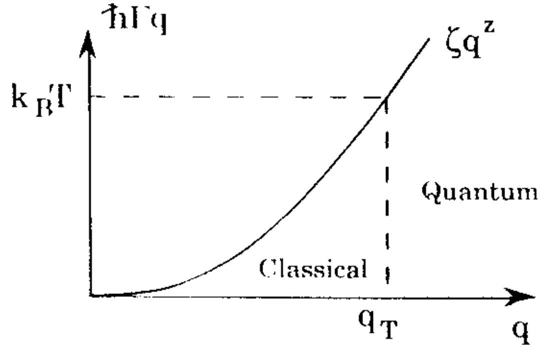
- As $\chi^{-1} \to 0$, (7.3) diverges at low q if

$$d_{eff} = d + z \leq 4. \tag{7.4}$$

- For $d_{eff} > 4$ (the upper critical dimension), mean field theory (or conventional perturbation theory) applies.

- Increase of the effective dimension from d to d + z is due to the sum over ν which corresponds to an imaginary 'time' range of finite size (for $T \neq 0$) of 0 to τ_o. Since $\Gamma \sim q^z$, this time is 'equivalent' (in the sense required in the Ginzburg criterion) to z space dimensions, so that the total is d + z.

8. *Temperature Dependence of the Mode Coupling Parameter*

- 

$z = n + 2$
for $\chi^{-1} \to 0$
$T \to 0$

for $q \leq q_T \sim T^{1/z}$, the modes are essentially classical.

- $$\frac{1}{\beta}\sum \chi_k = \text{'quantum'} + \frac{1}{\beta}\sum_{q<q_T} \chi_q, \tag{8.1}$$

so that for d = 3

$$\overline{m_T^2} \propto T^{1+\frac{1}{z}} \quad \text{as before.} \tag{8.2}$$

- Next consider sum $\frac{1}{\beta} \sum \chi_k^2$, (8.3)

then

$$\Delta b_T \sim T \sum_{q < q_T} \chi_q^2 \sim T^{1-\frac{1}{z}} \left(\sqrt{c\chi\, q_T^2} - 1\right). \tag{8.4}$$

- Thus, Δb_T could have a stronger T dependence at low T than $\overline{m_T^2}$. What is overall T dependence of $\chi^{-1}(T)$ as $T \to 0$? Connection to finite size scaling theory?

A1. *Quantum Extension of the Ginzburg Landau Model*

- Nyquist's Theorem can be expressed in the form

$$\overline{\left|m_q\right|^2} = \frac{1}{\beta} \sum \chi_k ,$$

where

$$k = (q, i\nu), \qquad \nu = \frac{2\pi|n|}{\tau_o}, \tag{A1.1}$$

$$\tau_o = \hbar\beta, \qquad n = 0,\ \pm 1,\ \pm 2,\ \ldots$$

- Introduce a new variable m(u), u = (r,τ),

$$m(u) = \frac{1}{\sqrt{u_o}} \sum m_k\, e^{ik\cdot u}, \tag{A1.2}$$

where

$$k \cdot u = q \cdot r - \nu\tau ,$$

$u_o = \upsilon_o \tau_o$, and $k = (q, \nu)$ (use iν in definition of k in χ_k.)

- Now

$$m_q(\tau) = \frac{1}{\sqrt{\tau_o}} \sum m_k\, e^{-i\nu\tau}, \tag{A1.3}$$

$$\overline{|m_q|^2} = \frac{1}{\tau_o} \sum \overline{|m_k|^2}. \tag{A1.4}$$

If

$$\overline{|m_k|^2} = \hbar \chi_k , \tag{A1.5}$$

then (A1.4) agrees with (1).

- Thus, m_k looks like a stochastic process anologous to m_q, but with both q and v indices and $\beta \to 1/\hbar$.
- This leads us to guess that the quantum availability model will be of the form

$$Z = Z_0 \sum e^{-A[m]/\hbar} , \tag{A1.6}$$

where A[m], the Euclidean Action, replaces $\hbar \beta F[m]$ of the classical model.

- We assume A[m] can be expanded in the Ginzburg Landau form

$$A[m] = \sum \frac{a_k}{2} |m_k|^2 + \frac{b}{4u_0} \sum m_1 \ldots m_4 + O[m^3] , \tag{A1.7}$$

where a_k and b are the parameters of the model.

- If b = 0

$$\overline{|m_k|^2} = \hbar a_k^{-1}. \tag{A1.8}$$

From (A1.5) a_k is thus χ_k^{-1} in the absence of mode coupling.

- In the Hartree approximation

$$A[m] \to \sum \frac{\chi_k^{-1}}{2} |m_k|^2 - \frac{3}{4} bu_0 \overline{m^2}^2 , \tag{A1.9a}$$

where, as in (3.5, 3.8),

$$\chi_k^{-1} = a_k + 3b \overline{m^2}, \tag{A1.9b}$$

$$\overline{m^2} = \frac{1}{u_0} \sum \overline{|m_k|^2} = \frac{1}{\beta u_0} \sum \chi_k . \tag{A1.9c}$$

- From an analysis identical to that in §2, we obtain (3.6) for Δb.
- Integrating over the m_k, we recover (3.7) for ΔF.
- The quantum model may also contain *non-local* terms third order in m_k which are disallowed by symmetry in the *classical* model (MPTIII).
- These results may be confirmed for the Hubbard Hamiltonian via the time-ordered operator formalism and the Hubbard-Stratonovich transformation. The latter also provides estimates of the parameters defining A[m] in terms of g(ε) and U.