Landau theory of phase transitions

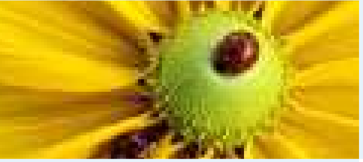
Landau's approach

- Landau has developed a very general phenomenological approach to the study of phase transitions.
-

Landau's approach

- Landau has developed a very general phenomenological approach to the study of phase transitions.
-
- The key idea is to identify some kind of "order parameter" whose value changes from zero to nonzero in the vicinity of a phase transition.
- For a spin system, we take the order parameter to be

$$m = \langle \sigma \rangle.$$ the magneic moment



Landau's approach

- Landau has developed a very general phenomenological approach to the study of phase transitions.
- We shall study his theory in the context of what we already know about magnetic systems, but the basic method is applicable to phase transitions in general.
- The key idea is to identify some kind of "order parameter" whose value changes from zero to nonzero in the vicinity of a phase transition.
- For a spin system, we take the order parameter to be

$$m = \langle \sigma \rangle, \text{theaverage magnetization.}$$

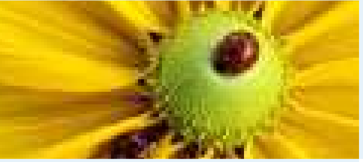
- If $T > T_c$, the spins are thermally disordered:

$$m = 0.$$

- If $T < T_c$, there is a nonvanishing magnetic order:

$$m \neq 0.$$

- For any T in the neighborhood of T_c, the order parameter m is a small quantity.

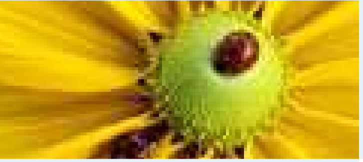


Quartic expansion

- Let us now neglect all powers m^k with $k > 4$ and focus on the general properties of the quartic expansion for the free energy A

$$A(T, m) = a(T) + \frac{1}{2}b(T)m^2 + \frac{1}{4}c(T)m^4,$$

where $b(T) = b_0(T - T_c)$ and $c(T) > 0$.

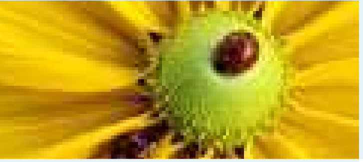


Quartic expansion

- Let us now neglect all powers m^k with $k > 4$ and focus on the general properties of the quartic expansion

$$A(T, m) = a(T) + \frac{1}{2}b(T)m^2 + \frac{1}{4}c(T)m^4,$$

  where $b(T) = b_0(T - T_c)$ and $c(T) > 0$.
- For large m, the m^4 term is dominant, so a minimum always exists.

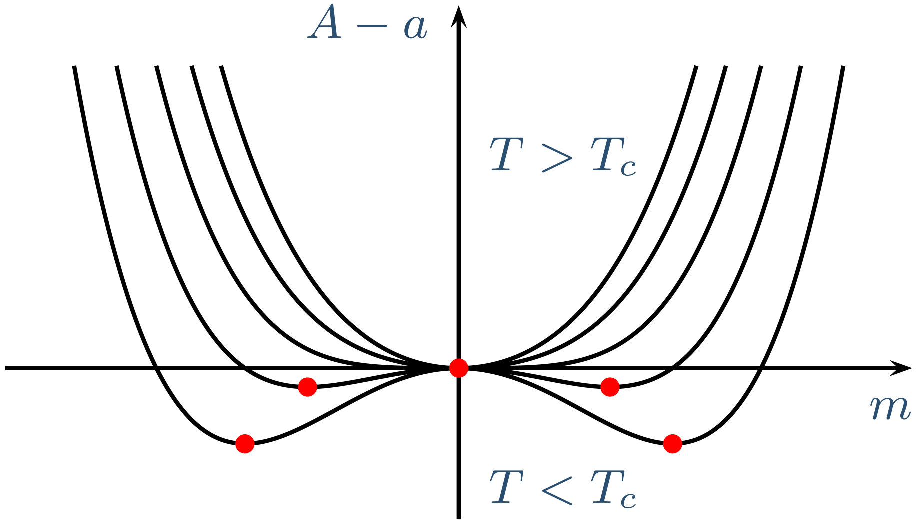


Quartic expansion

- Let us now neglect all powers m^k with $k > 4$ and focus on the general properties of the quartic expansion

$$A(T, m) = a(T) + \frac{1}{2}b(T)m^2 + \frac{1}{4}c(T)m^4,$$

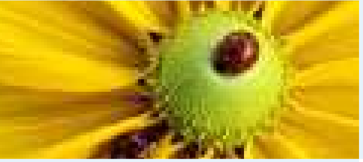
where $b(T) = b_0(T - T_c)$ and $c(T) > 0$.
- For large m, the m^4 term is dominant, so a minimum always exists.
- Depending on the sign of the m^2 term, there may be minima at either $m = 0$ or $m \neq 0$.



Location of minimum

- In thermal equilibrium, $m(T)$ takes on whatever value minimizes $A(T, m)$, hence

$$\frac{\partial A}{\partial m} = 0.$$



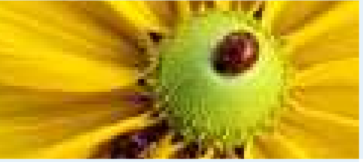
Location of minimum

- In thermal equilibrium, $m(T)$ takes on whatever value minimizes $A(T, m)$, hence

$$\frac{\partial A}{\partial m} = 0.$$

- Putting in $A = a + \frac{1}{2}bm^2 + \frac{1}{4}cm^4$, we get

$$\frac{\partial A}{\partial m} = bm + cm^3 = 0.$$



Location of minimum

- In thermal equilibrium, $m(T)$ takes on whatever value minimizes $A(T, m)$, hence

$$\frac{\partial A}{\partial m} = 0.$$

- Putting in $A = a + \frac{1}{2}bm^2 + \frac{1}{4}cm^4$, we get

$$\frac{\partial A}{\partial m} = bm + cm^3 = 0.$$

- The equilibrium solution with $m \neq 0$ is therefore given by

$$m(T) = \pm\sqrt{-\frac{b(T)}{c(T)}} \approx \pm\sqrt{\frac{b_0}{c(T_c)}}\,(T_c - T)^{1/2}.$$

- The qualitative behavior near T_c is thus

$$m(T) \propto (T_c - T)^{1/2},$$

which is just the mean-field result for magnetization.

- Let us now return to the general case

$$A(T,m) = a(T) + \frac{1}{2}b(T)m^2 + \frac{1}{4}c(T)m^4 + \frac{1}{6}d(T)m^6 + \cdots .$$

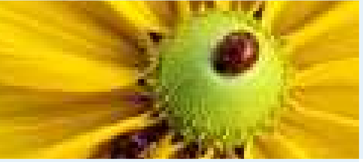
- For the Ising Hamiltonian, the quadratic coefficient $b(T)$ changes sign as a function of T.

Other types of phase transition

- Let us now return to the general case

$$A(T, m) = a(T) + \frac{1}{2}b(T)m^2 + \frac{1}{4}c(T)m^4 + \frac{1}{6}d(T)m^6 + \cdots .$$

- For the Ising Hamiltonian, the quadratic coefficient $b(T)$ changes sign as a function of T.
- What would happen in a more general case if $c(T)$ is the first coefficient to change sign?
- How would this affect the phase transition?



Other types of phase transition

- Let us now return to the general case

$$A(T,m) = a(T) + \frac{1}{2}b(T)m^2 + \frac{1}{4}c(T)m^4 + \frac{1}{6}d(T)m^6 + \cdots .$$

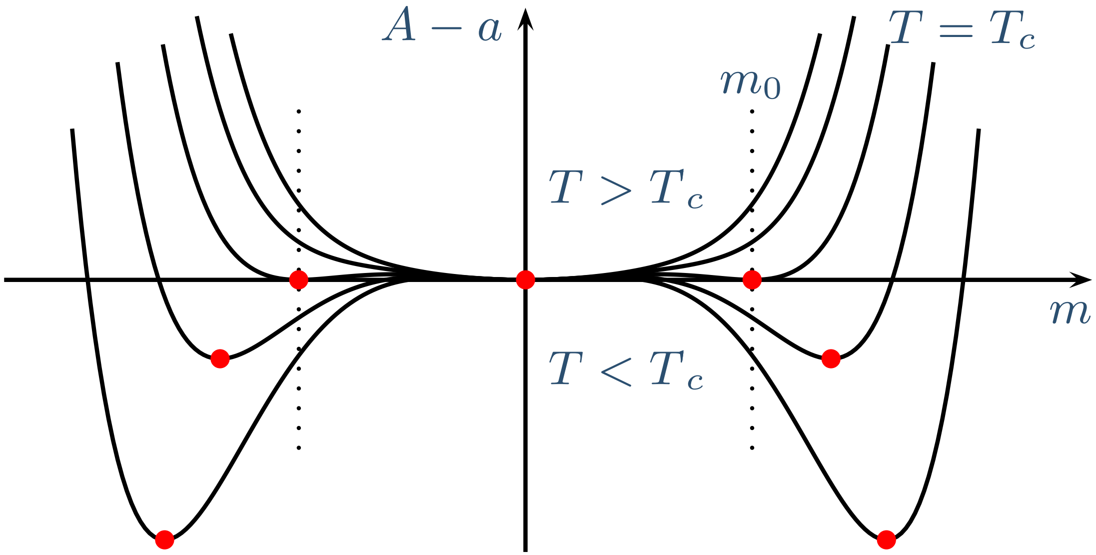
-

- What would happen in a more general case if $c(T)$ is the first coefficient to change sign?
- How would this affect the phase transition?
- To study this case, we approximate A as a sixth-order polynomial in m:

$$A(T,m) = a(T) + \frac{1}{2}b(T)m^2 + \frac{1}{4}c(T)m^4 + \frac{1}{6}d(T)m^6,$$

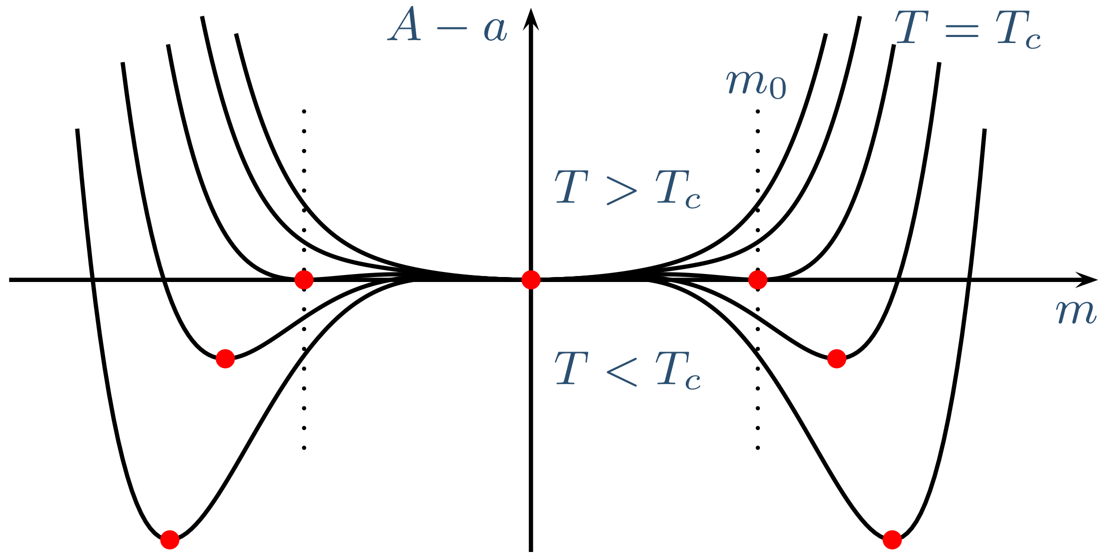
where in the temperature range of interest, $d(T) > 0$, $b(T) > 0$, and $c(T)$ may be either positive or negative.

- For sufficiently large negative values of $c(T)$, there may exist minima of $A(T,m)$ at both $m = 0$ and $m \neq 0$: at a different T'c



Free energy

- For sufficiently large negative values of $c(T)$, there may exist minima of $A(T, m)$ at both $m = 0$ and $m \neq 0$:

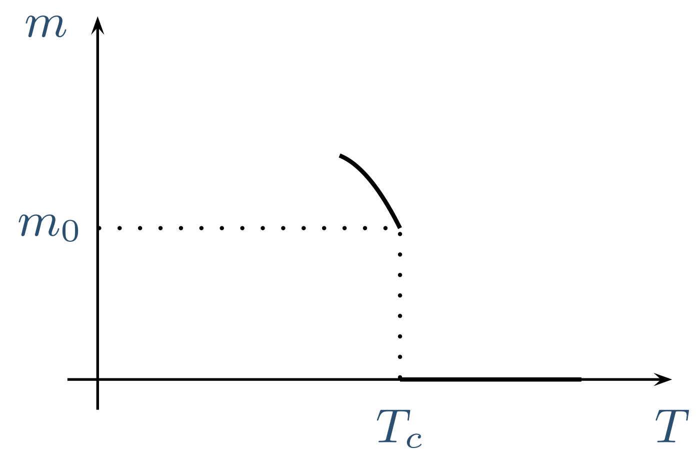


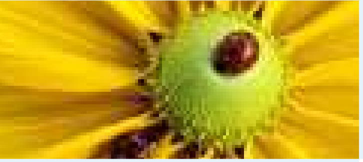
- For $T < T_c$, the minima with $m \neq 0$ are absolute minima, with free energies $A(T, m) < A(T, 0) = a(T)$.
- At the critical temperature $T = T_c$, the two sets of minima have the same free energy:

$$A(T_c, m_0) = A(T_c, 0) = a(T_c), \qquad m_0 \neq 0.$$

Order parameter

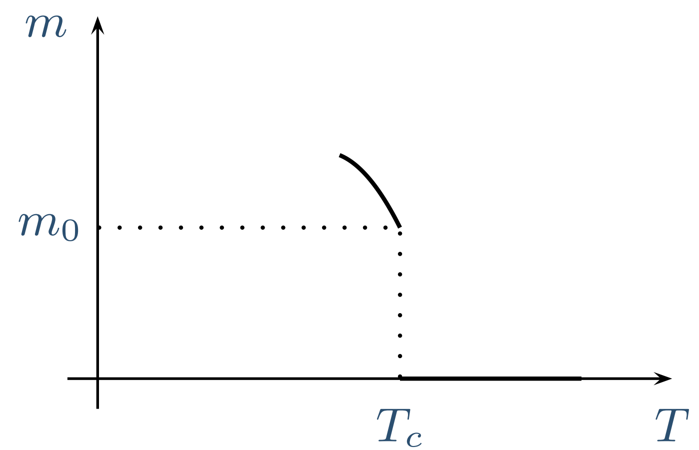
- The order parameter $m(T)$ therefore changes discontinuously from $m = 0$ to $m = m_0$ at $T = T_c$:





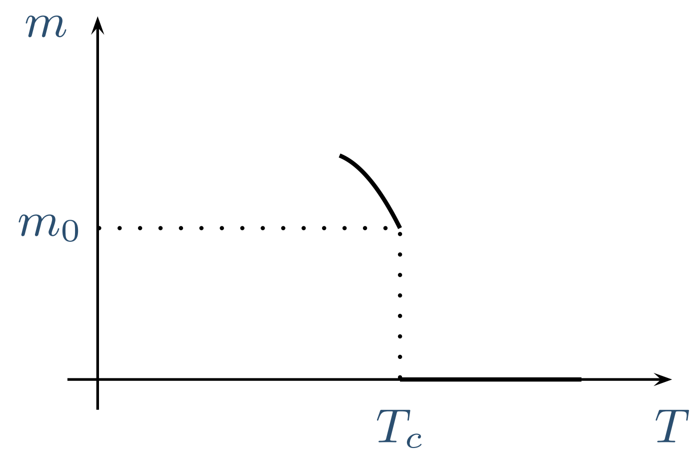
Order parameter

- The order parameter $m(T)$ therefore changes discontinuously from $m = 0$ to $m = m_0$ at $T = T_c$:



- This is known as a first-order phase transition.
- In a first-order phase transition, the equilibrium state shifts from one local minimum of $A(T, m)$ to another, with a discontinuous change of order parameter $m(T)$.

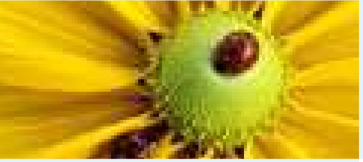
- The order parameter $m(T)$ therefore changes discontinuously from $m = 0$ to $m = m_0$ at $T = T_c$:



- This is known as a first-order phase transition.
- In a first-order phase transition, the equilibrium state shifts from one local minimum of $A(T, m)$ to another, with a discontinuous change of order parameter $m(T)$.
- By contrast, for a second-order phase transition, the position of the absolute minimum of $A(T, m)$ varies continuously with T.

Transition equations

- How do we determine the values of the critical parameters T_c and m_0 for a first-order phase transition?



Transition equations

- How do we determine the values of the critical parameters T_c and m_0 for a first-order phase transition?
- Any minimum of $A(T, m)$ must satisfy

$$\frac{\partial A}{\partial m} = bm + cm^3 + dm^5 = 0.$$

Transition equations

- How do we determine the values of the critical parameters T_c and m_0 for a first-order phase transition?
- Any minimum of $A(T, m)$ must satisfy

$$\frac{\partial A}{\partial m} = bm + cm^3 + dm^5 = 0.$$

- Hence, the minima are given by either $m = 0$ or

$$b + cm^2 + dm^4 = 0. \tag{1}$$

Transition equations

- How do we determine the values of the critical parameters T_c and m_0 for a first-order phase transition?
- Any minimum of $A(T, m)$ must satisfy

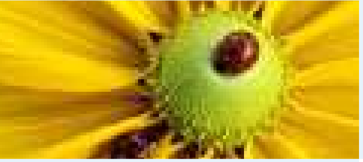
$$\frac{\partial A}{\partial m} = bm + cm^3 + dm^5 = 0.$$

- Hence, the minima are given by either $m = 0$ or

$$b + cm^2 + dm^4 = 0. \tag{1}$$

- The critical parameters T_c and m_0 must satisfy the additional condition

$$A(T_c, m_0) = A(T_c, 0) = a(T_c), \qquad m_0 \neq 0.$$



Transition equations

- How do we determine the values of the critical parameters T_c and m_0 for a first-order phase transition?
- Any minimum of $A(T, m)$ must satisfy

$$\frac{\partial A}{\partial m} = bm + cm^3 + dm^5 = 0.$$

- Hence, the minima are given by either $m = 0$ or

$$b + cm^2 + dm^4 = 0. \tag{1}$$

- The critical parameters T_c and m_0 must satisfy the additional condition

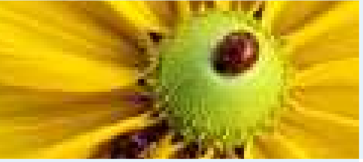
$$A(T_c, m_0) = A(T_c, 0) = a(T_c), \qquad m_0 \neq 0.$$

- This gives

$$\frac{1}{2}b(T_c)m_0^2 + \frac{1}{4}c(T_c)m_0^4 + \frac{1}{6}d(T_c)m_0^6 = 0,$$

and since $m_0 \neq 0$,

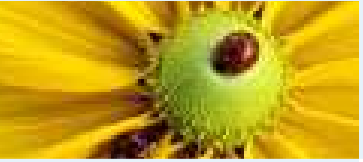
$$b(T_c) + \frac{1}{2}c(T_c)m_0^2 + \frac{1}{3}d(T_c)m_0^4 = 0. \tag{2}$$



Critical parameters

- By eliminating b, c, and d in turn from equations (1) and (2), we see that the critical parameters satisfy

$$m_0^2 = -\frac{3}{4}\frac{c(T_c)}{d(T_c)} = -4\frac{b(T_c)}{c(T_c)}, \qquad m_0^4 = 3\frac{b(T_c)}{d(T_c)}.$$

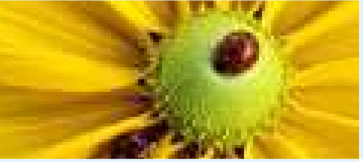


Critical parameters

- By eliminating b, c, and d in turn from equations (1) and (2), we see that the critical parameters satisfy

$$m_0^2 = -\frac{3}{4}\frac{c(T_c)}{d(T_c)} = -4\frac{b(T_c)}{c(T_c)}, \qquad m_0^4 = 3\frac{b(T_c)}{d(T_c)}.$$

- The last equation shows that for a phase transition of this type to occur, we must have both $d(T_c) > 0$ and $b(T_c) > 0$.



Critical parameters

- By eliminating b, c, and d in turn from equations (1) and (2), we see that the critical parameters satisfy

$$m_0^2 = -\frac{3}{4}\frac{c(T_c)}{d(T_c)} = -4\frac{b(T_c)}{c(T_c)}, \qquad m_0^4 = 3\frac{b(T_c)}{d(T_c)}.$$

- The last equation shows that for a phase transition of this type to occur, we must have both $d(T_c) > 0$ and $b(T_c) > 0$.
- Upon solving for c in the first two equations, we find

$$c(T_c) = -4\sqrt{\frac{b(T_c)d(T_c)}{3}},$$

which is the condition defining the critical temperature T_c.

- The value of m_0 can then be obtained from any of the equations above.

Critical parameters

- By eliminating b, c, and d in turn from equations (1) and (2), we see that the critical parameters satisfy

$$m_0^2 = -\frac{3}{4}\frac{c(T_c)}{d(T_c)} = -4\frac{b(T_c)}{c(T_c)}, \qquad m_0^4 = 3\frac{b(T_c)}{d(T_c)}.$$

- The last equation shows that for a phase transition of this type to occur, we must have both $d(T_c) > 0$ and $b(T_c) > 0$.
- Upon solving for c in the first two equations, we find

$$c(T_c) = -4\sqrt{\frac{b(T_c)d(T_c)}{3}},$$

which is the condition defining the critical temperature T_c.
- The value of m_0 can then be obtained from any of the equations above.
- Finally, for $T \le T_c$ [i.e., $c(T) \le c(T_c)$], we can find $m(T)$ by solving the quadratic equation (1):[3]

$$m^2 = \frac{-c + \sqrt{c^2 - 4bd}}{2d}.$$

[3] The positive root is the one that connects continuously with $m^2 = m_0^2$ at $T = T_c$.

Conclusions

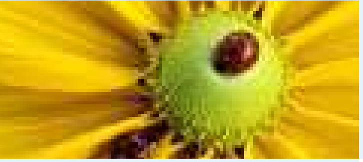
- The Landau theory thus provides a simple way of understanding the general features of phase transitions, independent of the details of any particular system.

Conclusions

- The Landau theory thus provides a simple way of understanding the general features of phase transitions, independent of the details of any particular system.
- We already know that the Landau theory cannot be exact (because it agrees with mean-field theory), but it provides extremely valuable qualitative insight in many situations.

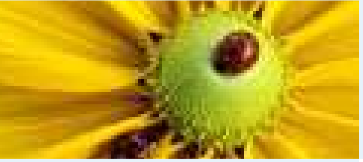
Conclusions

- The Landau theory thus provides a simple way of understanding the general features of phase transitions, independent of the details of any particular system.
- We already know that the Landau theory cannot be exact (because it agrees with mean-field theory), but it provides extremely valuable qualitative insight in many situations.
- A second-order phase transition occurs when the quadratic coefficient $b(T)$ changes sign, for positive $c(T)$.



Conclusions

- The Landau theory thus provides a simple way of understanding the general features of phase transitions, independent of the details of any particular system.
- We already know that the Landau theory cannot be exact (because it agrees with mean-field theory), but it provides extremely valuable qualitative insight in many situations.
- A second-order phase transition occurs when the quadratic coefficient $b(T)$ changes sign, for positive $c(T)$.
- A first-order phase transition occurs when the quartic coefficient $c(T)$ has a sufficiently large negative value, for positive $b(T)$ and $d(T)$.



Conclusions

- The Landau theory thus provides a simple way of understanding the general features of phase transitions, independent of the details of any particular system.
- We already know that the Landau theory cannot be exact (because it agrees with mean-field theory), but it provides extremely valuable qualitative insight in many situations.
- A second-order phase transition occurs when the quadratic coefficient $b(T)$ changes sign, for positive $c(T)$.
- A first-order phase transition occurs when the quartic coefficient $c(T)$ has a sufficiently large negative value, for positive $b(T)$ and $d(T)$.
- An example of a first-order phase transition is the crystallization of a liquid into a solid.
- In that case, the order parameter m is related to the spatial ordering that develops from the fluid state.

Order parameter for solid

density $\rho(r) = \sum_i \delta(r - r_i)$

Fourier transform

$$\rho(q) = \int dr\, \rho(r) e^{iq\cdot r} = \sum_j e^{iq\cdot r_j}$$

For solids , there are vectors G so that $G \cdot R_j = 2\pi n$ for some integer n.

For example, for $R_j = ja$, G= $2\pi/a$

$\rho(G) = \sum_j e^{iG\cdot u_j}$ is a good order parameter.