Possibility of anomalous fluctuations during structural phase transitions

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A theory is derived for phase transitions which result from particular features of the electron spectrum (congruent parts of the Fermi surface, particularly in quasi-one-dimensional systems). If the congruence is not perfect, or if the masses in two-band systems are greatly different, the fluctuations may occur over a broad temperature range. This result can explain, for example, the anomalies in the susceptibility, compressibility, and phonon spectra in A15 compounds.

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The Landau theory of phase transitions ignores inhomogeneous fluctuations of the order parameter. The range of applicability of this approximation (the average-field approximation) is determined by[1]

$$1 \gg |\tau| \gg \frac{b^2 T_c^2}{ac^3} \equiv \mathrm{Gi}, \tag{1}$$

where $\tau = (T - T_c)/T_c$, T_c is the transition temperature, and a, b, and c are coefficients in the expansion of the free energy in powers of the order parameter Δ:

$$F = a\tau |\Delta|^2 + \frac{b}{2}|\Delta|^4 + c|\vec{\nabla}\Delta|^2. \tag{2}$$

For superconductors the Ginzburg number is $\mathrm{Gi} \simeq 100\,(T_c/\epsilon_F)^4 \sim 10^{-14}$ (Ref. 2), and the fluctuation region is essentially unobservable (the Fermi energy is $\epsilon_F \gg T_c$). Phase transitions in electron systems which result from the presence of congruent parts of the Fermi surface, including Peierls transitions, have much in common with phase transitions in superconductors. In these systems (which exhibit an electron–hole pairing[3]), the ratio T_c/ϵ_F is also small. It might therefore seem that the fluctuation range should also be small, but this is not always the case. Let us examine, for example, the phase transition of a semimetal with a spectrum $\epsilon_1(\mathbf{p}) = (\mathbf{p}^2 - p_F^2)/2m_1$, $\epsilon_2(\mathbf{p}+\mathbf{w}) = -(\mathbf{p}^2 - p_F^2)/2m_2$ to the state of an excitonic dielectric. Such a transition may be accompanied by both structural distortions and the appearance of an antiferromagnetism.[3] In both cases the order parameter is the dielectric gap at the Fermi surface. An expansion corresponding to (2) can be constructed by a diagram perturbation theory, and the coefficients a, b, and c can be calculated in the same way:

$$a = N(0) = \frac{m p_F}{2\pi^2}, \qquad b = N(0)\frac{7\zeta(3)}{8(\pi T_c)^2}(1-\delta^2), \qquad c = bv_F^2(1-\delta^2), \tag{3}$$

where $\delta = (m_2 - m_1)/(m_1 + m_2)$, $m = 2m_1 m_2/(m_1 + m_2)$ and $v_F = p_F/m$. Using $T_c \simeq 0.57\,\Delta_0(1-\delta^2)^{1/2}$, $\Delta_0 = 2\epsilon_F \exp(-1/g)$, where g is the coupling constant, we find the Ginzburg number

$$\mathrm{Gi} \simeq 10\left(\frac{\Delta_0}{\epsilon_F}\right)^4 (1-\delta^2)^{-2}. \tag{4}$$

If the difference in masses is large, the fluctuation region may thus be quite large. With $m_2/m_1 \sim 100$ and $g \sim 0.3$, for example, Gi turns out to be of order unity, and the Landau theory is completely inapplicable.

A role similar to that of the mass difference may be played by a possible incomplete congruence of the Fermi surface, resulting from, for example, doping or an anisotropy. In quasi-one-dimensional systems, another possibility is a distortion of a flat Fermi surface by a hopping of electrons between chains.

To illustrate the situation, we consider a single-band metal with a spectrum $\epsilon(\mathbf{p}) = -\epsilon(\mathbf{p}+\mathbf{w}) \pm u$, where u is a constant, and where the $\pm$ correspond to different regions of solid angles. Mathematically, this model is completely analogous to a superconductor in a strong exchange field,[4] with the role of the exchange field being played here by[1)] u. We know that in this case the (T_c, u) phase diagram has a point $T_c(u) = \tilde{T}_c \simeq 0.54T_{c0}$, $u = \tilde{u} \simeq 1.06T_{c0}$ (T_{c0} is the transition temperature at $u = 0$), at which a second-order transition (at $T_c > \tilde{T}_c$) gives way to a first-order transition (at $T_c < \tilde{T}_c$). In other words, this is a tricritical point,[1] and we have a coefficient $b(\tilde{T}_c, \tilde{u}) = 0$. Fluctuations near such a point should be suppressed.[1] In this system, however, the coefficient c is equal to $v_F^2 b$, and it also vanishes at this point; i.e., in our case the tricritical point coincides with the so-called Lifshitz point.[5] It can be seen from (1) that the fluctuation region should expand as we approach the Lifshitz. point. It should be noted that we are restricting this discussion to the region $u < \tilde{u}$ (i.e., $T_c > \tilde{T}_c$), in which the second-order transition occurs from the metallic phase to a homogeneous dielectric phase, so that expression (1) applies. At $u > \tilde{u}$, the transition is to an inhomogeneous (incommensurable) phase, and condition (1) may take a different form. Formally, we have $\mathrm{Gi} = \infty$ precisely at the Lifshitz point. In this case, however, terms of the next higher order in Δ and its derivatives would have to be taken into account in (2), and these terms would limit the fluctuation growth.[5]

In both cases (the case of different masses and the case of incongruent Fermi surfaces), therefore, the growth of the fluctuations results from a decrease in the gradient term in (2), i.e., a decrease in the "stiffness" of the system. As a result, during structural transitions there is a softening of the phonons over a broad range of wave vectors. This effect can be seen particularly well in the case of a semimetal. The phonons which undergo the softening have momenta $\mathbf{q} = \mathbf{w}$ for which $\epsilon_1(\mathbf{p}) = -\epsilon_2(\mathbf{p}+\mathbf{w})$ (near the Fermi surface). If $m_2 \gg m_1$, this condition holds approximately for momenta $\mathbf{q}$ quite different from $\mathbf{w}$. In the limit $m_2 = \infty$, with an infinitesimally narrow level, this condition holds for all $\mathbf{q}$.

The effects discussed in this letter may be responsible for the anomalous temperature dependence which has been observed for the susceptibility and the compressibility in A15 compounds, and they may also be responsible for the anomalous softening

of the phonons over nearly the entire Brillouin zone.[6] We might also note in this connection that in Sm(Y)S compounds the frequencies of the longitudinal phonons, which soften (to a greater extent than those of the transverse phonons) at a phase transition to a state with a variable valence, lie below the frequencies of the transverse phonons (even at room temperature) nearly throughout the Brillouin zone.[7] This circumstance may also be related to the effect described above.

These effects may also occur during magnetic transitions, in particular, in chromium and its alloys, where spin waves would play the role of phonons.

Finally, we note that, because of the significant critical region in these systems, the fluctuational corrections should substantially change the relationship between T_c and Δ_0.

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[1)]We note in this connection that the effects which we are discussing here, i.e., the broad fluctuation region, should also occur in superconductors in a strong exchange field.

1. L. D. Landau and E. M. Lifshitz, Statisticheskaya fizika, Moscow, 1976 (Statistical Physics, Edison–Wesley, Reading, Mass).
2. V. L. Ginzburg, Fiz. Tverd. Tela (Leningrad) 2, 2031 (1960) [Sov. Phys. Solid State 2, 1824 (1960)].
3. Yu. V. Kopaev, in: Trudy FIAN (Proceedings of the P. N. Lebedev Physics Institute), Vol. 86, 1975, p. 3.
4. D. Saint-James, G. Sarma, and E. J. Thomas, Type II Superconductivity, Pergamon, New York, 1969 (Russ. transl. Mir. Moscow, 1970).
5. R. M. Hornreich, M. Luban, and S. Shtrikman, Phys. Rev. Lett. 35, 1678 (1975).
6. L. R. Testardi, M. Weger, and I. B. Goldberg, Superconducting Compounds with the β-Tungsten Structure (Russ. Transl. Mir, Moscow, 1977).
7. H. A. Mook, R. N. Nicklow, T. Penney, F. Holtzberg, and M. W. Shafer, Phys. Rev. B18, 2925 (1978).

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