Turning a first order quantum phase transition continuous by fluctuations: general flow equations and application to the nematic transition in two-dimensional electron systems

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We derive renormalization group equations which allow us to treat order parameter fluctuations near quantum phase transitions in cases where an expansion in powers of the order parameter is not possible. As a prototypical application, we analyze the nematic transition driven by a d-wave Pomeranchuk instability in a two-dimensional electron system. We find that order parameter fluctuations suppress the first order character of the nematic transition obtained at low temperatures in mean-field theory, so that a continuous transition leading to quantum criticality can emerge.

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Numerous itinerant electron systems undergo zero temperature quantum phase transitions as a function of a tunable control parameter such as pressure or doping [1–3]. Most interesting are continuous transitions associated with quantum critical fluctuations, which naturally lead to non-Fermi liquid behavior [4]. However, quantum phase transitions are frequently first order, such that critical fluctuations are absent [5].

In this letter we explore the possibility that a quantum phase transition which is first order in mean field theory, turns out to be actually continuous by virtue of order parameter fluctuations. As a prototypical example we consider the nematic transition [6] driven by a d-wave Pomeranchuk instability [7, 8] in two dimensions, which is presently being discussed in the context of cuprates [9], Sr₃Ru₂O₇ [10], and other correlated electron materials. Mean field studies of tight binding electrons on a square lattice indicate that this transition is typically discontinuous at zero temperature [11–13]. A continuous transition occurs only at
sufficiently high temperature, above a tricritical point. This feature is quite generic since the quartic coupling of the Landau free energy describing the transition at zero temperature is essentially determined by the curvature of the electronic density of states at the Fermi level, but with opposite sign. Due to the logarithmic divergence at the van Hove energy, the density of states typically has positive curvature in a broad window around the van Hove point, leading to a negative quartic coupling for the order parameter, and hence to a first order transition. A continuous transition at zero temperature is found only for judicious choices of hopping amplitudes and interactions [13].

A recent renormalization group (RG) analysis of a quantum Landau-Ginzburg-Wilson model with $\phi^4$ and $\phi^6$ interactions indicated that order parameter fluctuations can alter the order of the transition from first (in mean field theory) to second order [14]. However, that model is well defined only for a positive $\phi^6$-interaction, while, for example, the Landau energy for the nematic transition discussed above suffers from negative interactions not only at quartic order, but rather at any finite order $\phi^{2l}$. The minimum of the Landau energy associated with the first order transition and the ultimate increase at large values of $\phi$ cannot be accessed by an expansion around $\phi = 0$.

In such situations one would like to proceed without resorting to the usual expansion in powers of the order parameter field. The functional RG framework offers the possibility to approximate the order parameter interaction by a local potential without expanding it in powers of $\phi$ [15, 16]. In the following we will derive the functional flow equations for a general quantum Landau-Ginzburg-Wilson model for phase transitions in itinerant electron systems, and solve them for the specific case of a nematic transition in two dimensions. We find that fluctuations can indeed transform the first order transition obtained in mean field theory into a continuous one.

Our starting point is an action for the order parameter of the form

$$S[\phi] = \frac{1}{2} \int_q \phi_q \left( A_0 \frac{|\omega_n|}{|q|^z} + Z_0 q^2 \right) \phi_{-q} + U[\phi],$$  

(1)

where $\phi$ is a scalar order parameter field and $\phi_q$ with $q = (q, \omega_n)$ its momentum representation; $\omega_n = 2\pi n T$ with integer $n$ denotes the (bosonic) Matsubara frequencies. For the Matsubara sum and momentum integration we use the abbreviation $\int_q = T \sum_n \int \frac{d^d q}{(2\pi)^d}$. The prefactors $A_0$ and $Z_0$ are positive numbers. The dynamical exponent $z$ is restricted to
values \( z \geq 2 \). The potential \( U[\phi] \) is a functional of \( \phi \) which is local in space and time,

\[
U[\phi] = \int_0^{1/T} d\tau \int d^4r U(\phi(\mathbf{r}, \tau)) ,
\]

with a (so far) arbitrary real-valued function \( U(\phi) \). The momenta and frequencies contributing to \( S[\phi] \) are restricted by an ultraviolet cutoff \( \Lambda_0 \) to the region \( A_0 \frac{|\omega_n|}{|q|^{z-2}} + Z_0 q^2 \leq \Lambda_0^2 \).

An action of the form Eq. \( (1) \) can be derived from a fermionic model by introducing the order parameter as a Hubbard-Stratonovich field and subsequently integrating out the fermions \([17, 18]\). Usually \( U(\phi) \) is truncated at quartic order, such that only a (quadratic) mass term and the local \( \phi^4 \) interaction is kept, which is justified by power counting close to a continuous phase transition. Our essential generalization is that we do not truncate \( U(\phi) \) at all, to be able to deal with cases where an expansion in powers of \( \phi \) is not possible.

We integrate out fluctuations successively by computing the flow of the effective action \( \Gamma^\Lambda[\phi] \) from a functional RG flow equation. The effective action \( \Gamma^\Lambda[\phi] \) is the generating functional for one-particle irreducible vertex functions in the presence of an infrared cutoff \( \Lambda \). The cutoff is implemented by adding a regulator \( R^\Lambda \) to the inverse propagator. \( \Gamma^\Lambda[\phi] \) interpolates between the bare action \( S[\phi] \) for large \( \Lambda \) and the final effective action \( \Gamma[\phi] \) in the limit \( \Lambda \to 0 \). Its evolution is given by the exact functional flow equation \([19]\)

\[
\partial_\Lambda \Gamma^\Lambda[\phi] = \frac{1}{2} \text{tr} \left[ \frac{\dot{R}^\Lambda}{\Gamma^\Lambda_2[\phi] + R^\Lambda} \right] ,
\]

where \( \dot{R}^\Lambda = \partial_\Lambda R^\Lambda \), and \( \Gamma^\Lambda_2[\phi] = \delta^2 \Gamma^\Lambda[\phi] / \delta \phi^2 \). In momentum representation, the trace sums over momenta and frequencies: \( \text{tr} = \int_q \).

The exact effective action is a complicated functional of \( \phi \). We resort to an approximation of the flow based on the following ansatz:

\[
\Gamma^\Lambda[\phi] = \frac{1}{2} \int_q \phi_q \left( A \frac{|\omega_n|}{|q|^{z-2}} + Z q^2 \right) \phi_{-q} + U^\Lambda[\phi] ,
\]

with \( \Lambda \)-dependent parameters \( A \) and \( Z \) and a local potential \( U^\Lambda[\phi] \) of the form Eq. \( (2) \) with a \( \Lambda \)-dependent function \( U(\phi) \). A classical version of this ansatz, where Matsubara frequencies and the dynamical term are absent, has been used previously to analyze classical phase transitions \([15, 16]\). Inserting the ansatz \( (4) \) into the exact flow equation \( (3) \), and evaluating the resulting equation for uniform fields, one obtains the flow equation for \( U(\phi) \),

\[
\partial_\Lambda U(\phi) = \frac{1}{2} \int_q \dot{R}^\Lambda(q) G^\Lambda(q; \phi) ,
\]
where $G^\Lambda(q; \phi)$ is the regularized propagator in presence of a uniform field $\phi$,

$$G^\Lambda(q; \phi) = \left[ \Gamma^\Lambda_2(q; \phi) + R^\Lambda(q) \right]^{-1} = \left[ A \sqrt{\frac{\omega_n}{|q|^{d-2}}} + Z q^2 + U''(\phi) + R^\Lambda(q) \right]^{-1}. \quad (6)$$

Here $U''(\phi)$ is the second derivative of $U(\phi)$ with respect to $\phi$, such that the flow equation (5) is a partial differential equation.

The evolution of the parameters $A$ and $Z$ parametrizing the non-local quadratic term in the effective action is determined by the flow of $\Gamma^\Lambda_2(q; \phi)$,

$$\partial_\Lambda \Gamma^\Lambda_2(q; \phi) = \left[ \partial^3_\phi U(\phi) \right]^2 \int_p \hat{R}^\Lambda(p) [G^\Lambda(p; \phi)]^2 G^\Lambda(p + q; \phi) - \frac{1}{2} \left[ \partial^4_\phi U(\phi) \right] \int_p \hat{R}^\Lambda(p) [G^\Lambda(p; \phi)]^2. \quad (7)$$

The derivatives $\partial^3_\phi U(\phi)$ and $\partial^4_\phi U(\phi)$ correspond to local 3-point and 4-point vertices, respectively. We extract the $Z$-factor from the two-point vertex as

$$Z = \left[ \Gamma^\Lambda_2(\phi_0) \right]_{q=0},$$

where $\phi_0$ is the position of the global minimum of $U(\phi)$. The Laplacian $\Delta_q$ is defined at fixed $R^\Lambda$, that is, it does not act on the regulator $R^\Lambda(p + q)$ in $G^\Lambda(p + q)$ on the right hand side of Eq. (7). The flow of the $A$-factor could also be extracted from $\Gamma^\Lambda_2$, but it is of minor importance [20] and will be discarded here, that is, we set $A = A_0$.

As a regulator we choose a Litim-type [21] cutoff function

$$R^\Lambda(q) = \left[ Z (\Lambda^2 - q^2) - A|q|^{2-z}|\omega_n| \right] \theta \left[ Z (\Lambda^2 - q^2) - A|q|^{2-z}|\omega_n| \right], \quad (8)$$

which has the convenient feature that the regularized propagator becomes momentum- and frequency-independent in the integration region, that is, $G^\Lambda(q; \phi) = [Z \Lambda^2 + U''(\phi)]^{-1}$ for $A|q|^{2-z}|\omega_n| + Z q^2 < Z \Lambda^2$. The momentum integrations on the right hand side of the flow equations can be carried out analytically. The frequency summation in Eq. (5) is performed numerically.

The flow of $Z$ receives significant contributions only near a continuous phase transition at finite temperature, where non-Gaussian classical fluctuations generate an anomalous scaling dimension (given by the logarithmic derivative of $Z$ with respect to $\Lambda$) [20]. Note that quantum critical points at $T = 0$ are Gaussian for $d + z \geq 4$ [17]. We can therefore neglect the contributions from $\omega_n \neq 0$ to the flow of $Z$, and obtain

$$\frac{d \log Z}{d \log \Lambda} = -T[U''(\phi_0)]^2 \frac{S_{d-1}}{(2\pi)^d} \frac{\Lambda^{d-6}}{Z^4(1 + \tilde{\delta})^5} \frac{1}{d} \left[ 2(1 + \tilde{\delta}) - \frac{8}{d + 2} \right], \quad (9)$$
where \( \tilde{\delta} = U''(\phi_0)/(Z\Lambda^2) \) and \( S_{d-1} = 2\pi^{d/2}/\Gamma(d/2) \) is the area of the \((d-1)\)-dimensional unit sphere.

We now apply the flow equations to a specific model system, featuring a nematic transition driven by a d-wave Pomeranchuk instability. The model describes tight binding fermions on a square lattice with an attractive d-wave forward scattering interaction. Its Hamiltonian is given by \[ H = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} n_{\mathbf{k}} + \frac{1}{2L} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} f_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) n_{\mathbf{k}}(\mathbf{q}) n_{\mathbf{k}'}(-\mathbf{q}) , \]

where \( n_{\mathbf{k}}(\mathbf{q}) = \sum_{\sigma} \epsilon_{\mathbf{k-q}/2,\sigma} \epsilon_{\mathbf{k+q}/2,\sigma} \) and \( L \) is the number of lattice sites. For nearest and next-to-nearest neighbor hopping the kinetic energy reads \( \epsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y \). Its van Hove (saddle) points are situated at \( \mathbf{k} = (\pi,0) \) and \((0,\pi)\). The interaction has the form

\[ f_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) = -g(\mathbf{q}) d_{\mathbf{k}} d_{\mathbf{k}'} , \]

where \( d_{\mathbf{k}} = \cos k_x - \cos k_y \) is a form factor with \( d_{x^2-y^2} \) symmetry. The coupling function \( g(\mathbf{q}) \geq 0 \) has a maximum at \( \mathbf{q} = 0 \) and is restricted to small momentum transfers by a momentum cutoff. For sufficiently large \( g = g(0) \) the interaction drives a d-wave Pomeranchuk instability leading to a nematic state with broken orientation symmetry, which can be described by the order parameter

\[ \phi = \frac{g}{L} \sum_{\mathbf{k}} d_{\mathbf{k}} \langle n_{\mathbf{k}} \rangle . \]

The mean-field solution of the model \[ 10 \] has been analyzed in a series of articles \[ 11,13 \].

In the plane spanned by the chemical potential and temperature a nematic phase is formed below a dome-shaped transition line \( T_c(\mu) \) with a maximal transition temperature near van Hove filling. The phase transition is usually first order near the edges of the transition line, that is, where \( T_c \) is relatively low, and always second order at the roof of the dome.

Introducing an order parameter field via a Hubbard-Stratonovich transformation, integrating out the fermions, and keeping only the leading momentum and frequency dependences for small \( \mathbf{q} \) and \( \omega_n/|\mathbf{q}| \) leads to an action \( S[\phi] \) of the form Eq. \[ 11 \], with \( z = 3 \) and

\[ U(\phi) = \frac{\phi^2}{2g} - 2T \int \frac{d^2 k}{(2\pi)^2} \ln \left( 1 + e^{-(\epsilon_{\mathbf{k}} - \phi d_{\mathbf{k}} - \mu)/T} \right) . \]

The coefficients of a Landau expansion of this potential, \( U(\phi) = \frac{a_2}{2} \phi^2 + \frac{a_4}{4!} \phi^4 + \ldots \), are given by \( a_2 = g^{-1} - N_2(\mu) \) and \( a_{2l} = -\frac{\partial^{2l-2}}{\partial \mu^{2l-2}} N_{2l}(\mu) \) for \( l \geq 2 \), where \( N_{2l}(\mu) = \frac{2}{L} \sum_{\mathbf{k}} d_{\mathbf{k}}^{2l} \delta(\epsilon_{\mathbf{k}} - \mu) \) is
the density of states at the Fermi level with a d-wave form factor \([13]\). Since \(N_{2l}(\mu)\) diverges logarithmically at van Hove filling, \(a_{2l}\) is typically negative for \(l \geq 2\).

The coefficients \(A_0\) and \(Z_0\) in \(S[\phi]\) are related to the d-wave particle-hole bubble and the coupling function \(g(q)\) \([23]\). Note that \(A_0\) and \(Z_0\) are not involved in the mean-field solution of the model Eq. \(10\). \(A_0\) is associated with the Landau damping term in the bubble, and depends actually on the orientation of \(q\). We will neglect this \(q\)-dependence and insert a constant \(A_0\) corresponding to an angular average. While the bubble is fully determined by the kinetic energy \(\epsilon_k\), the choice of \(Z_0\) remains to a large extent arbitrary since it also depends on the momentum dependence of \(g(q)\). Since momenta \(q\) in the action \(S[\phi]\) correspond to momentum transfers in the underlying fermionic model, the ultraviolet cutoff \(\Lambda_0\) in \(S[\phi]\) limits momentum transfers in \(g(q)\) to \(|q| \leq \Lambda_0/\sqrt{Z_0}\).

We now present results for the nematic transition as obtained from the functional RG. The following parameters are the same in all quantitative plots: \(t = 1\), \(t' = -1/6\), \(g = 0.8\), \(A_0 = 1\), and \(Z_0 = 10\). In Fig. 1 we show an exemplary plot of the evolution of the flowing effective potential \(U(\phi)\) for \(\Lambda\) ranging from the ultraviolet cutoff \(\Lambda_0 = e^{-1} \approx 0.37\) to the final value \(\Lambda = 0\). The initial (mean-field) potential has a minimum at \(\phi_0 = 0.112\). The final potential exhibits spontaneous symmetry breaking with an order parameter \(\phi_0 = 0.102\). Fluctuations shift \(\phi_0\) toward a slightly smaller value compared to the mean-field solutions. Note the flat shape of \(U(\phi)\) for \(\phi < \phi_0\) at \(\Lambda = 0\), which is imposed by the convexity property of the grandcanonical potential \([24, 25]\). The final value of \(\phi_0\) can be obtained either by

![FIG. 1](image-url)
following the sequence of minima \( \phi_0^\Lambda \) until \( \Lambda \to 0 \), or by determining the point on the \( \phi \)-axis where the flat shape in the final potential \( U(\phi) \) terminates.

In Fig. 2 we present the transition line between normal and symmetry-broken phases for two choices of \( \Lambda_0 \). Compared to the corresponding mean-field result, the transition temperature is suppressed, with a larger reduction for larger \( \Lambda_0 \) (corresponding to a larger phase space for fluctuations). While the phase transition is of first order at low temperatures in mean-field theory, and also in the presence of fluctuations with a cutoff \( \Lambda_0 = e^{-1} \), for \( \Lambda_0 = 1 \) the transition is continuous down to \( T = 0 \), leading to quantum critical points \( \mu_c \) at the edges of the nematic dome. In Fig. 3 we show the order parameter \( \phi_0 \) at \( T = 0 \) as a function of \( \mu \) near the left edge of the transition lines in Fig. 2 for \( \Lambda_0 = e^{-1} \) and \( \Lambda_0 = 1 \). For the case \( \Lambda_0 = e^{-1} \) the jump of \( \phi_0 \) indicates a pronounced first order transition. By contrast, for \( \Lambda_0 = 1 \) the order parameter rises continuously, and the shape of \( \phi_0(\mu) \) exhibits the expected behavior of a Gaussian quantum critical point.

We note that the mean-field phase diagram is fully determined by the parameters \( t, t' \), and \( g \); the size of the phase boundary (in units of \( t \)) depends on \( g/t \), but its shape is very robust [12, 13]. The parameters \( A_0, Z_0, \) and \( \Lambda_0 \) determine the strength and phase space of fluctuations. The suppression of \( T_c \) and of the first order lines is stronger for larger \( \Lambda_0 \) and smaller \( A_0 \) and \( Z_0 \).

In summary, we have presented a renormalization group method which allows us to treat
order parameter fluctuations near quantum phase transitions in cases where an expansion in powers of the order parameter $\phi$ is not possible. We have derived flow equations for the full effective potential $U(\phi)$ in a local approximation. As a first application of the method, we have analyzed fluctuation effects on the nematic transition driven by a d-wave Pomeranchuk instability in two-dimensional itinerant electron systems. It turned out that order parameter fluctuations suppress the first order character of the nematic transition obtained at low temperatures in mean-field theory, such that a continuous transition associated with quantum criticality can emerge. Our flow equations may also be applied to a ferromagnetic transition with Ising symmetry and to other Pomeranchuk instabilities.

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