Crossover from BCS to Bose Superconductivity: Transition Temperature and Time-Dependent Ginzburg-Landau Theory

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We use functional integral formulation to study the finite temperature crossover from cooperative Cooper pairing to independent bound state formation and condensation, We show the inadequacy of mean field results for normal state properties obtained at the saddle point level as the coupling increases. The importance of quantum (temporal) fluctuations is pointed out and an interpolation scheme for T_c is derived from this point of view. The time-dependent Ginzburg-Landau (TDGL) equation near T_c is shown to describe a damped mode in the BCS limit, and a propagating one in the Bose limit. A singular point is identified at intermediate coupling where a simple TDGL description fails.

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The problem of the crossover [1,2] from BCS theory with cooperative Cooper pairing to the formation and condensation of composite bosons has attracted considerable attention [3–5] after the discovery of the high-T_c superconductors. Recently numerical simulations have clearly shown [4] that the intermediate coupling, crossover region displays highly anomalous correlations ("spin gap" behavior) in a degenerate Fermi system above T_c. More generally, the crossover question is also of interest for several other problems: excitonic condensates, superconductor-insulator transitions, and itinerant versus local-moment magnetism.

In this paper we study a continuum model of fermions with attractive interactions. We show that the saddle point approximation misses the qualitative physics of the intermediate and strong coupling normal state. The bosonic degrees of freedom, which become increasingly important with growing attraction, can only be adequately described by retaining the full frequency dependence of fluctuations about the normal state saddle point.

We first study the transition temperature. We show that a saddle point estimate T_0 gives increasingly incorrect results with coupling. In the strong coupling Bose limit T_0 is found to be related to the pair dissociation scale rather than the T_c ($\ll T_0$) at which coherence is established. Inclusion of Gaussian fluctuations about the trivial saddle point is shown to lead to the Nozières-Schmitt-Rink interpolation for T_c, which has a sensible strong coupling limit. To further elucidate the role of temporal fluctuations, we study the evolution of the time-dependent Ginzburg-Landau (TDGL) theory. In the BCS regime a damped mode with a small (order T_c/ϵ_F) propagating part is found, while in the Bose limit the mode is undamped. These two regimes are separated by a singular point at intermediate coupling where an energy scale, the chemical potential at T_c, vanishes, and even a linearized TDGL description fails. Finally, we briefly describe the evolution of the collective modes at $T=0$ with increasing coupling. Details will be given elsewhere [6].

We study fermions in a unit volume in 3D with a Hamiltonian density

$$H=\bar{\psi}_\sigma(x)\left[-\frac{\nabla^2}{2m}-\mu\right]\psi_\sigma(x) - g\bar{\psi}_\uparrow(x)\bar{\psi}_\downarrow(x)\psi_\downarrow(x)\psi_\uparrow(x)\,.$$

The chemical potential μ fixes the average density n. The partition function Z, at a temperature β^{-1}, is written as an imaginary time functional integral [7] with action $S=\int_0^\beta d\tau\int d\mathbf{x}[\bar{\psi}_\sigma(x)\partial_\tau\psi_\sigma(x)+H]$, where $x=(\mathbf{x},\tau)$ and $\hbar=k_B=1$. Introducing the usual Hubbard-Stratonovich field $\Delta(\mathbf{x},\tau)$, which couples to $\bar{\psi}\bar{\psi}$, and integrating out the fermions we obtain $Z=\int D\Delta D\bar{\Delta}\exp(-S_{\text{eff}}[\Delta,\bar{\Delta}])$. The effective action

$$S_{\text{eff}}[\Delta(x)]=\frac{1}{g}\int_0^\beta d\tau\int d\mathbf{x}|\Delta(x)|^2-\operatorname{Tr}\ln\mathbf{G}^{-1}[\Delta(x)] \tag{1}$$

is written in terms of the (inverse) Nambu propagator

$$\mathbf{G}^{-1}(x,x')=\begin{pmatrix} -\partial_\tau+\dfrac{\nabla^2}{2m}+\mu & \Delta(x) \\ \bar{\Delta}(x) & -\partial_\tau-\dfrac{\nabla^2}{2m}-\mu \end{pmatrix} \times\delta(x-x')\,,$$

and the trace in (1) is over space, imaginary time, and Nambu indices.

Below a certain temperature, which we denote by T_0 (rather than T_c for reasons which will become clear soon), the trivial saddle point $\Delta\equiv 0$ becomes unstable. This is defined by setting $\Delta=0$ in saddle point condition $\delta S_{\text{eff}}/\delta\Delta=0$. One then obtains the familiar gap equation $1/g=\sum_{\mathbf{k}}\tanh(\xi_{\mathbf{k}}/2T_0)/2\xi_{\mathbf{k}}$, where $\xi_{\mathbf{k}}=\varepsilon_{\mathbf{k}}-\mu$ with $\varepsilon_{\mathbf{k}}=|\mathbf{k}|^2/2m$.

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A BCS type cutoff cannot be used to access the strong coupling Bose regime. We thus use the s-wave scattering length a_s, defined by the low energy limit of the two-body problem in vacuum via $m/4\pi a_s = -1/g + \sum_{\mathbf{k}} (2\varepsilon_{\mathbf{k}})^{-1}$, to regulate the ultraviolet divergence in the gap equation. Eliminating the coupling g between these two equations we obtain

$$-\frac{m}{4\pi a_s} = \sum_{\mathbf{k}} \left[\frac{\tanh(\xi_{\mathbf{k}}/2T_0)}{2\xi_{\mathbf{k}}} - \frac{1}{2\varepsilon_{\mathbf{k}}} \right], \tag{2}$$

where a_s now plays the role of the coupling constant [8].

To solve the above equation for T_0 we need to first determine the chemical potential μ, as a function of the coupling and temperature, using $N = -\partial\Omega/\partial\mu$. The saddle point approximation for the thermodynamic potential, $\Omega_0 = S_{\text{eff}}[\Delta=0]/\beta$, leads to the number equation

$$n = n_0(\mu, T) \equiv \sum_{\mathbf{k}} \left[1 - \tanh\left(\frac{\xi_{\mathbf{k}}}{2T} \right) \right]. \tag{3}$$

We now estimate, at the saddle point level, T_0 as a function of the coupling g by solving (2) and (3); the two limiting cases can be solved analytically. In the weak coupling limit ($g \to 0$) we use $\mu \gg T_0$ to solve (3) yielding the result $\mu = \epsilon_F$, where $\epsilon_F = k_F^2/2m = (3\pi^2 n)^{2/3}/2m$ is the noninteracting Fermi energy. The solution of (2), for $1/k_F a_s \to -\infty$, is $T_0 = 8e^{-2}\gamma\pi^{-1}\epsilon_F \exp(-\pi/2k_F|a_s|)$, with $\gamma \simeq 1.781$. This is just the BCS result with ϵ_F playing the role of an effective cutoff [9].

In strong coupling the roles of the gap and number equations are reversed: The gap equation (2) determines μ, while the number equation (3) determines T_0 for $g \to \infty$. In this limit, $1/k_F a_s \to +\infty$ and one expects tightly bound pairs with binding energy $E_b = 1/ma_s^2$, and nondegenerate fermions with a large, *negative* chemical potential: $|\mu| \gg T$. From the gap equation (2) we obtain $\mu = -E_b/2$; i.e., the chemical potential for the fermions is one-half the pair binding energy. The strong coupling ($E_b/\epsilon_F \gg 1$) solution of (3) yields $T_0 \simeq E_b/2\ln(E_b/\epsilon_F)^{3/2}$.

This unbounded increase of the "transition temperature" with coupling is an artifact of the approximation, and as we shall see, there is no sharp phase transition at T_0. The trivial saddle point can only describe a normal state consisting of free fermions. In strong coupling T_0 is thus related to a pair-breaking scale T_{dissoc} defined as the temperature at which some fixed fraction of the bound pairs are dissociated. To estimate T_{dissoc} we use the condition $\mu_b = 2\mu_f$ for "chemical" equilibrium between bound pairs (bosons b) and unbound fermions (f): $b \rightleftharpoons f\uparrow + f\downarrow$. Further the bosons and fermions are nondegenerate and may be treated as classical ideal gases, leading to the result $T_{\text{dissoc}} \simeq E_b/\ln(E_b/\epsilon_F)^{3/2}$. The logarithmic term is an entropic contribution which favors broken pairs and leads to a dissociation temperature less than the binding energy E_b.

To include the effects of bound pairs in the strong coupling normal state, and to determine the evolution of T_c as a function of coupling, we look at Gaussian fluctuations about the trivial saddle point $\Delta(\mathbf{x}, \tau) = 0$. The action, expanded to second order in Δ, is given by $S_{\text{Gauss}} = S_{\text{eff}}[0] + \sum_{\mathbf{q}, iq_l} \Gamma^{-1}(\mathbf{q}, iq_l) |\Delta(\mathbf{q}, iq_l)|^2$, where $\Gamma^{-1} = 1/g - \chi^0_{\text{pair}}$ may be written as

$$\Gamma^{-1}(\mathbf{q}, iq_l) = \sum_{\mathbf{k}} \left[\frac{1 - n_{\mathbf{k}} - n_{\mathbf{k}+\mathbf{q}}}{iq_l - \xi_{\mathbf{k}} - \xi_{\mathbf{k}+\mathbf{q}}} + \frac{1}{2\varepsilon_{\mathbf{k}}} \right] - \frac{m}{4\pi a_s},$$

with $iq_l = i2l\pi/\beta$ and $n_{\mathbf{k}} = n_F(\xi_{\mathbf{k}})$, the Fermi occupation. The resulting expression for the thermodynamic potential $\Omega = \Omega_0 - \beta^{-1} \sum_{\mathbf{q}, iq_l} \ln \Gamma(\mathbf{q}, iq_l)$ is identical to the diagrammatic result of Nosières and Schmitt-Rink (NSR) [2]. Following NSR one can rewrite Ω in terms of a phase shift defined by $\Gamma(\mathbf{q}, \omega \pm i0) = |\Gamma(\mathbf{q}, \omega)| \exp[\pm i\delta(\mathbf{q}, \omega)]$. The number equation incorporating the effects of Gaussian fluctuations is given by

$$n = n_0(\mu, T) + \sum_{\mathbf{q}} \int_{-\infty}^{+\infty} \frac{d\omega}{\pi} n_B(\omega) \frac{\partial\delta}{\partial\mu}(\mathbf{q}, \omega), \tag{4}$$

where the "free" n_0 is defined in (3) and $n_B(\omega) = 1/[\exp(\beta\omega) - 1]$ is the Bose function.

Our next step is to see how the Gaussian fluctuations affect $T_c(g)$, the temperature at which long range order is established. This is defined by the simultaneous solution of (2) and (4). In weak coupling the results are essentially unaffected by the inclusion of Gaussian fluctuations in the number equation, since the second term in (4) is a small correction to the first one in this limit. Thus we find $\mu \simeq \epsilon_F$ and $T_c \simeq T_0$ for $g \to 0$.

On the other hand, the strong coupling results are greatly affected by the proper treatment of bound pairs in (4). To see this most clearly, note that the singularity structure of $\Gamma(\mathbf{q}, z)$ reflects the two-particle spectrum. For sufficiently large coupling (in 3D) Γ has an isolated pole representing the two-body bound state and a branch cut representing the continuum of two-particle excitations. For $g \to \infty$ there is a very large cost to break a pair, and the low energy physics for $T \ll T_{\text{dissoc}}$ is dominated by the pole. Thus $\Gamma(\mathbf{q}, iq_m) \simeq R(\mathbf{q})/[iq_m - \omega_b(\mathbf{q}) + 2\mu]$, with $\omega_b(\mathbf{q}) \simeq -E_b + |\mathbf{q}|^2/4m$ the dispersion for a pair. The partition function, after rescaling the Δ field, may be rewritten as $Z = Z_0 \int d\bar{\phi}\, d\phi \exp \sum_{\mathbf{q}, iq_l} \times \bar{\phi}_q (iq_l - \omega_b(\mathbf{q}) + 2\mu) \phi_q$, which is nothing but the partition function of a free Bose gas. Going beyond the Gaussian approximation, we find a repulsive two-body interaction between the bosons (see below). As is well known, this repulsion stabilizes the low temperature phase, but does not substantially affect the condensation temperature. From Z we obtain the strong coupling number equation $n = n_0 + \sum_{\mathbf{q}} n_B[\omega_b(\mathbf{q}) - 2\mu]$. The saddle point condition (2) is solved as before to obtain $\mu(T_c) = -E_b/2$. The n_0 in the equation above may then be ignored, and we find the Bose condensation temperature $T_c = [n/2\zeta(3/2)]^{2/3}\pi/m = 0.218\epsilon_F$, for bosons of mass $2m$ [10] and density $n/2$.

In Fig. 1 we plot a numerical solution of (2) and (4)

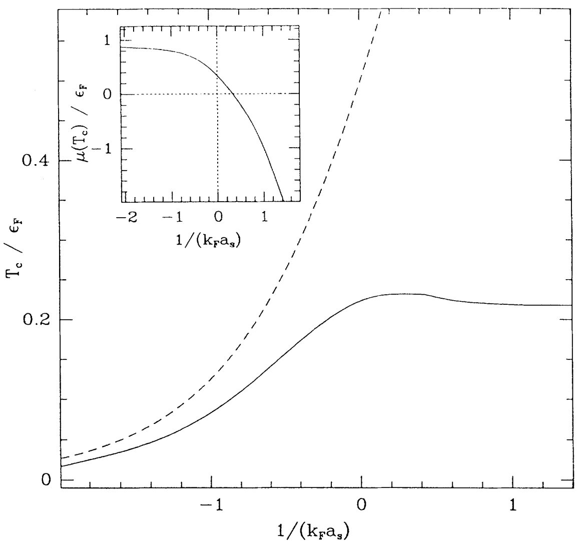

FIG. 1. T_c/ϵ_F [and in the inset $\mu(T_c)/\epsilon_F$] as a function of the coupling $x=1/k_F a_s$. The BCS limit corresponds to $x \to -\infty$ and the Bose regime to $x \gg 1$. The dashed line is the saddle point result (see text).

which smoothly interpolates between the two limiting cases described above.

To study the evolution of the TDGL we look at the equation $\delta S_{\rm eff}/\delta\Delta^*(q)=0$ near T_c for Δ slowly varying in space and time. We expand the action (1) to fourth order in $\Delta(q)$, where $q=(\mathbf{q}, iq_m)$, to obtain

$$S_{\rm eff}=\sum_q \frac{|\Delta(q)|^2}{\Gamma(q)}+\frac{1}{2}\sum_{q_1,q_2,q_3} b_{1,2,3}\Delta_1\Delta_2^*\Delta_3\Delta_{1-2+3}^*+\cdots .$$

We first look at the *static* part of the problem and make the expansion $\Gamma^{-1}(\mathbf{q},0)=a+c|\mathbf{q}|^2/2m+\cdots$. It is straightforward to show that

$$a=-\frac{m}{4\pi a_s}+\sum_{\mathbf{k}}\left[\frac{1}{2\varepsilon_{\mathbf{k}}}-\frac{X}{2\xi_{\mathbf{k}}}\right],$$

$$c=\sum_{\mathbf{k}}\left[\frac{X}{4\xi_{\mathbf{k}}^2}-\frac{\beta Y}{8\xi_{\mathbf{k}}}+\left(\beta^2 XY+\frac{\beta Y}{\xi_{\mathbf{k}}}-\frac{2X}{\xi_{\mathbf{k}}^2}\right)\frac{(\mathbf{k}\cdot\hat{\mathbf{n}})^2}{8m\xi_{\mathbf{k}}}\right],$$

where $X=\tanh(\beta\xi_{\mathbf{k}}/2)$, $Y={\rm sech}^2(\beta\xi_{\mathbf{k}}/2)$, and $\mathbf{k}\cdot\hat{\mathbf{n}}=|\mathbf{k}|\cos\theta$. Further, the coefficient of the nonlinear term is

$$b\equiv b(0,0,0)=\sum_{\mathbf{k}}\left[\frac{X}{4\xi_{\mathbf{k}}^3}-\frac{\beta Y^2}{8\xi_{\mathbf{k}}^2}\right]. \tag{5}$$

These results are similar to the recent work of Drechsler and Zwerger [5] who, however, did not study the nontrivial frequency dependence to be discussed next.

We next turn to the time dependence of the linearized TDGL equation. This requires a careful examination [6,11] of Gaussian fluctuations about the broken symmetry solution, and a simple low frequency expansion is obtained only when $\Delta(T)\ll\omega$. In this case one needs to expand $Q(iq_l)\equiv\Gamma^{-1}(\mathbf{q}=0,iq_l)-\Gamma^{-1}(0,0)$ in powers of ω after analytic continuation. It is easy to see that $Q(\omega+i0^+)=Q'(\omega)-iQ''(\omega)$ with

$$Q'(\omega)=\kappa\omega\mathcal{P}\int_0^\infty d\epsilon\frac{\sqrt{\epsilon}\tanh[(\epsilon-\mu)/2T_c]}{2(\epsilon-\mu)(\omega-2\epsilon+2\mu)},$$

$$Q''(\omega)=\kappa 2^{-3/2}\pi(2\mu+\omega)^{1/2}\tanh(\omega/4T_c)\Theta(2\mu+\omega),$$

where $\kappa=N(\epsilon_F)/\sqrt{\epsilon_F}$. A low frequency ($\omega\ll T_c$) expansion of Q is possible both in the BCS and Bose limits, where the condition $\omega\ll|\mu|$ is automatically satisfied. Note, however, that for the intermediate coupling a_s^* for which $\mu(T_c)=0$ the expansion breaks down since $\omega=0$ coincides with the branch point of $\Gamma(\mathbf{q}=0,z)$. This then corresponds to a singular point in the evolution from Cooper pairs to composite bosons where an energy scale $\mu(T_c)$ goes through zero. An analytical inspection of the pole structure of $\Gamma^{-1}(\mathbf{q},z)$ indicates that $1/a_s^*>0$; i.e., the coupling at which TDGL theory fails is always more attractive than the threshold for a two-body bound state in vacuum [8]. (See also Fig. 1, inset.) However, the condition $\Delta(T)\ll\omega$ together with $\omega\ll\min(T_c,|\mu(T_c)|)$ implies that our TDGL results are not valid in a small region about $\mu(T_c)=0$ where $|\mu|<\Delta$.

For $\Delta\ll\omega\ll\min(T_c,|\mu(T_c)|)$ the expansion $Q(\omega+i0^+)=-d\omega+\cdots$ yields

$$d=\sum_{\mathbf{k}}\frac{\tanh(\beta\xi_{\mathbf{k}}/2)}{4\xi_{\mathbf{k}}^2}+i\frac{\pi}{8}\kappa\beta\sqrt{\mu}\Theta(\mu). \tag{6}$$

Fourier transforming to $(\mathbf{x},t)$ we obtain the TDGL equation

$$\left(a+b|\Delta(\mathbf{x},t)|^2-\frac{c}{2m}\nabla^2-id\frac{\partial}{\partial t}\right)\Delta(\mathbf{x},t)=0, \tag{7}$$

where the coefficients are given above. We next discuss in detail the two analytically tractable limits.

In weak coupling, we find $a=N(\epsilon_F)\ln(T/T_c)$, $b=7\zeta(3)N(\epsilon_F)/8\pi^2T_c^2$, $c=7\zeta(3)N(\epsilon_F)\epsilon_F/12\pi^2T_c^2$, and $d=[i\pi N(\epsilon_F)/8T_c][1-i(2T_c/\pi\epsilon_F)]$. By rescaling the order parameter $\Psi=\sqrt{2c}\Delta$ one obtains the conventional TDGL equation with characteristic length scale $\xi(T)=\xi_0\varepsilon^{-1/2}$ and time scale $\tau(T)=\tau_0\varepsilon^{-1}$ with $\xi_0\simeq v_F/T_c$ ($\sim\xi_{\rm pair}$, the pair size), and $\tau_0\simeq 1/T_c$, where $\varepsilon=|T-T_c|/T_c\ll 1$. The width of the Ginzburg region is $(T_c/\epsilon_F)^4$. The dynamics of Ψ is overdamped reflecting the continuum of fermionic excitations into which a pair can decay. There is in addition an $O(T_c/\epsilon_F)$ propagating part since the model is not particle-hole symmetric [12].

As the coupling increases, we see from (6) that the coefficient of the propagating piece grows while that of the damped part diminishes. Beyond the singular point at $\mu(T_c)=0$, an essentially propagating mode is obtained. The fermionic excitations now have a gap in the normal state, and the damping of the bosonic mode is ignored at this level of approximation [13]. In the extreme strong coupling limit $d=\pi N(\epsilon_F)/8\sqrt{\epsilon_F|\mu|}$ with $\mu\simeq -E_b/2$, and defining $\Psi_0=\sqrt{d}\Delta$ we can rewrite (7) as $-\tilde{\mu}\Psi_0+U|\Psi_0|^2\Psi_0-(2M)^{-1}\nabla^2\Psi_0-i\partial_t\Psi_0=0$. This is simply the Gross-Pitaevski equation for a dilute gas of bosons of mass $M=2m$ with a repulsive interaction $U=4\pi a_b/M$ characterized by a (boson) scattering length $a_b=2a_s>0$ with $n_b a_b^3 \ll 1$, where $n_b=n/2\sim k_F^3$ (in terms of the k_F of the constituent fermions).

The chemical potential of the bosons controls the phase transition via the change in sign of $\tilde{\mu}=E_b-2|\mu|$. The prefactors of the divergent length and time scales at this transition are given by $\xi_0 \simeq k_F^{-1}/\sqrt{k_F a_s} \gg \xi_{\rm pair} \simeq a_s$ and $\tau_0 \simeq T_c^{-1}/k_F a_s$, respectively. These are both much longer than the microscopic scales because of the diluteness condition $k_F a_s \ll 1$. Consequently, the Ginzburg region ($\varepsilon \ll k_F a_s$) is again small in strong coupling.

We have also extended the analysis to the broken symmetry state [6]. For $T \ll T_c$ Gaussian fluctuations make only a small correction to the saddle point results even for strong coupling, since the nontrivial saddle point already includes the nonperturbative effects of bound state formation and condensation (in marked contrast to the normal state results). In addition to recovering the ground state crossover [1], we have also studied the collective modes. Unlike the regime close to T_c with its singular point when $\mu(T_c)=0$, a well-defined TDGL equation is obtained for all couplings at $T=0$ [14]. Using this we find that the Anderson-Bogoliubov mode in the BCS limit evolves smoothly into the Bogoliubov sound mode for the dilute Bose gas. Note that the repulsion between bosons discussed above is crucial for the collective mode spectrum.

We have studied the crossover from Cooper pairs to composite bosons in a 3D Fermi system with attractive interactions. The functional integral approach was shown to lead to useful approximations for all couplings and temperatures, even in the absence of a small parameter. Our results demonstrate the importance of quantum (temporal) fluctuations in the intermediate and strong coupling normal state [15]. An accurate treatment of these fluctuations is therefore crucial for a full understanding of the deviations [4] from Fermi liquid behavior with increasing coupling.

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[8] As a function of g, $1/a_s$ increases monotonically from $-\infty$ for $g\rightarrow 0^+$ to $+\infty$ for $g\rightarrow\infty$. Beyond the two-body bound state threshold in vacuum ($1/a_s=0$), a_s is the "size" of this bound state with binding energy $E_b=1/ma_s^2$; see Ref. [3].

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[10] The result is quite different for lattice fermions. In the $U<0$ Hubbard model for $|U|/t\gg 1$ the bosons have an effective mass U/t^2 thus leading to a strong coupling $T_c\sim t^2/U$. See, e.g., R. Micnas, J. Ranninger, and S. Robaszkiewicz, Rev. Mod. Phys. **62**, 113 (1990).

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[13] Even in a purely bosonic system the dynamics of the order parameter will be damped sufficiently close to T_c [see P. Hohenberg and B. I. Halperin, Rev. Mod. Phys. **49**, 435 (1977), Sec. VI E]. Our analysis, however, is restricted to be valid only outside the critical region.

[14] In this case a nonzero Δ precludes a vanishing energy scale and the low frequency expansion of the effective action is well defined for all couplings.

[15] Our 3D results also shed light on the difficulties faced by analytical calculations of the crossover problem in 2D [S. Schmitt-Rink, C. M. Varma, and A. Ruckenstein, Phys. Rev. Lett. **63**, 445 (1989); A. Tokumitu, K. Miyake, and K. Yamada, Prog. Theor. Phys. Suppl. **106**, 63 (1992)]. While incorporating the temporal fluctuations one is also forced to include the spatial ones, which at the Gaussian level destroy long range order in 2D.