The effect of different 3-D QED vertex ansaetze on critical coupling

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Abstract

We study the semi-metal/insulator phase transition in graphene using a Schwinger-Dyson approach. We consider various forms of vertex ansaetze to truncate the hierarchy of Schwinger-Dyson equations. We define a Ball-Chiu type vertex that truncates the equations without violating gauge invariance. We show that there is a family of these vertices, parametrized by a continuous parameter that we call $a$, all of which satisfy the Ward identity. We have calculated the critical coupling of the phase transition using different values of $a$. We have also tested a common approximation in which only the first term in the Ball-Chiu ansatz is included. This vertex is independent of $a$, and, although it is not gauge invariant, it has been used many times in the literature because of the numerical simplifications it provides. We have found that, with a one-loop photon polarization tensor, the results obtained for the critical coupling from the truncated vertex and the full vertex with $a = 1$ agree very well, but other values of $a$ give significantly different results. We have also done a fully self-consistent calculation, in which the photons are backcoupled to the fermion degrees of freedom, for one choice $a = 1$. Our results show that when photon dynamics are correctly taken into account, it is no longer true that the truncated vertex and the full Ball-Chiu vertex with $a = 1$ agree well. The conclusion is that traditional vertex truncations do not really make sense in a system that does not respect Lorentz invariance, like graphene, and the need to include vertex contributions self-consistently is likely inescapable.

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I. INTRODUCTION

Graphene has been studied by many physicists since its discovery, in part because of its technological applications, and also because of its interest to theorists. The lattice structure of graphene produces a fermion dispersion relation that is linear near the lowest energies, called Dirac points. The low energy dynamics is well described by a continuum quantum field theory called reduced QED in which the electronic quasi-particles have a linear dispersion relation and are restricted to move in the two-dimensional plane of the graphene sheet, while the photons are free to move in three dimensions [1, 2].

The coupling constant in the effective theory is dimensionless and non-perturbatively large, which is part of the reason that graphene is interesting to theorists. Several different methods are available to study non-perturbative systems. In this paper we use Schwinger-Dyson (SD) equations, one of the most commonly used continuum non-perturbative approaches, and study some issues that arise when the method is applied to study graphene.

For a given theory, the SD equations provide a coupled infinite hierarchy of integral equations for non-perturbative dressing functions that describe the modification of the bare theory by the interactions. The set of equations has to be truncated in a way that respects gauge invariance, and includes the essential physics that is relevant to the problem at hand. The truncated equations involve a coupled set of dressing functions, each of which has support on a three or four-dimensional momentum phase space. In the case of graphene, the number of dressing functions is larger than in standard QED because the condition $v_F \neq c$ breaks Lorentz invariance. The number of dressing functions increases further in an anisotropic situation, where the $x$ and $y$ eigenvalues of the Fermi velocity tensor differ.

SD equations cannot be solved analytically, and numerical solutions are noto-
riously difficult to obtain. For this reason, many different approximations are in common use. In this paper we discuss these approximations, and the different motivations and justifications for each. We explore their relative importance, with particular emphasis on the choice of the vertex ansatz that is used to truncate the SD equations. We focus on the critical coupling at which graphene goes through a quantum phase transition from a semi-metal state to an insulating state. The value of this coupling is of great interest because the ability to produce an insulating state would have enormous significance in the development of graphene based electronic devices.

The Ball-Chiu (BC) ansatz was introduced 40 years ago \[3, 4\] and has been used in many calculations in Lorentz invariant theories to truncate the SD equations in a way that preserves gauge invariance. The low energy effective theory that describes graphene is not Lorentz invariant, and we therefore use a modification of the conventional BC vertex that truncates the SD equations of this theory without violating gauge invariance. We show that for the theory we use to describe graphene, there is no unique way to construct a BC-type vertex using only the contraint that the Ward identity must be satisfied. There is a family of ansaetze, parametrized by a continuous parameter that we call $a$, all of which satisfy the Ward identity. Our calculations show that the value of the critical coupling for the phase transition depends fairly strongly on the choice of the parameter $a$. This result shows that a correct formulation of the calculation will likely require self-consistently determined vertex functions.

We emphasize that the value of the critical coupling produced by any calculation based on an effective theory is not expected to be exact, since there are potentially important screening effects that are necessarily ignored. The point of this work is to explore the validity of the SD approach in the context of graphene and determine directions for future work.
We work in Euclidian space throughout this paper. We use the notation $P_\mu = (p_0, \vec{p})$, $P^2 = p_0^2 + \vec{p}^2$, and similarly for other momentum variables. We define $Q = K - P$ and use the shorthand $dK = dk_0 dk_1 dk_2 / (2\pi)^3$. We use natural units: $\hbar = c = 1$.

II. NOTATION

The bare Feynman rules for the low energy effective theory we use to describe graphene (in covariant gauge) are

\[ S^{(0)}(P) = -\left[i\gamma_\mu M_{\mu\nu} P_\nu \right]^{-1} \]
\[ G^{(0)}_{\mu\nu}(P) = \left[ \delta_{\mu\nu} - \frac{P_\mu P_\nu}{P^2} (1 - \chi) \right] \frac{1}{2\sqrt{P^2}} \]
\[ \Gamma^{(0)}_\mu = M_{\mu\nu} \gamma_\nu \]

(1)

where $M = (1, v_F, v_F)_{\text{diag}}$. The photon propagator for reduced QED is obtained by integrating out momentum modes perpendicular to the plane of the graphene sheet [1, 2]. It corresponds to a nonlocal action because the photon propagates outside the plane of the graphene sheet. The inverse dressed propagators are defined as

\[ S^{-1} = S^{(0)}^{-1} + \Sigma \]  
\[ G^{-1} = G^{(0)}^{-1} + \Pi_{\mu\nu} \]  

(2)

(3)

where $\Sigma$ and $\Pi_{\mu\nu}$ are the fermion self-energy and photon polarization tensor.

These dressing functions can be decomposed using a set of projection operators, each of which is multiplied by a different scalar function. The theory that describes graphene involves more dressing functions than standard QED, because the (non-unity) Fermi-velocity breaks Lorentz invariance. In standard QED the fermion self-energy can be written $\Sigma = -i(A - 1) \slash{P} + D$ where the functions $A$ and $D$ are
momentum dependent dressing functions that reduce to $A = 1$ and $D = 0$ in a bare massless theory. The photon polarization tensor can be written as the product of a four-dimensionally transverse projection operator and one dressing function, as $\Pi_{\mu\nu} = (\delta_{\mu\nu}P^2 - P_\mu P_\nu)\bar{\Pi}$. To describe graphene, these expressions must be modified. For electrons in graphene, the self-energy is defined as

$$\Sigma = -i\gamma^\mu M_{\mu\alpha}(F_{\alpha\nu} - \mathbb{I}_{\alpha\nu})P_\nu + D$$

where $F = (Z, A, A)_{\text{diag}}$. It is easy to see that in the limit $v_F = 1$ and $Z = A$, equation (4) reduces to the conventional covariant expression. The photon polarization tensor in graphene is written in terms of two dressing functions, which correspond to coefficients of two projection operators. These two projectors are transverse and longitudinal with respect to the momentum three-vector, while both are four-dimensionally transverse as required by gauge invariance. The three components of the fermion self-energy (equation (4)) satisfy integral equations that are calculated by taking the appropriate projections of its SD equation. In the limit $v_F \ll 1$ the contribution of the three-dimensionally transverse component of the photon propagator to all three components of $\Sigma$ is suppressed by a factor $v_F^2$, and the only component of the photon propagator that is needed to calculate the fermion dressing functions is

$$G_{00} = \delta_{\mu0}\delta_{\nu0}G_{\mu\nu} = \frac{p^2}{P^2} \frac{1}{2\sqrt{P^2} + \frac{p^2}{P^2}\Pi_{00}}. \quad (5)$$

This means that only one component of the polarization tensor needs to be calculated, which leaves a total of four dressing functions ($Z, A, D, \Pi_{00}$).

The effect of an anisotropic fermi velocity has been considered by several authors. The motivation is that anisotropy could reduce the critical coupling and make the insulating state easier to realize. One introduces an additional fermion dressing
function, so that the function $A$ gets replaced by two functions $A_1$ and $A_2$. The definition of the fermion self-energy is obtained from (4) using $M = (1, v_1, v_2)_{\text{diag}}$ and a non-diagonal definition of the matrix $F$ of the form

$$F = \begin{pmatrix} Z & 0 & 0 \\ 0 & A_1 & A_2 \\ 0 & -A_2 & A_1 \end{pmatrix}. \quad (6)$$

We define the fermi-velocity $v_F = \sqrt{v_1 v_2}$, the anisotropy parameter $\eta = v_1/v_2$, and the coupling $\alpha = e^2/(4\pi v_F)$. The naive definition $F = (Z, A_1, A_2)_{\text{diag}}$ does not reproduce the isotropic result in the limit $v_1 = v_2 = v_F$; furthermore, the naive diagonal definition renormalizes the anisotropy, while the correct form renormalizes the Fermi velocity (and principle axes) but not the anisotropy \cite{5}.

The conclusion to date is that anisotropy likely increases the critical coupling \cite{5–7}. However, the most sophisticated calculations that have so far been done rely on a vertex ansatz that is not fully gauge invariant (see discussion below). One of the goals of this paper is to determine how reliable this kind of vertex ansatz is.

III. SCHWINGER-DYSON EQUATIONS

The SD integral equations for the fermion self-energy and photon polarization tensor are

$$\Sigma(p_0, \vec{p}) = e^2 \int dK G_{\mu\nu}(q_0, \vec{q}) M_{\mu\tau} \gamma_{\tau} S(k_0, \vec{k}) \Gamma_{\nu} \quad (7)$$

$$\Pi_{\mu\nu}(p_0, \vec{p}) = -e^2 \int dK \text{Tr} [S(q_0, \vec{q}) M_{\mu\tau} \gamma_{\tau} S(k_0, \vec{k}) \Gamma_{\nu}] \quad (8)$$

where $\Gamma_{\mu}$ is a three-point function that will be discussed below. As discussed in section \cite{11} in the limit $v_F \ll 1$ we need only the zero-zero component of the photon
propagator and photon polarization tensor. We discuss below two further approximations that can be applied to the photon propagator.

1. The Coulomb approximation means that the frequency dependence of the bare propagator is dropped. This is a very common approximation, especially in the condensed matter community, and is motivated by the idea that the photon velocity is much greater than the fermion velocity. The zero-zero component of the photon propagator in equation (5) becomes

\[ G_{00}^{\text{coulomb}} = \frac{1}{2\sqrt{p^2 + \Pi_{00}}}. \]  

(9)

2. The one-loop approximation means that the function \( \Pi_{00} \) is replaced by the result of a one-loop calculation where the integrand is constructed with bare lines and vertices. This is also a common approximation and is motivated by the vanishing fermion density of states at the Dirac points. The one-loop result for the zero-zero component of the polarization tensor is

\[ \Pi_{00}^{\text{1loop}}(p_0, \vec{p}) = \frac{\pi \alpha}{v_F} \frac{p^2 v_F^2}{\sqrt{P_{\mu} M_{\mu \rho} M_{\rho \nu} P_{\nu}}}. \]  

(10)

Next we discuss the vertex function \( \Gamma_\mu \) that appears in equations (7, 8). The full hierarchy of SD equations provides an integral equation for this vertex function in terms of a four-point function. As is well known, the coupled nature of the equations requires that some truncation is introduced. The equation for the three-vertex is extremely difficult to solve, and therefore we will use an ansatz that expresses this vertex in terms of the fermion dressing functions, so that the two equations (7, 8) form a closed set. The BC vertex [3, 4] is constructed to satisfy the Ward identity, which
in our notation is written $-iQ_{\mu}\Gamma_\mu(P, K) = S^{-1}(P) - S^{-1}(K)$, and truncates the SD equations without violating gauge invariance. In general there are components of the vertex which are transverse (give zero when contracted with $Q_{\mu}$) which cannot be determined from gauge invariance. Various modifications of the BC vertex that include transverse contributions have been used in QED \[8–10\]. The BC vertex can be generalized to a Lorentz non-invariant system in a straightforward way. The authors of \[11\] used the ansatz

$$\Gamma_\mu(P, K) = \frac{1}{2} \left[ F(p_0, \vec{p}) T_{\mu\alpha} + F(k_0, \vec{k}) T_{\mu\alpha} \right] M_{\alpha\beta} \gamma_\beta$$

(11)

motivated by the idea that this is the simplest extension of the BC vertex that satisfies the Ward identity. However, it is easy to see that the ansatz in (11) will satisfy the Ward identity if the factor multiplying the square bracket is changed as

$$\frac{(P + K)_\mu}{P^2 - K^2} \to \frac{\tilde{M}(a)_{\mu\lambda} \tilde{M}(a)^{\lambda\nu}(P + K)_\nu}{(PMMP - K\tilde{M}MK)}$$

(12)

where $\tilde{M}(a)_{\mu\nu} = (1, a, a)_{\text{diag}}$ and $a$ is any real number, and we have used the short-hand notation $PMMP = P_\mu \tilde{M}(a)_{\mu\lambda} \tilde{M}(a)_{\lambda\nu} P_\nu$ (and likewise for $K$). The original ansatz in (11) corresponds to $\tilde{M}(1) = I$. A more natural choice might be $\tilde{M}(v_F) = M$. Any value of $a$ is equally valid from the point of view of gauge invariance.

In many SD calculations the term in square brackets in (11) is dropped. This is usually called the BC$_1$ approximation for the vertex:

$$\Gamma_\mu^{\text{Short}}(P, K) = \frac{1}{2} \left[ F(p_0, \vec{p}) T_{\mu\alpha} + F(k_0, \vec{k}) T_{\mu\alpha} \right] M_{\alpha\beta} \gamma_\beta.$$  

(13)

This expression does not satisfy the Ward identity, but is numerically much easier to work with. The point is that the denominator $1/(P^2 - K^2) = 1/(p^2_0 + p^2 - k^2_0 - k^2)$
has singularities along a curve in the domain of the integral over \((k_0, k)\) for which 
\[ P^2 - K^2 = 0. \] These singularities are integrable, but they are difficult to deal with numerically. We can also see that the square bracket in (11) will go to zero at 
\( (p_0 = k_0, p = k) \), and perhaps other places along the curve defined by the equation 
\[ P^2 = K^2. \] The non-perturbative fermion dressing functions do not have simple symmetry properties that would allow us to identify the curves along which the square bracket in the BC vertex is zero. We note that in a Lorentz invariant calculation, where the fermion dressing functions depended on only one variable, the cancellation of the zeros in the numerator and denominator occur at one easily identifiable point in the domain of the integral. The integrals obtained using a non-covariant BC vertex are numerically much more difficult to calculate, and we further expect that some choices of the value of \( a \) could be numerically more stable than others. We point out that the authors of [11] (using the value \( a = 1 \)) found that dropping the second term in (11) had virtually no effect on the critical coupling that was obtained from the calculation. It therefore seems possible that the issue described above could have no practical significance. In fact it turns out that results can be strongly dependent on the value of the parameter \( a \).

The full set of SD equations are calculated by substituting equations (9, 10, 11, 12) into (7, 8), multiplying by the appropriate projection operators, and contracting over all indices. The procedure is straightforward but very lengthy. All calculations were done using FORM [12]. The results, for \( a = 1 \), are given in Appendix A.

IV. RESULTS

To explore the dependence of the critical coupling on the value of \( a \), we begin by adopting a very simple approximation in which all fermion dressing functions other than \( D \) are set to their bare values \( Z = A = 1 \). We also use the Coulomb approxima-
tion and the one-loop photon polarization tensor instead of self-consistently solving the photon SD. These approximations are known to give unrealistically large values for the critical coupling. The point of these calculations is only to test the effect of the value of $a$ in the simplest possible way. Figure 1 shows that reducing $a$ reduces the critical coupling, and the dependence is fairly strong. In Table I we give the critical coupling for each value of $a$. The second number in the bracket indicates the error for each result. The numerical method we use to find a value of the critical coupling and its error is explained in Appendix B.

![Graph showing the condensate as a function of the coupling](image)

**FIG. 1:** The condensate as a function of the coupling, from a calculation including only one dressing function.

| $a$     | 1/300  | 1/100  | 1/75   | 1/50   |
|---------|--------|--------|--------|--------|
| $\alpha_c$ | (0.74, 0.09) | (2.22, 0.17) | (2.94, 0.11) | (4.41, 0.14) |

**TABLE I:** The critical couplings for different values of $a$, obtained from the results shown in figure 1.

Next we solve the coupled set of equations for all three fermion dressing functions.
but again using the Coulomb approximation and the one-loop approximation for the photon self-energy. In figure 2 we show the results for three choices of the parameters \((a, \eta)\). The figure shows once again that the form of the vertex ansatz has a significant effect on the critical coupling, in fact, larger than the shift in the critical coupling obtained by introducing anisotropy. However, the direction is the opposite of what we saw in figure 1 - reducing \(a\) increases the critical coupling. We also comment that values of \(a\) smaller than \(1/50\) do not converge without using a huge number of lattice points, (see section III for a discussion of this point). The corresponding results for the critical coupling are shown in Table II.

![Graph](image)

**FIG. 2:** The condensate as a function of the coupling using the vertex in equations (11, 12). The red curve is \((a, \eta) = (1, 1)\), orange is \((a, \eta) = (1, 0.3)\), and blue is \((a, \eta) = (1/50, 1)\).

| \((a, \eta)\) | (1,1)     | (1,0.3)   | (1/50,1)  |
|----------------|-----------|-----------|-----------|
| \(\alpha_c\)   | (2.999, 0.068) | (3.814, 0.073) | (4.204, 0.029) |

**TABLE II:** The critical couplings for different values of \((a, \eta)\) from the results shown in figure 2.
Another important thing to check is the effect of using the one-loop approximation for the polarization tensor. The polarization tensor should be determined self-consistently from its integral equation, which is given in the last line of equation (A3). In [13] it was found, using the BC$_1$ vertex in equation (13), that the effect of using a self-consistently determined photon polarization tensor reduced the coupling fairly dramatically (from 3.19 to 1.99). Figure 3 shows $D(0)$ versus $\alpha$ for the approximate BC$_1$ vertex, and the full BC vertex with $a = 1$, in both cases with and without the one-loop approximation for the polarization tensor. The figure shows that when the photon degrees of freedom are backcoupled, the result from the approximate vertex does not agree well with the full BC vertex. The corresponding results for the critical coupling are shown in Table III.

![Figure 3: The condensate versus the coupling using the BC$_1$ vertex, and the full BC vertex with $a = 1$, with and without backcoupling.](image)

|       | BC backcoupled | BC$_1$ backcoupled | BC 1-loop | BC$_1$ 1-loop |
|-------|----------------|-------------------|-----------|---------------|
| $\alpha_c$ | (1.782, 0.065) | (2.085, 0.037) | (3.19, 0.19) | (3.199, 0.092) |

TABLE III: The critical couplings for the data shown in figure 3.
V. CONCLUSIONS

We have studied the semi-metal/insulator phase transition in graphene by solving a set of coupled Schwinger-Dyson equations. The full set of equations is numerically prohibitively difficult to solve, and for this reason many different approximations are common in the literature. We have studied the effect of some of these approximations, with particular emphasis on possible choices of the ansatz for the three-point vertex function, which is introduced to truncate the hierarchy of SD equations. We have shown that there is no unambiguous way to extend the definition of the Ball-Chiu vertex for a theory in which Lorentz invariance is broken, like graphene. There is a family of vertices, parametrised by a continuous variable (that we call $a$), all of which satisfy the Ward identity. Our calculations show that the value of the critical coupling depends strongly on the value of $a$. The conclusion is that to predict the critical coupling, one must include a true non-perturbative three-vertex. This could be done either by truncating the SD equations by introducing some ansatz for the four-point function, or using a three-particle reducible (3PI) effective action approach. We note that one advantage of working with the 3PI effective action is that all truncations occur at the level of the action, which means that gauge invariance is automatically preserved to the level of the truncation [14, 15]. While it is true that the renormalization of NPI actions is a notoriously difficult problem [16, 17], the issue becomes largely trivial for a theory defined in less than four dimensions, like graphene. A 3PI effective action approach might be a promising method to study phase transitions in graphene when starting from a continuum field theory.
Appendix A: The SD equations

The SD equations for an anisotropic theory, obtained with a BC vertex ansatz are given in equation (A3). These expressions were calculated from equations (7, 8) by defining the appropriate projection operators and contracting over Lorentz and Dirac indices. All calculations were done using FORM [12]. The denominator of the fermion propagator is written

\[
S_p = p_0^2 Z_p^2 + v_1^2 (p_1 A_1 + p_2 A_2)^2 + v_2^2 (p_2 A_{2p} - p_1 A_{2p})^2 + D_p^2.
\]  

The subscript \(D\), for each dressing function, indicates a difference function defined as, for example

\[
Z_D = \frac{Z_P - Z_K}{P_\mu \tilde{M}(a)_{\mu\rho} M(a)_{\rho\nu} + K_\mu \tilde{M}(a)_{\mu\rho} M(a)_{\rho\nu} K_\nu}
\]  

and similarly for all fermion dressing functions. In the integral equation for \(\Pi_{00}\) we used the notation \(Z_{QD}\) to indicate the function in equation (A2) with \(P\) replaced by \(Q\), and similarly for the other fermion dressing functions. The subscript \(S\) represents the sum of two dressing functions, for example \(Z_S = Z_P + Z_K, Z_{SQ} = Z_Q + Z_K\), etc. We note that all dependence on the parameter \(a\) appears in equation (A2), and all dependence on the anisotropy parameter is in equation (A1). The parameter \(\chi\) should be set to zero to obtain the equations that correspond to the truncated vertex in equation (13), and one otherwise. The isotropic limit corresponds to \(\eta = 1\) and
\[ A_2 = 0. \]

\[
Z(P) = 1 + 2\alpha v_F \int \frac{dK}{S_k} q^4 \frac{(k_0 Z_K ((k_0 + p_0)^2 \chi Z_D + Z_S) + 2D_D \chi D_K (k_0 + p_0))}{2p_0 (Q^2)^{3/2}} \left(2q^2 + \sqrt{Q^2 \Pi_Q^{00}}\right)
\]

\[
A_1(P) = 1 - 2\alpha v_F \int \frac{dK}{S_k} \frac{q^4}{2p^2 (Q^2)^{3/2}} \left(2q^2 + \sqrt{Q^2 \Pi_Q^{00}}\right) \left(A_{2K} (k_2 p_1 - k_1 p_2) ((k_0 + p_0)^2 \chi Z_D + Z_S) + \right.
\]

\[
+ A_{1K} \bar{k} \cdot \bar{p} \left((k_0 + p_0)^2 \chi Z_D + Z_S\right) + 
\]

\[
k_0 (-\chi) (k_0 + p_0) Z_K \left(A_{2D} (k_2 p_1 - k_1 p_2) + A_{1D} \left(\bar{k} \cdot \bar{p} + p^2\right)\right)
\]

\[
A_2(P) = 2\alpha v_F \int \frac{dK}{S_k} \frac{q^4}{2p^2 (Q^2)^{3/2}} \left(2q^2 + \sqrt{Q^2 \Pi_Q^{00}}\right) \left(k_0 (-\chi) (k_0 + p_0) Z_K (A_{2D} (k \cdot p + p^2)
\]

\[- (k_2 p_1 - k_1 p_2) A_{1D}) + A_{2K} k \cdot p (\chi Z_D (k_0 + p_0)^2 + Z_S) - (k_2 p_1 - k_1 p_2) A_{1K} (\chi Z_D (k_0 + p_0)^2
\]

\[+ Z_S)\right)
\]

\[
D(P) = 2\alpha v_F \int \frac{dK}{S_k} \frac{q^4 (D_K (\chi Z_D (k_0 + p_0)^2 + Z_S) - 2D_D k_0 \chi (k_0 + p_0) Z_K)}{q^2 (Q^2)^{3/2}} \left(2Q^4 \Pi_Q^{00}\right)
\]

\[
\Pi_{00}(P) = -16\alpha v_F \int \frac{dK}{S_k S_q} 2\chi D_K D_Q (k_0 + q_0)^2 Z_{DQ} - 2k_0 q_0 \chi (k_0 + q_0)^2 Z_K Z_Q Z_{DQ} - 
\]

\[
4k_0 \chi D_Q D_{DQ} (k_0 + q_0) Z_K - 4q_0 \chi D_K D_{DQ} (k_0 + q_0) Z_Q + 2D_K D_Q Z_{SQ} - 2k_0 q_0 Z_K Z_Q Z_{SQ}\right).
\]

(A3)

**Appendix B: Numerics**

In this section we give a brief summary of the main aspects of our numerical procedure.

All integrations were done using a Gauss-Legendre method. We used spherical coordinates, so that there are two independent variables \((p_0, |\vec{p}|)\) and three integration variables \((k_0, |\vec{k}|, x = \hat{p} \cdot \hat{k})\). The \(k_0\) and \(k\) integrations were done on a logarithmic scale to increase sensitivity to the small momentum part of the phase space where the dressing functions change most. Interpolations were done using a combination of
linear interpolation, in regions where the function to be interpolated was fairly flat, and Pade approximates, in regions the function changed more sharply. Convergence was obtained with \((N_{p_0} = 30, N_p = 30)\) points in the external momentum space and \((N_{k_0} = 100, N_k = 100, N_x = 36)\) internal grid points. Adequate computational speed was acheived by parallelizing the code using MPI.

To calculate the critical coupling from a given set of data that gives the value of the condensate \(D(0)\) for different values of the coupling \(\alpha\), we use the following procedure. We invert the array to obtain a numerical representation of \(\alpha[D(0)]\), construct an interpolated function, and extrapolate to find the critical coupling \(\alpha_c \equiv \alpha[0]\). In all cases, the data that we need to interpolate is very smooth, and different interpolation methods give results for the critical coupling that agree to very high precision.

It is clear however that the accuracy of the result for the critical coupling does not depend on the accuracy of the interpolated function. For example, if the last three points on the blue curve in figure 2 were missing, the extrapolated critical alpha would be much too small. Numerically however, the last points are the most difficult to calculate because of the phenomena called critical slowing down, which occurs when the solution is very close to the trivial solution for which the dressing function \(D(p)\) is zero over its full domain. One way to quantify the error in the extrapolated result for the critical coupling would be to remove the last calculated point, and compare with the previous result. If the data stopped at a point where the curvature of the data was large, this would give a significantly different critical coupling. However, if the last few points in the data give a line that is fairly straight but not close to vertical, this procedure will indicate a small error even though the extrapolated critical alpha will not be very accurate. An alternative estimate is the absolute difference between the extrapolated result and the smallest value of \(\alpha\) in the data set. The error calculated this way is related to the inverse slope of the data at small \(\alpha\); it will be small if the curve drops steeply to the horizontal axis, and large
if the curve is fairly flat.

In all of the calculations we have done, the absolute difference of the extrapolated value and the smallest calculated value is larger than the error obtained by removing the last point, and all of the errors given in the results section are absolute difference errors. We also note that in this calculation the error is always positive, because the critical coupling produced by the extrapolation can only be smaller than the true critical coupling.

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