

Electron-electron interactions in the vacuum polarization of graphene

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We discuss the effect of electron-electron interactions on the static polarization properties of graphene beyond RPA. Divergent self-energy corrections are naturally absorbed into the renormalized coupling constant α . We find that the lowest-order vertex correction, which is the first nontrivial correlation contribution, is finite, and about 30% of the RPA result at strong coupling $\alpha \sim 1$. The vertex correction leads to further reduction of the effective charge. Finite contributions to dielectric screening are expected in all orders of perturbation theory.

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I. INTRODUCTION AND MOTIVATION

Graphene is a two-dimensional (2D) allotrope of carbon on a honeycomb lattice with one electron per π orbital (half filling). Its bare electronic spectrum is described in terms of a linearly dispersing, massless, chiral Dirac field ($\Psi_{\mathbf{p}}$). Since its isolation a few years ago¹ it was realized that graphene displays a number of unique properties that are at odds with the standard theory of metals.¹⁻³ One of the most important unresolved questions in graphene is the role of electron-electron interactions.⁴⁻¹² Even though, due to the vanishing of the density of states at the Fermi energy, the electron-electron interactions are expected to remain unscreened and strong; it is not clear what is their influence on the properties of graphene.

In the present work we study the influence of the electron-electron interactions on the static dielectric function of graphene at half filling. We perform calculations to one order beyond the conventional random-phase approximation (RPA) vacuum polarization bubble by including self-energy and vertex corrections into the polarization loop. Our main finding is that vertex contributions become important in the coupling regime $\alpha \sim 1$, which in turn means that other non-RPA contributions should also be included. We were mainly motivated by the question of whether the interactions can significantly affect the screening properties. This issue is particularly relevant in graphene for two reasons: (1) The effective coupling constant α (see the precise definition below) in graphene is large, $\alpha \sim 1$, and thus interactions are expected to be generically important, and (2) in spite of the above, to the best of our knowledge, no clear signatures of interaction effects have been observed so far in graphene. For example, measurements of the compressibility¹³ have not detected electron correlation effects. In addition, screening of external charged impurities introduced in graphene is also expected to be sensitive to interaction effects, at least on the theoretical level,¹⁴⁻¹⁷ and could be relevant for interpretation of recent experiments on charged impurity scattering.¹⁸ It is thus generally important to investigate the problem of how the correlations affect the effective charge of the carriers in graphene, which is determined by the vacuum polarization. We will assume that graphene at half filling (i.e., when the chemical potential crosses the Dirac point) remains a homogeneous gas of quasiparticles, which in itself is not necessar-

ily an innocent assumption due to the possibility of puddles, ripples, etc.³ However, we assume that the system is homogeneous as the importance of the above effects is still unsettled.

Our starting point is the low-energy Hamiltonian of graphene which can be written as (we use units such that $\hbar = 1$),

$$H = \sum_{\mathbf{p}} \Psi_{\mathbf{p}}^{\dagger} (v|\mathbf{p}| \hat{\sigma}_{\mathbf{p}} - \mu \hat{\sigma}_0) \Psi_{\mathbf{p}} + H_I, \quad (1)$$

where v is the Fermi velocity, μ is the chemical potential away from half filling, $\hat{\sigma}_0 = \hat{I}$ is the 2×2 identity matrix, $\hat{\sigma}_{\mathbf{p}} \equiv \hat{\sigma} \cdot \mathbf{p} / |\mathbf{p}| = (\hat{\sigma}_x p_x + \hat{\sigma}_y p_y) / |\mathbf{p}|^{-1}$, and $\hat{\sigma}_x, \hat{\sigma}_y$ are Pauli matrices. The first term in the Hamiltonian (1) reflects the effective Lorentz invariance that exists in the noninteracting problem at low energies and gives rise to bizarre electronic behavior analogous to the one found in quantum electrodynamics (QED).¹⁹

In Eq. (1), H_I is the electron-electron interaction,

$$H_I = \frac{1}{2} \sum_{\mathbf{p}} \hat{n}_{\mathbf{p}} V_{\mathbf{p}} \hat{n}_{-\mathbf{p}}, \quad \hat{n}_{\mathbf{p}} \equiv \sum_{\mathbf{q}} \Psi_{\mathbf{q}+\mathbf{p}}^{\dagger} \Psi_{\mathbf{q}}, \quad (2)$$

where

$$V_{\mathbf{p}} = \frac{2\pi e^2}{|\mathbf{p}|} \quad (3)$$

is the Fourier transform of the Coulomb potential in 2D. The relative strength of the Coulomb interactions to the kinetic energy is determined by graphene's "fine-structure constant" $\alpha \equiv e^2/v$. Unlike QED, the Dirac fermion velocity is much smaller than the speed of light c , and hence the Coulomb field can be treated as instantaneous ($v \approx 10^6$ m/s). As a result, the Coulomb interaction breaks the Lorentz invariance of the problem leading to fundamental differences between the graphene problem and QED. From now on we absorb the dielectric constant of the medium ϵ into the definition of the effective charge e . For example, in the typical case of graphene on a SiO₂ substrate with dielectric constant $\epsilon \approx 4$, we have $e^2 = 2e_0^2/(1+\epsilon)$, where e_0 is the charge of the electron. Keeping in mind that $e_0^2/v \approx 2.2$, one then finds the coupling constant $\alpha \approx 0.9$.²⁰ Nevertheless, even in this situation when the relation $\alpha \ll 1$ is not strictly satisfied, pertur-

bation theory is expected to give a good indication for the behavior of physical quantities.

The rest of the paper is organized as follows. Section II deals with corrections to the polarization loop arising from the dressing of the electron propagators. In Sec. III the true interaction (correlation) insertion, the vertex correction, is examined. Section IV contains our conclusions.

II. SELF-ENERGY CORRECTIONS TO THE POLARIZATION

We concentrate on the most interesting case of zero Fermi energy ($\mu \rightarrow 0$), when the low-energy physics is controlled by the proximity to the Dirac point.

The free Dirac Green's function is

$$\hat{G}(\mathbf{k}, \omega) = \frac{1}{\omega \hat{\sigma}_0 - v|\mathbf{k}| \hat{\sigma}_k + i \hat{\sigma}_0 0^+ \text{sign}(\omega)}. \quad (4)$$

The interaction effects lead to the dressed Green's function $\hat{G}^{-1} \rightarrow \hat{G}^{-1} - \hat{\Sigma}$, where the self-energy $\hat{\Sigma}$ is a sum of two terms with different matrix structure: $\hat{\Sigma} = \hat{\Sigma}_0 + \hat{\Sigma}$, $\hat{\Sigma}_0 \propto \hat{\sigma}_0$, $\hat{\Sigma} \propto \hat{\sigma}_k$. At Hartree-Fock (HF) level (first order in α) a divergent contribution appears, due to the long-range nature of the Coulomb interaction⁴ where $\Lambda \sim 1/a \gg k$ is an ultraviolet cutoff (a is the lattice spacing). One finds

$$\hat{\Sigma}^{(1)}(|\mathbf{k}|) = (\alpha/4)(v|\mathbf{k}|) \hat{\sigma}_k \ln(\Lambda/|\mathbf{k}|), \quad (5)$$

which implies that the effective velocity changes $v \rightarrow v[1 + (\alpha/4)\ln(\Lambda/|\mathbf{k}|)]$, and grows without bound at low energies $|\mathbf{k}|/\Lambda \rightarrow 0$. This should in principle lead to anomalies in thermodynamic and spectral properties of graphene.^{4,21} From a theoretical viewpoint, most importantly, the single logarithmic behavior was found to persist to second order of perturbation theory as well,⁶ and consequently this is expected to be the case to all orders, reflecting the fairly simple (at least at weak coupling) renormalization structure of the theory.

We now turn to the calculation of the static polarization, $\Pi(\mathbf{q}) \equiv \Pi(\mathbf{q}, \omega=0)$. The frequency variable in $\Pi(\mathbf{q})$ is omitted from now on. The bare polarization bubble (without any interaction lines in the loop) is known to be

$$\Pi^{(0)}(\mathbf{q}) = -i \sum_{\mathbf{k}} \int \frac{d\omega}{2\pi} \text{Tr}\{\hat{G}(\mathbf{k}, \omega) \hat{G}(\mathbf{k} + \mathbf{q}, \omega)\} = -|\mathbf{q}|/(4v). \quad (6)$$

From now on the trace stands for summation over spin (s), valley (v), and pseudospin (Pauli matrix σ) indices, i.e.,

$$\text{Tr} = \sum_{s,v} \text{Tr}_{\sigma} = 4 \text{Tr}_{\sigma}. \quad (7)$$

The momentum sums are performed as $\sum_{\mathbf{k}} = \int d^2k / (2\pi)^2$.

Next, we calculate the bubble dressing due to the electron-electron interactions to first order in α . The two diagrams at this order are shown in Fig. 1. We write the total polarization as

$$\Pi(\mathbf{q}) = \Pi^{(0)}(\mathbf{q}) + \Pi^{(1)}(\mathbf{q}) + \Pi^{(2)}(\mathbf{q}), \quad (8)$$

where $\Pi^{(1)}$ and $\Pi^{(2)}$ stand for the contributions of Fig. 1(a) and Fig. 1(b), respectively.

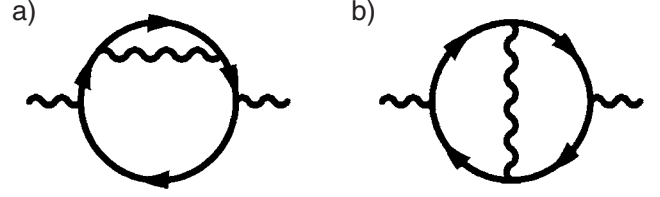


FIG. 1. First-order interaction corrections to the polarization bubble. (a) Self-energy correction and (b) vertex correction. The explicit form of these diagrams is given by Eqs. (9) and (19). The wavy line represents the Coulomb interaction, Eq. (3).

The self-energy dressing of Fig. 1(a) can be written as (the factor of 2 originates from the two possible insertions)

$$\begin{aligned} \Pi^{(1)}(\mathbf{q}) = & -2i \sum_{\mathbf{k}} \int \frac{d\omega}{2\pi} \text{Tr}\{\hat{G}(\mathbf{k}, \omega) \hat{G}(\mathbf{k} + \mathbf{q}, \omega) \\ & \times \hat{G}(\mathbf{k}, \omega) \hat{\Sigma}(\mathbf{k}, \omega)\}. \end{aligned} \quad (9)$$

At lowest order, the self-energy is simply the Hartree-Fock one, meaning that in Eq. (9) we replace

$$\hat{\Sigma}(\mathbf{k}, \omega) \rightarrow \hat{\Sigma}^{(1)}(\mathbf{k}) = i \sum_{\mathbf{p}} \int \frac{d\omega_1}{2\pi} \hat{G}(\mathbf{p}, \omega_1) V_{\mathbf{k}-\mathbf{p}}. \quad (10)$$

The large logarithm present in $\hat{\Sigma}^{(1)}(\mathbf{k})$ at low momenta, Eq. (5), is expected to appear also in some form in $\Pi^{(1)}(\mathbf{q})$.

Let us define the following quantities which appear in our results from now on:

$$\Delta(\mathbf{k}, \mathbf{q}) \equiv 1 - \frac{\hat{\mathbf{k}} \cdot (\mathbf{k} + \mathbf{q})}{|\mathbf{k} + \mathbf{q}|}, \quad \hat{\mathbf{k}} \equiv \mathbf{k}/|\mathbf{k}|, \quad (11)$$

$$E(\mathbf{k}, \mathbf{q}) \equiv v(|\mathbf{k}| + |\mathbf{k} + \mathbf{q}|). \quad (12)$$

After performing the frequency, and then momentum integrations in Eq. (9), and using the self-energy from Eq. (10), we obtain

$$\begin{aligned} \Pi^{(1)}(\mathbf{q}) = & 4 \sum_{\mathbf{k}, \mathbf{p}} V_{\mathbf{k}-\mathbf{p}} (\hat{\mathbf{k}} \cdot \hat{\mathbf{p}}) \frac{\Delta(\mathbf{k}, \mathbf{q})}{[E(\mathbf{k}, \mathbf{q})]^2} \\ = & \frac{\alpha}{16} \frac{|\mathbf{q}|}{v} \ln(\Lambda/|\mathbf{q}|), \quad \Lambda/|\mathbf{q}| \gg 1. \end{aligned} \quad (13)$$

This result means that the large logarithm in $\Pi^{(1)}(\mathbf{q})$ simply reflects the renormalization of the Fermi velocity, i.e., this divergence is not independent, but can be simply reabsorbed into the velocity by replacing $v \rightarrow v[1 + (\alpha/4)\ln(\Lambda/|\mathbf{q}|)]$ in the one-loop result $\Pi^{(0)}(\mathbf{q}) = -|\mathbf{q}|/(4v)$. Due to the simple logarithmic structure of the theory this is expected to hold to all orders of perturbation theory, i.e., all self-energy corrections lead to a replacement of the coupling α in all final expressions with the “running” coupling $\alpha(q)$, accounting for the velocity renormalization. We therefore assume that the velocity renormalization procedure is performed in all higher order diagrams. At finite small chemical potential $\mu \ll \Lambda$, which is the case in any realistic experimental situation, the divergence is cut off, $\ln(\Lambda/|\mathbf{q}|) \rightarrow \ln(\Lambda/\mu)$. Due to the slow

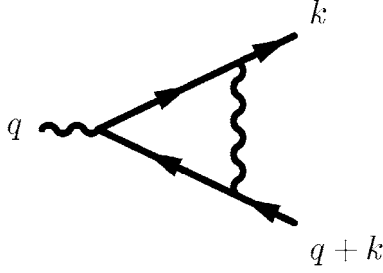


FIG. 2. First-order interaction correction to the vertex $\hat{\Gamma}(k;q)$, given by Eq. (14).

variation of the logarithmic function or possible other factors (such as strong dielectric screening), no significant variation of the velocity has been found in experiment.³

An interesting effect, related to the interaction contribution $\Pi^{(1)}(\mathbf{q})$, Eq. (13), was recently discussed in Ref. 16 within the renormalization group (RG) approach. Our calculation, leading to Eq. (13), provides an explicit perturbative confirmation of the RG results. If we imagine an external Coulomb impurity with charge $Z > 0$, probing the polarization of the vacuum, then the induced charge density, in momentum space, is $\rho_{\text{ind}}(\mathbf{q}) = ZV_{\mathbf{q}}\Pi(\mathbf{q})$. Here $\Pi(\mathbf{q}) = \Pi^{(0)}(\mathbf{q}) + \Pi^{(1)}(\mathbf{q})$. While the first term leads to induced charge $\rho_{\text{ind}}^{(0)}(\mathbf{q}) = -Z\alpha(\pi/2)$, localized in real space at the impurity site and with a screening sign, the interaction term $\rho_{\text{ind}}^{(1)}(\mathbf{q}) = Z\alpha^2(\pi/8)\ln(\Lambda/|\mathbf{q}|)$ has an opposite sign and decays as an inverse power law ($1/r^2$, with logarithmic corrections). This peculiar behavior simply reflects, however, the renormalization (increase) of the Fermi velocity at low momenta, which leads to suppression of screening at large distances.

III. VERTEX CORRECTIONS TO THE POLARIZATION BUBBLE

We proceed with the calculation of the vertex correction in Fig. 1(b). Before evaluating this expression, it is useful to examine the (possible) singularity structure separately in the vertex operator, shown in Fig. 2. For simplicity we use the notation $\hat{\Gamma}(k;q)$ which stands for the more conventionally used form $\hat{\Gamma}(k, k+q; q)$, where the variables denote both frequency and momenta (q is the bosonic momentum/frequency).

Since the Coulomb interaction is nonretarded, we have the simple expression

$$\hat{\Gamma}(\mathbf{k}; \mathbf{q}, \omega) = i \sum_{\mathbf{p}} \int \frac{d\omega_1}{2\pi} \hat{G}(\mathbf{p}, \omega_1) \hat{G}(\mathbf{p} + \mathbf{q}, \omega_1 + \omega) V_{\mathbf{k}-\mathbf{p}}. \quad (14)$$

After evaluating the frequency integral, the result is a sum of off-diagonal and diagonal parts (with respect to the Pauli-matrix indexes) $\hat{\Gamma} = \hat{\Gamma}^{(o)} + \hat{\Gamma}^{(d)}$. More explicitly,

$$\hat{\Gamma}^{(o)}(\mathbf{k}; \mathbf{q}, \omega) \propto \sum_{\mathbf{p}} V_{\mathbf{k}-\mathbf{p}} (\hat{\sigma}_{\mathbf{p}} - \hat{\sigma}_{\mathbf{p}+\mathbf{q}}) \left(\frac{1}{E(\mathbf{p}, \mathbf{q}) + \omega} - \frac{1}{E(\mathbf{p}, \mathbf{q}) - \omega} \right). \quad (15)$$

We are interested only in the zero-frequency limit (and only in the real part of $\hat{\Gamma}$, since the imaginary part does not contribute to the polarization). In this case the off-diagonal piece vanishes identically, $\hat{\Gamma}^{(o)}(\mathbf{k}; \mathbf{q}, \omega=0) = 0$. This is expected to be the case since the Coulomb interaction is diagonal and thus the vertex cannot generate a static contribution with a different matrix structure. On the other hand the diagonal part is finite in the same limit

$$\hat{\Gamma}^{(d)}(\mathbf{k}; \mathbf{q}, \omega=0) \propto \sum_{\mathbf{p}} V_{\mathbf{k}-\mathbf{p}} (1 - \hat{\sigma}_{\mathbf{p}} \hat{\sigma}_{\mathbf{p}+\mathbf{q}}) \frac{1}{E(\mathbf{p}, \mathbf{q})}. \quad (16)$$

An explicit evaluation shows that $\hat{\Gamma}^{(d)}(\mathbf{k}; \mathbf{q}, \omega=0)$ does not have any divergent contributions. For example, at $|\mathbf{k}| \ll |\mathbf{q}|$,

$$\hat{\Gamma}^{(d)}(\mathbf{k}; \mathbf{q}, 0) \propto \alpha \text{ const}, \quad |\mathbf{k}| \ll |\mathbf{q}|, \quad (17)$$

while in the opposite limit

$$\hat{\Gamma}^{(d)}(\mathbf{k}; \mathbf{q}, 0) \propto \alpha (|\mathbf{q}|/|\mathbf{k}|), \quad |\mathbf{q}| \ll |\mathbf{k}|. \quad (18)$$

For our purposes the exact formulas are not important (we also do not show the dependence on the angle between \mathbf{k}, \mathbf{q}); our main conclusion at this stage is that the vertex does not have any divergent parts. We have also examined diagrams of higher order, such as “ladder” and “crossed” ladder vertex corrections, and have found that all of them are finite. Therefore the vertex insertions into the polarization function are expected to give a finite contribution to that quantity, and below we evaluate the lowest-order vertex correction numerically.

It is clear that a Ward identity relating divergent contributions in the self-energy and in the vertex does not hold here, unlike conventional QED where Lorentz (and gauge) invariance guarantees cancellation between vertex and self-energy corrections,²² and charge is renormalized only through simple polarization loops in the photon propagator. On the other hand, in graphene, where the only nontrivially renormalized quantity is the velocity v , both the polarization operator and the vertex operator do not show any independent divergencies.

The diagram of Fig. 1(b) now reads

$$\Pi^{(2)}(\mathbf{q}) = -i \sum_{\mathbf{k}} \int \frac{d\omega}{2\pi} \text{Tr} \{ \hat{G}(\mathbf{k}, \omega) \hat{\Gamma}(\mathbf{k}; \mathbf{q}, 0) \hat{G}(\mathbf{k} + \mathbf{q}, \omega) \}, \quad (19)$$

where the full expression for $\hat{\Gamma}$ from Eq. (14) should be used. An explicit calculation, starting by evaluation of the energy integrations, leads to the result

$$\Pi^{(2)}(\mathbf{q}) = -\frac{1}{4} \text{Tr} \sum_{\mathbf{k}, \mathbf{p}} V_{\mathbf{k}-\mathbf{p}} \frac{(1 - \hat{\sigma}_{\mathbf{p}+\mathbf{q}} \hat{\sigma}_{\mathbf{p}})(1 - \hat{\sigma}_{\mathbf{k}} \hat{\sigma}_{\mathbf{k}+\mathbf{q}})}{E(\mathbf{k}, \mathbf{q})E(\mathbf{p}, \mathbf{q})}. \quad (20)$$

Taking into account

$$\hat{\sigma}_{\mathbf{k}} \hat{\sigma}_{\mathbf{p}} = \frac{1}{|\mathbf{k}||\mathbf{p}|} [\mathbf{k} \cdot \mathbf{p} + i\hat{\sigma}_3(\mathbf{k} \times \mathbf{p})_z], \quad (21)$$

where $(\mathbf{p} \times \mathbf{q})$ stands for a vector product, we then arrive at the final formula

$$\Pi^{(2)}(\mathbf{q}) = -2 \sum_{\mathbf{k}, \mathbf{p}} \frac{V_{\mathbf{k}-\mathbf{p}}}{E(\mathbf{k}, \mathbf{q})E(\mathbf{p}, \mathbf{q})} \left\{ \Delta(\mathbf{k}, \mathbf{q})\Delta(\mathbf{p}, \mathbf{q}) + \frac{(\mathbf{p} \times \mathbf{q})_z(\mathbf{k} \times \mathbf{q})_z}{|\mathbf{p}||\mathbf{k}||\mathbf{p}+\mathbf{q}||\mathbf{k}+\mathbf{q}|} \right\}. \quad (22)$$

It is clear on dimensional grounds that $\Pi^{(2)}(\mathbf{q})$ is linear in $|\mathbf{q}|$. This is in fact the case for polarization diagrams in all orders of perturbation theory. The four-dimensional integrals, appearing in Eq. (22), cannot be evaluated analytically. We have found, as expected in light of our previous discussion of the vertex function, that the expressions converge in the ultraviolet limit. After computing the integrals numerically, we obtain the following result for the combination $V_{\mathbf{q}}\Pi^{(2)}(\mathbf{q})$, which appears in the dielectric function,

$$\frac{2\pi e^2}{|\mathbf{q}|} \Pi^{(2)}(\mathbf{q}) = -0.53\alpha^2. \quad (23)$$

Adding also the one-loop RPA result, we have finally (where \mathcal{E} is the static dielectric constant, defined by the formula below)

$$V_{\mathbf{q}}^{\text{eff}} = \frac{V_{\mathbf{q}}}{1 - V_{\mathbf{q}}\Pi(\mathbf{q})} = \frac{V_{\mathbf{q}}}{\mathcal{E}}, \quad (24)$$

$$\mathcal{E} = 1 + \frac{\pi}{2}\alpha + 0.53\alpha^2 + O(\alpha^3). \quad (25)$$

We conclude that, at $\alpha \sim 1$, the vertex correction is more than 30% of the one-loop result. It also has a screening sign, i.e., it reduces the effective charge. One also expects that finite contributions will appear to all orders in α . However, resummation of perturbation theory by simple means seems impossible, as the contributions in question are finite and accumulate over a wide range of momenta in the corresponding diagrams (rather than within a specific integration window, from where divergent parts typically originate, and thus can be easily collected). Even though the vertex contribution is a sizable one, two remarks are in order: (1) It does not change drastically the structure of the theory, apart from con-

tributing toward further screening of the interactions, and (2) the fact that perturbation theory is used with the intention of being applied at a rather strong coupling is in itself questionable. Nevertheless, perturbation theory provides a clear indication that a significant contribution to screening exists beyond the conventional one-loop RPA result. On the other hand, in the weak-coupling regime, $\alpha \ll 1$, RPA is parametrically well justified as far as the static polarization properties are concerned (although the RPA is not justified for the self-energy⁶).

IV. DISCUSSION AND CONCLUSIONS

It is also useful to compare our results to the situation in ordinary metals with a finite Fermi surface. Certain approximations are typically used to account for vertex corrections, such as the Hubbard form of the dielectric function. When extrapolated to low momentum, the vertex contribution tends to decrease the screening length,²³ i.e., it reduces further the range of the interactions. Naturally in graphene, where the screening length is infinite (for the case of zero chemical potential considered here), the vertex correction affects directly the effective charge, without changing the shape of the Coulomb potential.

Finally we mention two recent related works, discussing interaction effects, that appeared while the present paper was being prepared. In Ref. 24, the effect of self-energy and vertex corrections to lowest order (α) on the minimal conductivity in graphene was discussed, with the conclusion that the corrections are of order 1%. Dynamical polarization properties were studied in Ref. 25, where the vertex diagrams were found to have logarithmically singular contributions near the threshold $\omega \sim vq$, leading to the possibility of a plasmon mode.

In summary, we have shown that vertex corrections can have a sizable effect on the static vacuum polarization diagrams in the regime of strong coupling, while for small coupling their importance diminishes parametrically. The self-energy corrections are naturally absorbed into the renormalization of the Fermi velocity. The non-RPA vertex diagram at lowest order of perturbation theory was found to decrease the effective charge, meaning that in principle, correlation effects at higher order must also be taken into account. Thus the ultimate asymptotic behavior of the static polarization function for $\alpha \sim 1$ remains an open problem.

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