

Velocity renormalization in graphene from lattice Monte Carlo

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We compute the Fermi velocity of the Dirac quasiparticles in clean graphene at the charge neutrality point for strong Coulomb coupling α_g . We perform a Lattice Monte Carlo calculation within the low-energy Dirac theory, which includes an instantaneous, long-range Coulomb interaction. We find a renormalized Fermi velocity $v_{FR} > v_F$, where $v_F \simeq c/300$. Our results are consistent with a momentum-independent v_{FR} which increases approximately linearly with α_g , although a logarithmic running with momentum cannot be excluded at present. At the predicted critical coupling α_{gc} for the semimetal-insulator transition due to excitonic pair formation, we find $v_{FR}/v_F \simeq 3.3$, which we discuss in light of experimental findings for v_{FR}/v_F at the charge neutrality point in ultra-clean suspended graphene.

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1. Introduction

Graphene, a two-dimensional membrane of carbon atoms with unique electronic properties, is characterized by a low-energy spectrum of Dirac quasiparticles, with a Fermi velocity $v_F \simeq 1/300$ of the speed of light in vacuum [1, 2]. As the strength of the Coulomb interaction between the quasiparticles is controlled by $\alpha_g \equiv e^2/(4\pi\epsilon v_F) \simeq 2.2/\epsilon$, the role of interactions can be enhanced to the point that graphene may resemble Quantum Electrodynamics (QED) in a strongly coupled regime [3]. In particular, the unscreened, long-range Coulomb interaction in graphene leads to non-trivial velocity renormalization effects. At weak coupling, a logarithmic running $v_F(n)/v_F(n_0) = 1 + (\alpha_g/4) \ln(n_0/n)$ with carrier density n is found [4], such that v_{FR} is expected to become large in the vicinity of the Dirac point ($n = 0$). On the experimental side, logarithmic velocity renormalization is most prominent in ultra-clean suspended graphene [6] and on boron nitride (BN) substrates [7], with $v_{FR}/v_F \simeq 2 - 3$ in the former case, where $\epsilon = 1$.

Electron-electron interactions may also trigger a semimetal-insulator transition due to excitonic pairing of quasiparticles and holes at a critical coupling α_{gc} . For graphene, Lattice Monte Carlo (LMC) has been applied to the Dirac theory using a contact Thirring interaction [8] and a long-range Coulomb interaction [9–11], and to the tight-binding Hamiltonian using interactions of the Hubbard [12–14] and Coulomb [15–17] types. For the Dirac theory, $\alpha_{gc} \simeq 1.11 \pm 0.06$ was found [9], to be compared with $\alpha_{gc} \simeq 0.9 \pm 0.2$ in the tight-binding + Coulomb approach [16]. While such a transition has not yet been observed, the empirical $v_{FR}/v_F \simeq 2 - 3$ in suspended graphene is indicative of interaction-induced spectral changes [3, 6].

2. Lattice Monte Carlo

The LMC treatment of graphene uses the linearized low-energy Hamiltonian [18, 19] with an instantaneous Coulomb interaction, such that $A_\mu \equiv (A_0, \vec{0})$. This gives the Euclidean (continuum) action

$$S_E \equiv \frac{1}{2g^2} \int d^3x dt (\partial_i A_0)^2 + \sum_{a=1}^{N_f} \int d^2x dt \bar{\psi}_a D[A_0] \psi_a, \quad (2.1)$$

where $g^2 \equiv e^2/\epsilon$, with $\epsilon \equiv (1 + \kappa)/2$ for a substrate with dielectric constant κ . Here, ψ_a is a four-component Dirac field in $2 + 1$ dimensions with $\bar{\psi} \equiv \psi^\dagger \gamma_0$, A_0 is the gauge (photon) field in $3 + 1$ dimensions, and $N_f = 2$ for a graphene monolayer. The Dirac operator is

$$D[A_0] = \gamma_0(\partial_0 + iA_0) + v_F \sum_{k=1}^2 \gamma_k \partial_k + m_0, \quad (2.2)$$

where the γ_μ satisfy the Euclidean Clifford algebra $\{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu}$, and the bare fermion mass m_0 provides an infrared regulator for modes that would be massless when the $U(2N_f)$ chiral symmetry of Eq. (2.1) is spontaneously broken. The lattice version of Eq. (2.1) is formulated in terms of “staggered” fermions, *i.e.* one-component Grassmann variables $\chi, \bar{\chi}$, which partially retain the $U(2N_f)$ chiral symmetry of Eq. (2.1) at finite lattice spacing (for staggered fermions in odd dimensions, see Ref. [20]). The fermionic part of Eq. (2.1) is given for $N_f = 2$ in terms of staggered fermions by $\sum_{\mathbf{n}, \mathbf{m}} \bar{\chi}_{\mathbf{n}} K_{\mathbf{n}, \mathbf{m}}[\theta_0] \chi_{\mathbf{m}}$, where $\mathbf{n} \equiv (n_0, n_1, n_2) = (t, x, y)$ and \mathbf{m} denote lattice sites on

a 2 + 1 dimensional fermion “brane”. This square space-time lattice embedded in a cubic lattice should not be understood as a tight-binding theory. The staggered Dirac operator is

$$K_{\mathbf{n},\mathbf{m}}[\theta_0] = \frac{1}{2a}(\delta_{\mathbf{n}+\mathbf{e}_0,\mathbf{m}}U_{0,\mathbf{n}} - \delta_{\mathbf{n}-\mathbf{e}_0,\mathbf{m}}U_{0,\mathbf{m}}^\dagger) + \frac{\lambda}{2a}\sum_i \eta_{\mathbf{n}}^i(\delta_{\mathbf{n}+\mathbf{e}_i,\mathbf{m}} - \delta_{\mathbf{n}-\mathbf{e}_i,\mathbf{m}}) + m_0 \delta_{\mathbf{n},\mathbf{m}}, \quad (2.3)$$

where $\eta_{\mathbf{n}}^1 = (-1)^{n_0}$, $\eta_{\mathbf{n}}^2 = (-1)^{n_0+n_1}$, with \mathbf{e}_i a unit vector in lattice direction i . The invariance of Eq. (2.1) under spatially uniform, time-dependent gauge transformations is retained by the gauge links $U_0 \equiv \exp(i\theta_0)$. We perform LMC calculations for $v_F = 1$ (thus $g^2 \rightarrow g^2/v_F$) and $a/a_x = 1$, where $a \equiv a_t$ is the temporal lattice spacing, and thus $\lambda = 1$. At non-zero α_g , we have $\lambda_R \equiv v_{FR}(a/a_x)_R$ from which v_{FR}/v_F can be obtained, once the asymmetry $(a/a_x)_R$ is known.

We compute the renormalized λ_R and m_R from the staggered fermion propagator $C_f(t, x, y) \equiv \langle \chi(t, x, y) \bar{\chi}(t_0, x_0, y_0) \rangle = \langle K_{\mathbf{n},\mathbf{n}_0}^{-1} \rangle$ on an $N_x^2 \times N_t$ space-time lattice with $N_{x,t}/4$ integer. Here \mathbf{n}_0 is an arbitrary point of reference, and the brackets denote an average over ensembles of gauge field configurations, obtained as a function of $\beta \equiv v_F/g^2 = 1/(4\pi\alpha_g)$ and m_0 , with the Hybrid Monte Carlo algorithm. From $C_f(t, x, y)$, we form $C_{ft}(t, p_1, p_2) \equiv \sum_{x,y} \exp(-ip \cdot x) C_f(t, x, y)$, for momenta $p_i = 2\pi n/N_x$, with $n = -N_x/4, \dots, N_x/4$, $t = 0, \dots, N_t - 1$, and summation over even lattice sites, defined by $(-1)^{t+x+y} = 1$. The expression for the “temporal correlator” C_{ft}^R with renormalized m_R , λ_R and wave function renormalization Z_R (for $a = 1$) is [21]

$$C_{ft}^R(t, p_1, p_2) = Z_R G_t(p_1, p_2), \quad (2.4)$$

for $t = 0, 2, \dots, N_t - 2$, and

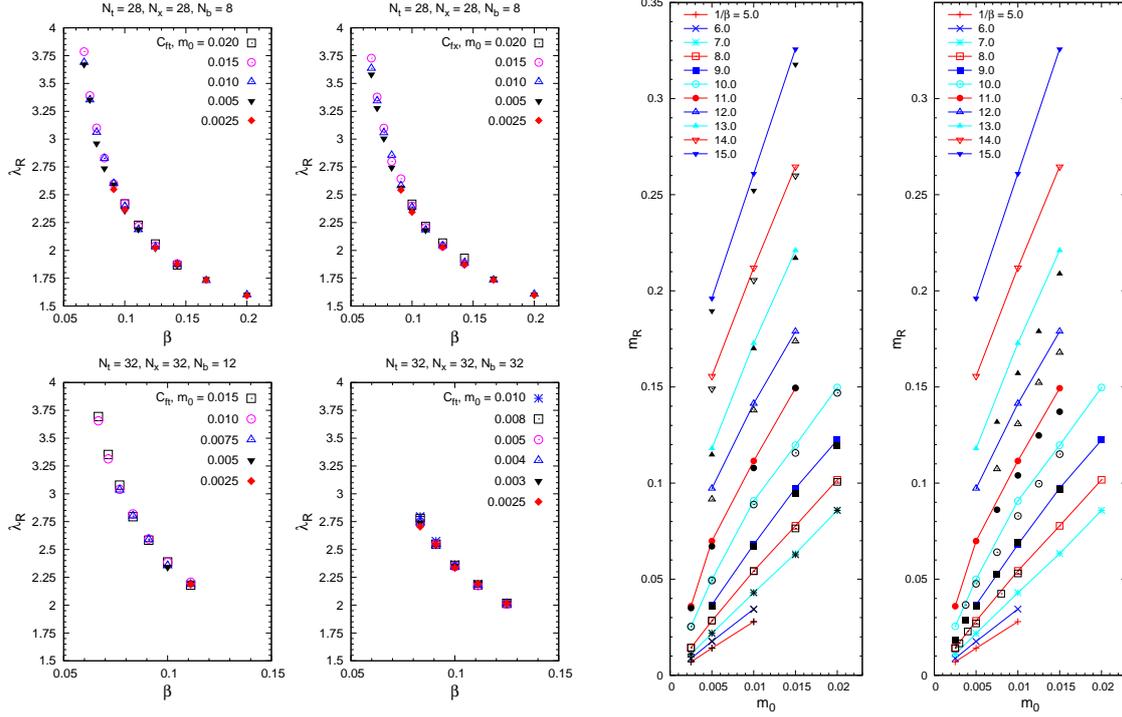
$$C_{ft}^R(t, p_1, p_2) = -\frac{Z_R}{2m_R} \left[\exp(iB_0) G_{t+1}(p_1, p_2) - \exp(-iB_0) G_{t-1}(p_1, p_2) \right], \quad (2.5)$$

for $t = 1, 3, \dots, N_t - 1$, with anti-periodic boundary conditions. The function $G_t(p_1, p_2)$ is

$$G_t(p_1, p_2) \equiv \frac{N}{C^2(\mu_t) - B^2(B_0)} \times \left[A(B_0)C(\mu_t) \cos(B_0 t^*) \sinh(\mu_t t^*) + B(B_0)D(\mu_t) \sin(B_0 t^*) \cosh(\mu_t t^*) + iA(B_0)C(\mu_t) \sin(B_0 t^*) \sinh(\mu_t t^*) - iB(B_0)D(\mu_t) \cos(B_0 t^*) \cosh(\mu_t t^*) \right], \quad (2.6)$$

where $A(x) \equiv \cos(xN_t/2)$, $B(x) \equiv \sin(xN_t/2)$, $C(x) \equiv \cosh(xN_t/2)$, $D(x) \equiv \sinh(xN_t/2)$, $t^* \equiv N_t/2 - t$, $N \equiv 2m_R/\sinh(2\mu_t)$, and $\sinh^2(\mu_t) \equiv m_R^2 + \lambda_R^2 \sin^2(p_1) + \lambda_R^2 \sin^2(p_2)$. This expression for C_{ft}^R includes a constant “background field” $B_0 \equiv \langle \theta_0 \rangle$, as $\langle \theta_0 \rangle \neq 0$ in a finite volume. B_0 is roughly bounded by $\pm\pi/N_t$ [21], and the imaginary part of C_{ft}^R vanishes for $B_0 \rightarrow 0$.

We also define the fermion “spatial correlator” $C_{fx}(x, \omega, p_2) \equiv \sum_{t,y} \exp(-ip \cdot x) C_f(t, x, y)$, for $\omega = 2\pi(n - 1/2)/N_t$ (due to the anti-periodic temporal boundary conditions), $n = -N_t/4, \dots, N_t/4$, spatial slices $x = 0, \dots, N_x - 1$, and summation over even lattice sites. The expression for C_{fx}^R can be inferred from C_{ft}^R . The function $G_x(\omega, p_2)$ is obtained from Eq. (2.6) by first exchanging $\sin \leftrightarrow \cos$, followed by $t \rightarrow x$, $N_t \rightarrow N_x$, $\mu_t \rightarrow \mu_x$ and $B_0 \rightarrow 0$. In addition, we have $m_R \rightarrow m_R/\lambda_R$ in Eq. (2.5), $m_R \rightarrow m_R/\lambda_R^2$ in the expression for N , and $\sinh^2(\mu_x) \equiv m_R^2/\lambda_R^2 + \sin^2(\omega + B_0)/\lambda_R^2 + \sin^2(p_2)$. Unlike Eqs. (2.4) and (2.5), C_{fx}^R is real-valued, with periodic boundary conditions.



(a) λ_R as a function of $\beta \equiv 1/(4\pi\alpha_g)$ and m_0 , as obtained from C_{ft} and C_{fx} on $28^3 \times 8$ (upper panels), $32^3 \times 12$ and 32^4 (lower panels) lattices. Note that the dependence on m_0 is negligible, and that the results obtained from C_{ft} and C_{fx} agree closely.

(b) Left panel: m_R as a function of $\beta^{-1} \equiv 4\pi\alpha_g$ and m_0 , obtained from C_{ft} (colored connected symbols) and C_{fx} (black unconnected symbols) on a $28^3 \times 8$ lattice. Right panel: m_R obtained from C_{ft} on $28^3 \times 8$ (colored connected symbols) and $32^3 \times 12$ lattices (black unconnected symbols).

Figure 1: LMC calculation of λ_R and m_R (for $a = 1$). All lines are intended as a guide to the eye, and statistical errors are comparable to the size of the symbols.

3. Results

In Fig. 1(a), we show λ_R as obtained from a chi-square fit of Eqs. (2.4) and (2.5) to LMC data. While Eq. (2.1) is gauge invariant, C_{ft} and C_{fx} are not, and thus a gauge fixing condition is imposed on each configuration in order to obtain stable results. For C_{ft} , a correlated fit is performed for all (t, p_1, p_2) , and in the case of C_{fx} for all (x, ω, p_2) . The fitted parameters are m_R , λ_R , B_0 and Z_R . Our lattices have $N_t = N_x$, and the length of the “bulk” dimension (where only the photons propagate) is denoted N_b . We use the notation $N_x^3 \times N_b$, and simply N_x^4 when $N_b = N_t = N_x$. On the $28^3 \times 8$ lattice, LMC data is available for (inverse) lattice couplings $5.0 \leq \beta^{-1} \leq 15.0$, and for bare quasiparticle masses $0.0025 \leq m_0 \leq 0.020$, with slightly more restrictive data sets on the $32^3 \times 12$ and 32^4 lattices. We find that λ_R increases monotonically as a function of α_g from the non-interacting value of unity, with no appreciable differences between λ_R as obtained from C_{ft} and C_{fx} . We find the dependence on m_0 to be almost negligible. Finite size effects for λ_R are small, and the fitted values of B_0 agree closely with $\langle \theta_0 \rangle$.

In Fig. 1(b), we show the physical quasiparticle mass m_R as a function of β^{-1} and m_0 , with emphasis on asymmetries between the temporal and spatial correlations, and on finite size effects.

As Eq. (2.1) treats space and time asymmetrically, the spatial and temporal correlation lengths ξ may exhibit unequal critical scaling, such that $\xi_s \propto |\beta - \beta_c|^{-\nu_s}$ and $\xi_t \propto |\beta - \beta_c|^{-\nu_t}$. The dynamical critical exponent $z \equiv \nu_t/\nu_s$ is an important characteristic of a quantum critical point (QCP), and implies that the dispersion relation is modified to $E \propto p^z$. At large N_f , Ref. [5] predicted $z \simeq 0.8$ for graphene in the strong-coupling limit. However, arguments have also been put forward which indicate $z = 1$ for a QCP with $d < 4$ in theories with a long-range Coulomb interaction [23]. From Fig. 1(b), we find that the values of m_R obtained from C_{ft} and C_{fx} agree very closely for $\beta^{-1} \leq 11.0$, which is consistent with $z \simeq 1$. We also find no sign of non-linear dispersion. A more accurate analysis is possible following Ref. [8], in terms of the equation of state (EOS)

$$m_0 = A(\beta - \beta_c) m_R^{(\delta \cdot \beta_m^{-1})/\nu_t} + B m_R^{\delta \cdot \beta_m/\nu_t}, \quad (3.1)$$

for m_R computed from C_{ft} , where δ and β_m are critical exponents characterizing the QCP at $\beta = \beta_c$. An analogous EOS with $\nu_t \rightarrow \nu_s$ can be given for m_R as obtained from C_{fx} . We also find from Fig. 1(b) that finite size effects are under control for $\beta^{-1} \leq 9.0$, but not for smaller β (stronger coupling), especially in the region of the phase diagram where a dynamically generated gap exists, and $\lim_{m_0 \rightarrow 0} m_R \neq 0$. In principle, Eq. (3.1) can be used to compute z and m_R in the limit $m_0 \rightarrow 0$, *i.e.* the gap in the quasiparticle spectrum. The lattice spacing asymmetry $(a/a_x)_R$ could then be inferred by measuring the gap in terms of temporal and spatial correlations. For reliable conclusions, such an EOS analysis should be combined with an extrapolation to infinite volume, similar to that of Ref. [22] for QED₄. For the present analysis, we note from Fig. 1(b) that the values of m_R computed from C_{ft} and C_{fx} differ by no more than $\simeq 10\%$ at the smallest values of β . Assuming this trend persists in the limits of infinite volume and vanishing m_0 , we find $1.0 \leq (a/a_x)_R \leq 1.1$ over the range of α_g studied. In the absence of substantial indications for $(a/a_x)_R \neq 1$, we take λ_R as a measure of v_{FR}/v_F .

4. Conclusions

In Fig. 2, we summarize our LMC results for v_{FR}/v_F as a function of $\alpha_g \equiv 1/(4\pi\beta)$, and compare with available experimental data. Throughout our analysis, we have assumed that v_{FR} is constant, while in reality we should expect it to run logarithmically with the momentum p and diverge at the Dirac point, according to $v_F(p)/v_F(p_0) = 1 + (\alpha_g/4) \ln(p_0/p)$, where p_0 is the momentum scale at which $v_{FR} = v_F$. At present, we cannot distinguish between this and the simpler expression $v_{FR}/v_F = 1 + C\alpha_g$, and much larger lattices appear to be required to detect a logarithmic running of the Fermi velocity with p . On the other hand, we find a pronounced dependence of v_{FR}/v_F on α_g . We find that v_{FR} increases linearly with α_g from the non-interacting value v_F up to $\alpha_g \simeq 0.5$, above which the increase becomes more rapid. At the predicted critical coupling $\alpha_{gc} \simeq 1.1$, we find $v_{FR}(\alpha_{gc})/v_F \simeq 3.3$ within our present linearized treatment of the velocity renormalization. Since all of the empirical $v_{FR}(p=0)/v_F$ fall short of this, we find a plausible explanation for the non-observation of excitonic insulating phases in graphene monolayers. We note that the result of Ref. [6] is tantalizingly close to $\simeq 3.3$, which suggests that further refinements in the quality of suspended graphene may suffice to trigger the excitonic instability. It would be of interest to study the logarithmic running of v_{FR} with momentum on larger lattices.

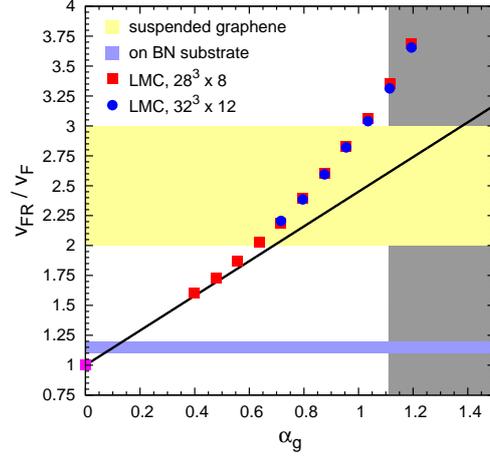


Figure 2: Plot of $v_{FR}(\alpha_g)/v_F$ for asymmetry $(a/a_x)_R \simeq 1$. The black line is $v_{FR}/v_F = 1 + C\alpha_g$, and the predicted insulating phase occurs for $\alpha_g > \alpha_{gc}$ (gray shaded area). We find a linear dependence of v_{FR}/v_F on α_g up to $\alpha_g \simeq 0.5$ (solid black line). Note that $v_{FR}(\alpha_g = 0)/v_F \equiv 1$. Horizontal bands indicate empirical data on $v_{FR}(p=0)/v_F$ from Ref. [6] (suspended graphene) and Ref. [7] (on BN substrate). Note that the expected logarithmic momentum-dependence of v_{FR}/v_F cannot be resolved on present lattices.

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