Graphene and graphene-type systems

Stability of Dirac liquids with strong Coulomb interaction

Dirac liquid is linear in momentum low-energy electronic spectrum (semimetallic state). Is it stable against the strong long-range part of Coulomb interaction? To suppress short-range correlations consider flat-top potential at short-range, \( V(r < 2a) = U(2a) \), and Coulomb otherwise.

Dimensionless parameter \( \epsilon_0 = e^2 f(0) / \epsilon F(0) = \sqrt{a} / (2 \pi a_0) \) (where \( a_0 \) is about 2.2 in suspended graphene).

Introduce effective coupling constant \( \alpha_{c} \alpha_{p} \), where \( \alpha_{c} \) is the Fermi velocity. 2d Dirac fermions cannot screen the Coulomb part and quasiparticle properties get strongly renormalized.

**Renormalization of \( \alpha_{l} \)**

The scale \( \alpha_{l} \) renormalizes to 0:

- 1st-order: \( \alpha_{c} \) renormalizes to 0
- 2nd-order: \( c \alpha_{l} > 0.8 \) RG flows towards strong coupling

A: With increasing the system size, the effective coupling \( \alpha_{l} \) always flows towards 0; i.e., the 2d Dirac liquid is an asymptotically free T=0 state (I. Tupitsyn and N. Prokof'ev, PRL 118, 026403 (2017)).

**BDMC**

The BDMC result in higher orders (BDMCn; BDMC1) converges to the DMRG answer.

- 2nd-order in \( \alpha_{l} = \alpha_{p} \)
- High-order expansion is required.

**Jellium model for electrons**

- Known issue with the GW approximation: Incorrect prediction of dielectric response, \( \varepsilon(\omega) = 1 - (4\pi e^2 / \hbar^2) \) \( \Pi(k, \omega) \).
- Key finding: At small momenta the polarization function is orders of magnitude larger than expected from \( n^2 / m^{1/2} \) and \( 4\pi e^2 / \hbar^2 \) \( \Pi(k, \omega) \) tends to diverge. The problem can be traced back to the fact that the GW approximation does not respect the dynamic particle number conservation law, implying that \( \Pi(k=0, \omega) \) should be constant (\( \Pi = \gamma (1 - V(k)) \) and \( \gamma (k=0, \omega) = (\varepsilon(0)) \n(0) \)).
- Workaround: Enforce physical behavior by performing simple transformation before calculating the dielectric response: \( \Pi(k, \omega) \rightarrow 1 \Pi(k, \omega) - \[1(0, \omega) + 1(0, 0) n_\omega \] + \) in higher orders calculations the correction term vanishes.

**Hydrogen chain**

- Equation of state in TDL, STO 6-31G basis

The BDMC result in higher orders (BDMC; BDMC \( = \) sc-GW(\( H^0 \)) \( \rightarrow \) DMRG answer.

- The difference between the two sc-GW answers can be used as an estimate of the method accuracy (see Figure).

Full interaction tensor and cut-offs: Dependence of interactions on two site differences \( u=(i, j) \) and \( v=(k, l) \) can be radially simplified \( u=0 \) and \( v=0 \) represent the “density-dipole” part of the interaction potential. We found that energies per atom obtained with unrestricted summation over \( (u, v) \) (in the Dyson equation for screened effective interaction \( W \)) and with \( u^2 + v^2 = 2 \) coincide at the level of \( \sim 10^3 \) even at the smallest values of lattice constant \( R \).

- Rigorous correction to sc-GW(\( H^0 \)) is needed.