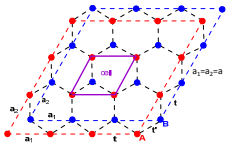
Systems with long-range forces

I.S. Tupitsyn, and N.V. Prokof'ev
University of Massachusetts, Amherst, USA

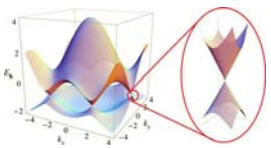
SIMONS FOUNDATION

Graphene and graphene-type systems

Honeycomb lattice



Bare dispersion with Dirac points



Hamiltonian: $U(r) \propto e^2/r$

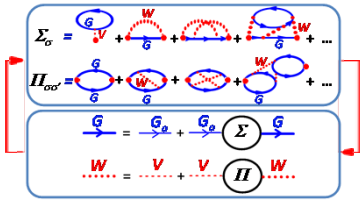
$$H_0 = -t \sum_{<ij>\sigma} (a^\dagger_{i\sigma} b_{j\sigma} + h.c.)$$

$$H_{int} = \frac{1}{2} \sum_{i,j,\sigma,\sigma'} U(|\mathbf{r}_i - \mathbf{r}_j|)\, n_{i\sigma} n_{j\sigma'}$$

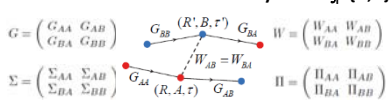
$$H_{SB} = \sum_{\sigma} m_\sigma \left(\sum_{i\in A} a^\dagger_{i\sigma} a_{i\sigma} - \sum_{i\in B} b^\dagger_{i\sigma} b_{i\sigma} \right)$$

Chiral symmetry breaking term

Skeleton diagrammatic representation



Each i^{th} vertex is characterized by index ξ_i={A,B}

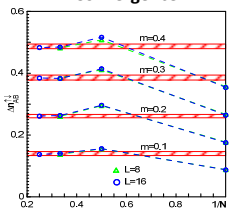


Benchmarking the BDMC technique: Semimetal-Insulator transition

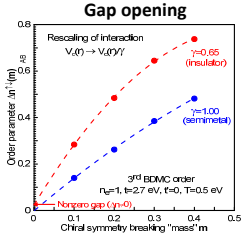
(against the Hybrid MC results: M.V. Ulybyshev et al, PRL 111, 056801 (2013))

Order parameter: $\Delta n^{\uparrow\downarrow}_{AB}(m) = (n^\uparrow_A - n^\downarrow_A) - (n^\uparrow_B - n^\downarrow_B)$

Convergence



Gap opening



To reproduce the Hybrid Monte Carlo results, we had to go to 3rd BDMC order (N=3); 1st order schemes (GW or RPA) are inadequate.

Stability of Dirac liquids with strong Coulomb interaction

Dirac liquid = 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 $\alpha_0 = e^2/v_F^{(0)}$, $v_F^{(0)} = \sqrt{3}at/2$ (α_0 is about 2.2 in suspended graphene).

Introduce effective coupling constant $\alpha = e^2/v_F$, *where* v_F is the Fermi velocity. 2d Dirac fermions cannot screen the Coulomb part and quasiparticle properties get strongly renormalized.

Q: Renormalization of $\alpha(l)$ with the scale of distance $l=ln(L/a)$?

Perturbation Theory

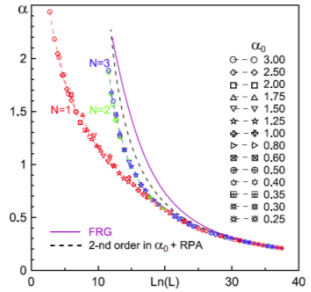
1st-order: α *renormalizes to 0 as* $\sim Ln^{-1}(L)$ *with system size L*

2nd-order: *at* $\alpha > \alpha_c \approx 0.8$ *RG flows towards strong coupling*

RPA: α *renormalizes to 0*

And the correct answer is … ? High-order expansion is required.

BDMC RG flow of α with system size L



A: With increasing the system size, the effective coupling α 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)).

Jellium model for electrons

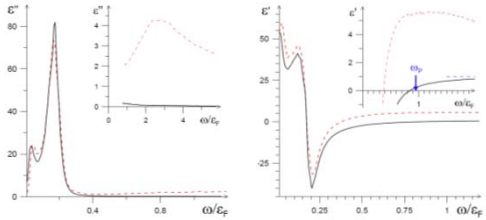
$$H = \sum_{i=1}^{N} \left\{ \frac{\mathbf{p}_i^2}{2m} - \mu \right\} + \sum_{i<j}^{N} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}$$ on the homogeneous positive background $n_+ = n_e$

Known issue with the GW approximation: Incorrect prediction of dielectric response, $\varepsilon(k, \omega) = 1 - (4\pi e^2/k^2)\,\Pi(k, \omega)$.

Key finding: At small momenta the polarization function is orders of magnitude larger than expected from $nk^2/m\omega_n^2$, and $(4\pi e^2/k^2)\Pi(k, \omega)$ 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 $\Pi(k=0,\tau)$ should be constant ($\Pi = -\chi/(1-V\chi)$ and $\chi(k=0,\tau) = \langle N(0)\, N(\tau)\rangle$).

Workaround: Enforce physical behavior by performing simple transformation before calculating the dielectric response: $\Pi(k, \omega_n) \rightarrow \Pi(k, \omega_n) - \Pi(0, \omega_n) + \Pi(0,0)\delta_{n,0}$. In higher orders calculations the correction term vanishes.

Result of correction (r_s=1, k/k_F=0.1, T/ε_F=0.02)



Analytical continuation of $\varepsilon(k,\omega_n)$. Red dashed line: original GW. Black solid line: corrected GW spectrum.

After correction, the high-frequency tail of Im ε(k, ω) = ε" gets suppressed by nearly two orders of magnitude and the plasmon mode gets correctly reproduced with 10% accuracy (K. Van Houcke, I.S. Tupitsyn, A.S. Mishchenko, and N.V. Prokof'ev, arXiv:1607.01183).

Hydrogen chain

$$H = -\sum_{i,j,\alpha,\beta,\sigma} t_{i,j}^{\alpha,\beta}(\sigma)\, a^\dagger_{i,\alpha,\sigma} a_{j,\beta,\sigma} + \frac{1}{2} \sum_{i,j,k,l} \sum_{\alpha,\beta,\gamma,\delta} \sum_{\sigma,\sigma'} U_{i,j,k,l}^{\alpha,\beta,\gamma,\delta}(\sigma,\sigma')\, a^\dagger_{i,\alpha,\sigma}\, a^\dagger_{k,\gamma,\sigma'} a_{l,\delta,\sigma'}\, a_{j,\beta,\sigma}$$

with $t_{i,j}^{\alpha,\beta}$ and $U_{i,j,k,l}^{\alpha,\beta,\gamma,\delta}$ being the hopping and bare interaction matrix elements in the chosen basis ({i,j,k,l} – site/atom indices; {α,β,γ,δ} – orbital indices; {σ,σ'} - spins).

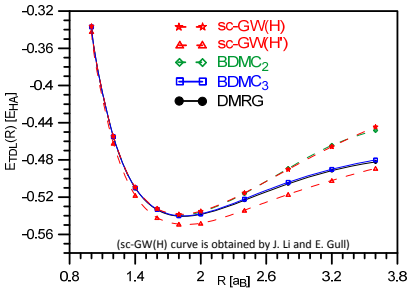
The configuration space of skeleton diagrams is sampled stochastically in BDMC, starting from vertex corrections to the sc-GW. The sc-GW result depends on **zero Hamiltonian terms that create or annihilate two electrons in the same state**. In **H'** these terms are explicitly dropped; **H** and **H'** have identical properties in exact solution.

H - "material science" choice; H' - lattice community approach

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 radically simplified (u=0 and v=0 represent the "density-density" 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*=v*=2 coincide at the level of ~10^{-5} even at the smallest values of lattice constant R.

Equation of state in TDL, STO-6G basis



The BDMC result in higher orders (BDMC$_n$; BDMC$_1$ ≡ sc-GW(H')) converges to the DMRG answer.

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