Prospects of Density-Potential Functional Theory for 2D Materials

Martin-I. Trappe[1,2] – **Shaffique Adam**[1,3]

[1] Centre for Advanced 2D Materials, NUS, Singapore
[2] Centre for Quantum Technologies, NUS, Singapore
[3] Yale-NUS College, Singapore

NUS National University of Singapore | Centre for Advanced 2D Materials

CQT | Centre for Quantum Technologies

Density-Potential Functional Theory

DPFT in position space

$$E[n,\mu] = E_{\text{kin}}[n] + \int (\mathrm{d}\boldsymbol{r})\, V_{\text{ext}}(\boldsymbol{r})\, n(\boldsymbol{r}) + E_{\text{int}}[n] + \mu \left(N - \int (\mathrm{d}\boldsymbol{r})\, n(\boldsymbol{r}) \right)$$

Legendre transform via $V(\boldsymbol{r}) = \mu - \dfrac{\delta E_{\text{kin}}[n]}{\delta n(\boldsymbol{r})}$ $\quad E_1[V-\mu] = E_{\text{kin}}[n] + \int (\mathrm{d}\boldsymbol{r})\, (V-\mu)\, n$

$$E[V,n,\mu] = E_1[V-\mu] + \int (\mathrm{d}\boldsymbol{r})\, (V_{\text{ext}} - V)\, n + E_{\text{int}}[n] + \mu N$$

Output: particle density of interacting system

Input: Noninteracting potential

→ Self-consistent ground-state solutions:

$$n(\boldsymbol{r}) = \frac{\delta E_1[V-\mu]}{\delta V(\boldsymbol{r})}$$

$$V(\boldsymbol{r}) = V_{\text{ext}}(\boldsymbol{r}) + \frac{\delta E_{\text{int}}[n]}{\delta n(\boldsymbol{r})}$$

$$N = \int (\mathrm{d}\boldsymbol{r})\, n(\boldsymbol{r})$$

Output: (effectively noninteracting) potential with interactions implicitly included

Suzuki-Trotter Approximations

$$E_1 = \mathrm{tr}\{(H-\mu)\Theta(\mu - H)\}$$

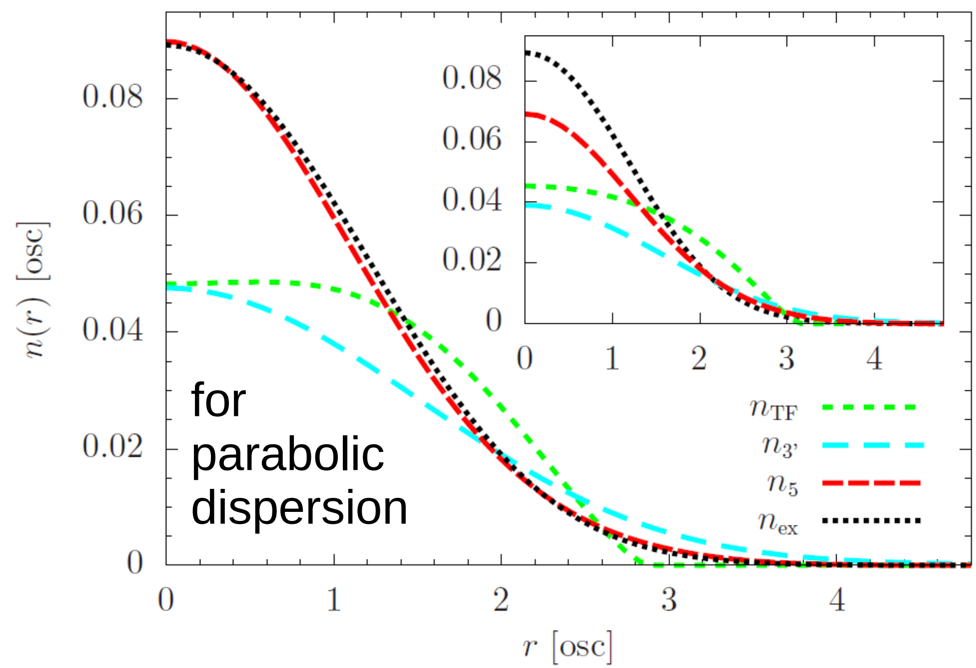
$$\Rightarrow n(\boldsymbol{r}) = \langle \boldsymbol{r} | \Theta(\mu - H) | \boldsymbol{r} \rangle$$

$$= \int_{-\infty}^{\mu} \mathrm{d}E \int \frac{\mathrm{d}t}{2\pi\hbar}\, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}E\,t} \langle \boldsymbol{r} | \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H\,t} | \boldsymbol{r} \rangle$$

n_{TF} from $\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H\,t} \approx \mathrm{e}^{-\frac{\mathrm{i}t}{\hbar}T}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}t\,V}$

$$\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H\,t} \approx \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\frac{t}{2}T}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}t\,V}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\frac{t}{2}T}$$

Hooke's atom   arXiv:1709.01719

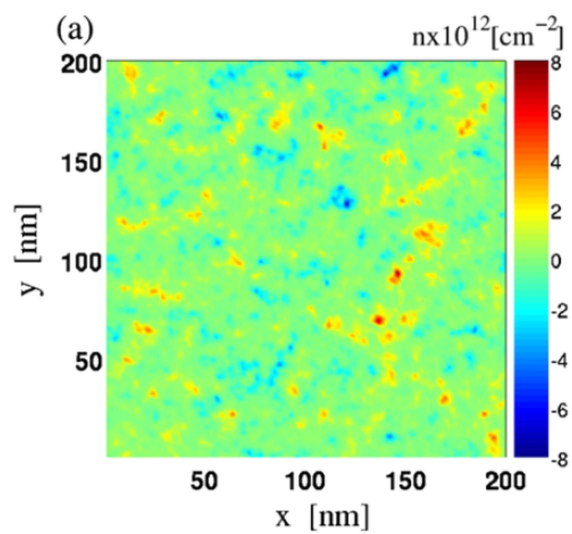


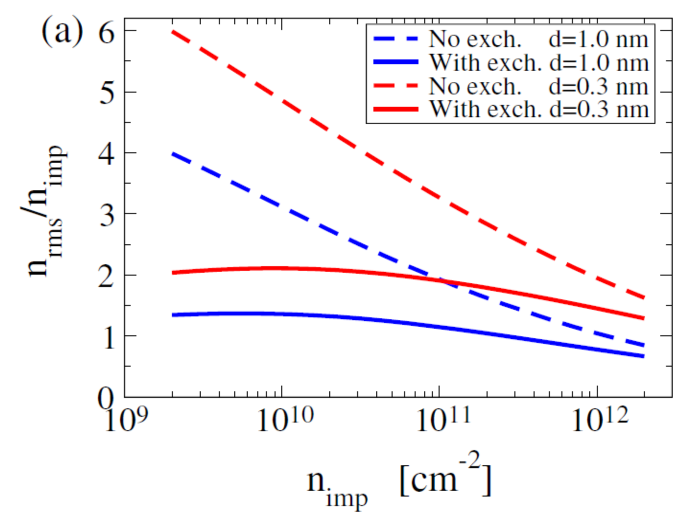
for linear dispersion:

$$n_{\mathrm{2D}}^{\mathrm{ST3}}(\boldsymbol{r}) = \int (\mathrm{d}\boldsymbol{r}')\, f\big(V(\boldsymbol{r}+\boldsymbol{r}')\big)\; {}_0F_1\big(2; g(V(\boldsymbol{r}+\boldsymbol{r}'), \boldsymbol{r}')\big)$$

Electron-Hole puddles in graphene
[TF + Quantum corrections]

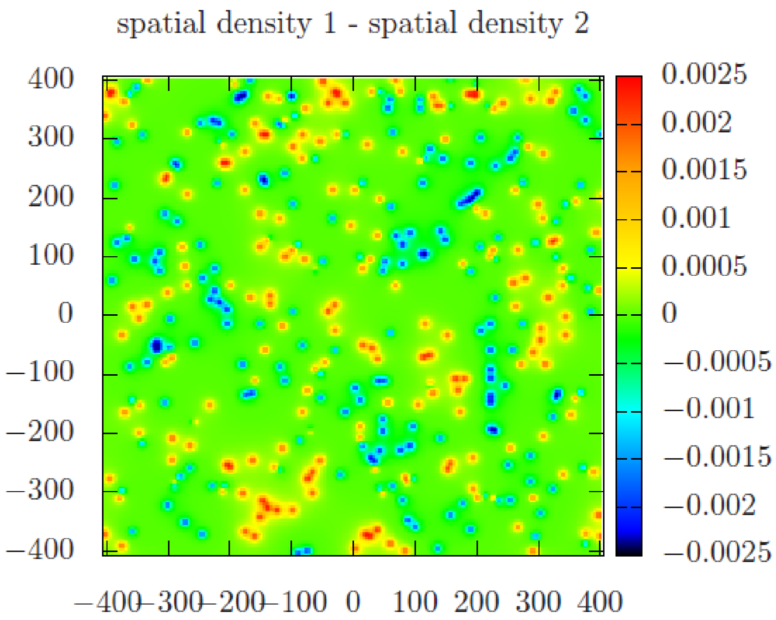
compare to Rossi, Das Sarma
PRL **101**, 166803 (2008)
[TF + Exchange]

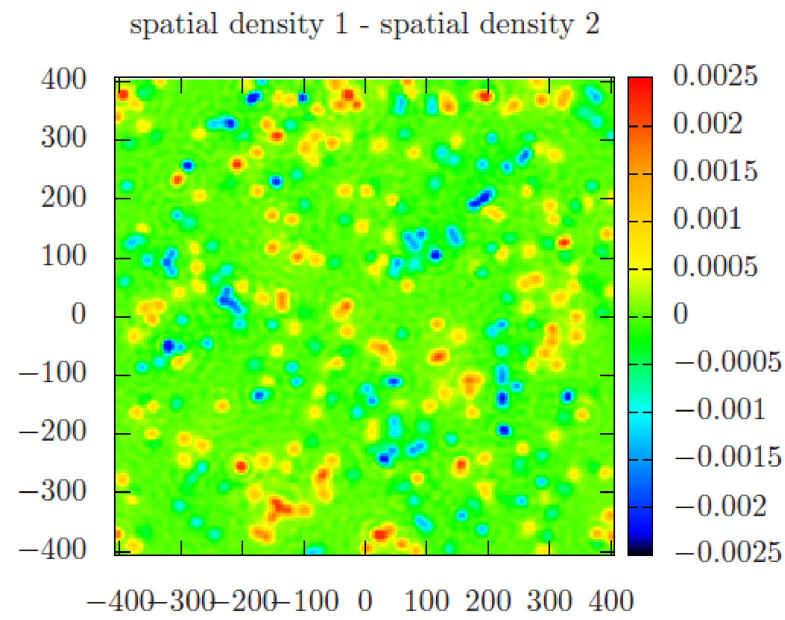




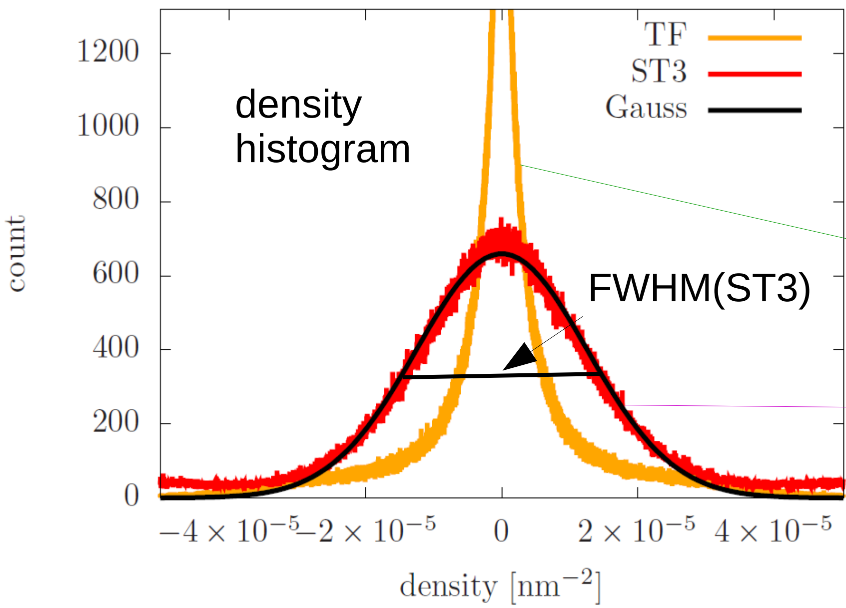
Example: Electron-Hole Puddles beyond Thomas-Fermi

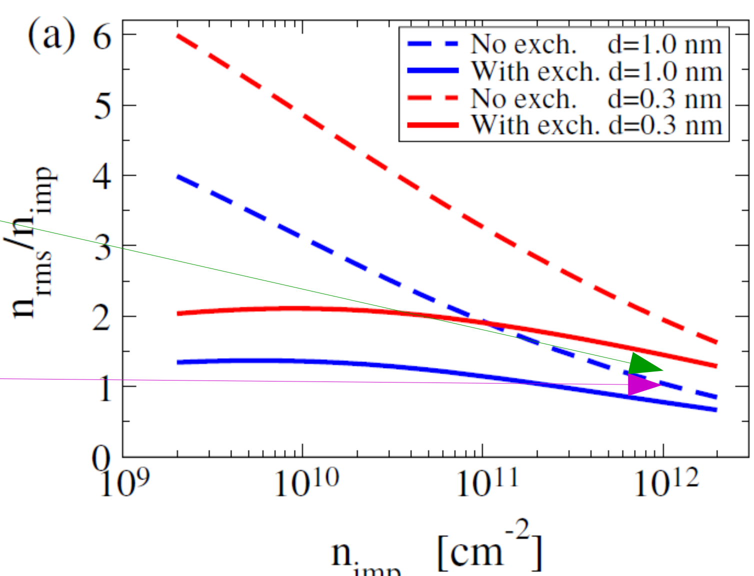
TF





ST3





Rossi & Das Sarma
PRL **101**, 166803 (2008)

NUS National University of Singapore · Centre for Advanced 2D Materials

Centre for Quantum Technologies · National University of Singapore

Direct Band Structure Renormalization

DPFT in position space $E[n,\mu] = E_{\text{kin}}[n] + \int (\mathrm{d}\boldsymbol{r})\, V_{\text{ext}}(\boldsymbol{r})\, n(\boldsymbol{r}) + E_{\text{int}}[n] + \mu \left(N - \int (\mathrm{d}\boldsymbol{r})\, n(\boldsymbol{r}) \right)$

DPFT in momentum space $\tilde{E}[\rho,\mu] = \int (\mathrm{d}\boldsymbol{p})\, T_{\text{kin}}(\boldsymbol{p})\, \rho(\boldsymbol{p}) + \tilde{E}_{\text{ext}}[\rho] + \tilde{E}_{\text{int}}[\rho] + \mu \left(N - \int (\mathrm{d}\boldsymbol{p})\, \rho(\boldsymbol{p}) \right)$

Input: Noninteracting dispersion relation

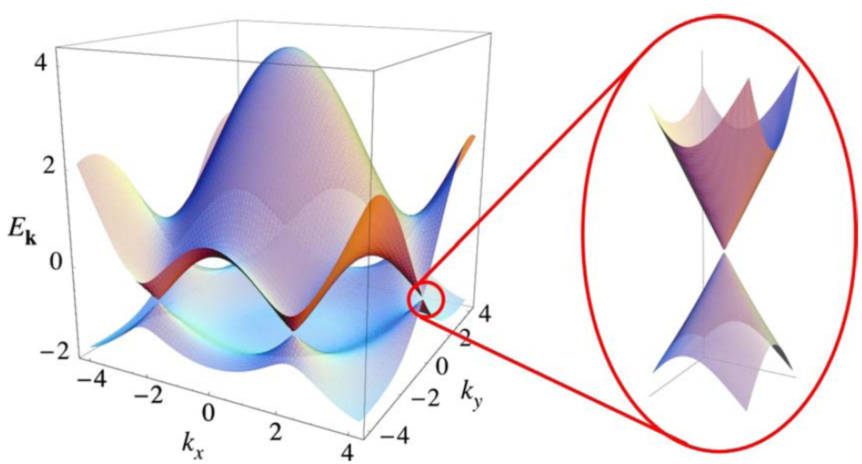
Self-consistent ground-state solutions:

$$\rho(\boldsymbol{p}) = \frac{\delta \tilde{E}_1[T-\mu]}{\delta T(\boldsymbol{p})}$$

$$T(\boldsymbol{p}) = T_{\text{kin}}(\boldsymbol{p}) + \frac{\delta \tilde{E}_{\text{int}}[\rho]}{\delta \rho(\boldsymbol{p})}$$

$$N = \int (\mathrm{d}\boldsymbol{p})\, \rho(\boldsymbol{p})$$

Output: <u>Interacting</u> band structure



[Castro Neto et al, RMP 81, 109 (2009)]

for two bands

$$\rho_{1/2}(\boldsymbol{p}) = \frac{\delta \tilde{E}_1}{\delta T_{1/2}(\boldsymbol{p})}$$

$$T_{1/2}(\boldsymbol{p}) = T_{\text{kin},1/2}(\boldsymbol{p}) + \frac{\delta \tilde{E}_{\text{int}}[\rho_1,\rho_2]}{\delta \rho_{1/2}(\boldsymbol{p})}$$

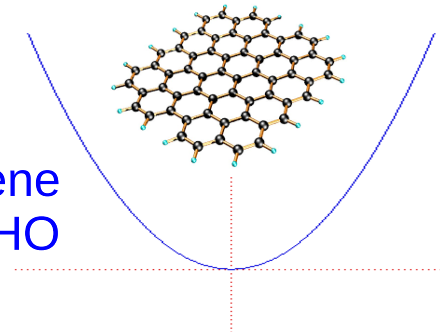
Interaction Contribution from Wigner Function

$$n(\boldsymbol{r}) = \frac{g}{(2\pi\hbar)^D}\int \mathrm{d}\boldsymbol{p}\, w_{\boldsymbol{r}}(Q(\boldsymbol{p}))$$

Wigner function in TF approximation

$$\rho(\boldsymbol{p}) =: \frac{g}{(2\pi\hbar)^D}\int \mathrm{d}\boldsymbol{r}\, w_{\boldsymbol{r}}(Q(\boldsymbol{p})) = \tilde{g}\,\mu\,\log[1+e^{Q}] =: f(Q)$$

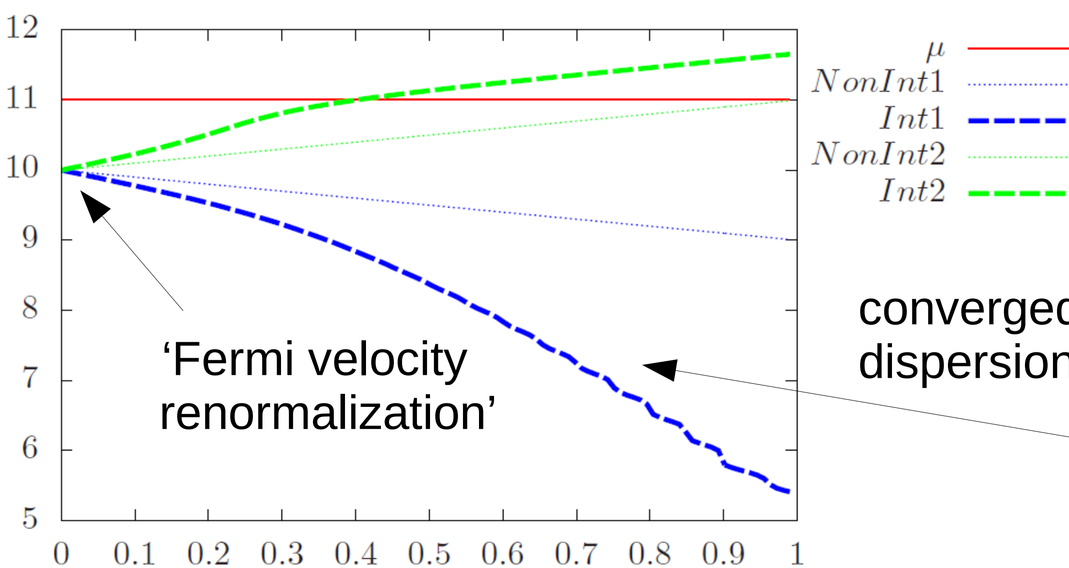
graphene in HO



e.g. $$\tilde{E}_{\mathrm{int}}[\rho] := \frac{1}{2}\int \mathrm{d}\boldsymbol{r}\,\mathrm{d}\boldsymbol{r}'\,\frac{n(\boldsymbol{r})\,n(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|} = \frac{g^2}{2(2\pi\hbar)^{2D}}\int \mathrm{d}\boldsymbol{r}\,\mathrm{d}\boldsymbol{r}'\,\mathrm{d}\boldsymbol{p}\,\mathrm{d}\boldsymbol{p}'\,\frac{w_{\boldsymbol{r}}[Q(\boldsymbol{p})]\,w_{\boldsymbol{r}'}[Q(\boldsymbol{p}')]}{|\boldsymbol{r}-\boldsymbol{r}'|}$$

$$= \frac{g^2}{2(2\pi\hbar)^{2D}}\int \mathrm{d}\boldsymbol{r}\,\mathrm{d}\boldsymbol{r}'\,\mathrm{d}\boldsymbol{p}\,\mathrm{d}\boldsymbol{p}'\,\frac{w_{\boldsymbol{r}}[f^{-1}(\rho(\boldsymbol{p}))]\,w_{\boldsymbol{r}'}[f^{-1}(\rho(\boldsymbol{p}'))]}{|\boldsymbol{r}-\boldsymbol{r}'|}$$

$$\Longrightarrow \frac{\delta\tilde{E}_{\mathrm{int}}[\rho]}{\delta\rho(\boldsymbol{p})}$$



converged dispersion

renormalized dispersion

$$T_{1/2}(\boldsymbol{p}) = T_{\mathrm{kin},1/2}(\boldsymbol{p}) + \frac{\delta\tilde{E}_{\mathrm{int}}[\rho_1,\rho_2]}{\delta\rho_{1/2}(\boldsymbol{p})}$$

self-consistent solutions for $\rho_{1/2}(\boldsymbol{p})$