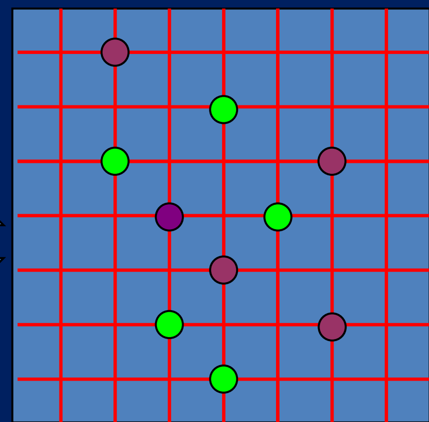
Pseudogap from Path Integral Monte Carlo (PIMC) on the Lattice

Coordinate space

L – limit for the spatial correlations in the system

$k_{cut} = \frac{\pi}{\Delta x}$; Δx



Periodic boundary conditions imposed

$Volume = L^3$

$lattice\ spacing = \Delta x$

- Spin up fermion

- Spin down fermion

External conditions:

T - temperature

μ - chemical potential

UV momentum cutoff $\Lambda_{\rm UV} = \frac{\pi}{\Delta x}$

IR momentum cutoff $\Lambda_{\rm IR} = \frac{2\pi}{L}$

$\frac{\hbar^2 \Lambda_{IR}{}^2}{2m} << \varepsilon_F, \ \Delta << \frac{\hbar^2 \Lambda_{UV}{}^2}{2m}$

$$\hat{H} = \hat{T} + \hat{V} = \int d^3r \sum_{s=\uparrow\downarrow} \hat{\psi}_s{}^\dagger(\vec{r}) \left(-\frac{\hbar^2 \Delta}{2m} \right) \hat{\psi}_s(\vec{r}) \ - \ g \int d^3r \ \hat{n}_\uparrow(\vec{r}) \hat{n}_\downarrow(\vec{r})$$

$$\hat{N} = \int d^3r \ \left(\hat{n}_\uparrow(\vec{r}) + \hat{n}_\downarrow(\vec{r}) \right); \ \ \hat{n}_s(\vec{r}) = \hat{\psi}_s{}^\dagger(\vec{r}) \hat{\psi}_s(\vec{r})$$

Pairing gap

Spectral weight function: $A(\vec{p},\omega)$

$$G^{ret/adv}(\vec{p},\omega)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}d\omega'\frac{A(\vec{p},\omega')}{\omega-\omega'\pm i0^{+}}$$

$$G(\vec{p},\tau)=-\frac{1}{2\pi}\int_{-\infty}^{+\infty}d\omega\, A(\vec{p},\omega)\frac{e^{-\omega\tau}}{1+e^{-\beta\omega}}$$

From Monte Carlo calcs.

$$G(\vec{p},\tau)=\frac{1}{Z}Tr\{e^{-(\beta-\tau)(\hat{H}-\mu\hat{N})}\hat{\psi}_{\uparrow}(\vec{p})e^{-\tau(\hat{H}-\mu\hat{N})}\hat{\psi}^{+}_{\uparrow}(\vec{p})\}$$

Constraints:

$$A(\boldsymbol{p},\omega)\geq 0,\qquad \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}A(\boldsymbol{p},\omega)=1,\quad \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}A(\boldsymbol{p},\omega)\frac{1}{1+\exp(\omega\beta)}=n(\boldsymbol{p}),$$

Maximum entropy method

From Bayes' theorem: $P(A|G) \propto P(G|A)P(A)$

A priori probability: $P(A) \propto \exp(\alpha S)$

Relative entropy: $S(\mathcal{M}) = \sum_{k=1}^{n_A} \Delta\omega \left[A(\omega_k) - \mathcal{M}(\omega_k) - A(\omega_k) \ln \left(\frac{A(\omega_k)}{\mathcal{M}(\omega_k)} \right) \right]$

Likelihood function: $P(G|A) \propto \exp\left(-\frac{1}{2}\chi^2\right)$ $\chi^2 = \sum_{i=1}^{n_\tau} \left(\frac{\tilde{\mathcal{G}}_{\tau_i} - \mathcal{G}(\tau_i)}{\sigma_{\tau_i}} \right)^2$ $\mathcal{G}(\tau_i) = \sum_{k=1}^{n_A} \frac{e^{-\omega_k \tau_i}}{1 + e^{-\omega_k \beta}} A_k \Delta\omega.$

Maximum entropy method: $\min_{A(\omega)} \left(\frac{1}{2}\chi^2 - \alpha S \right)$

SVD method

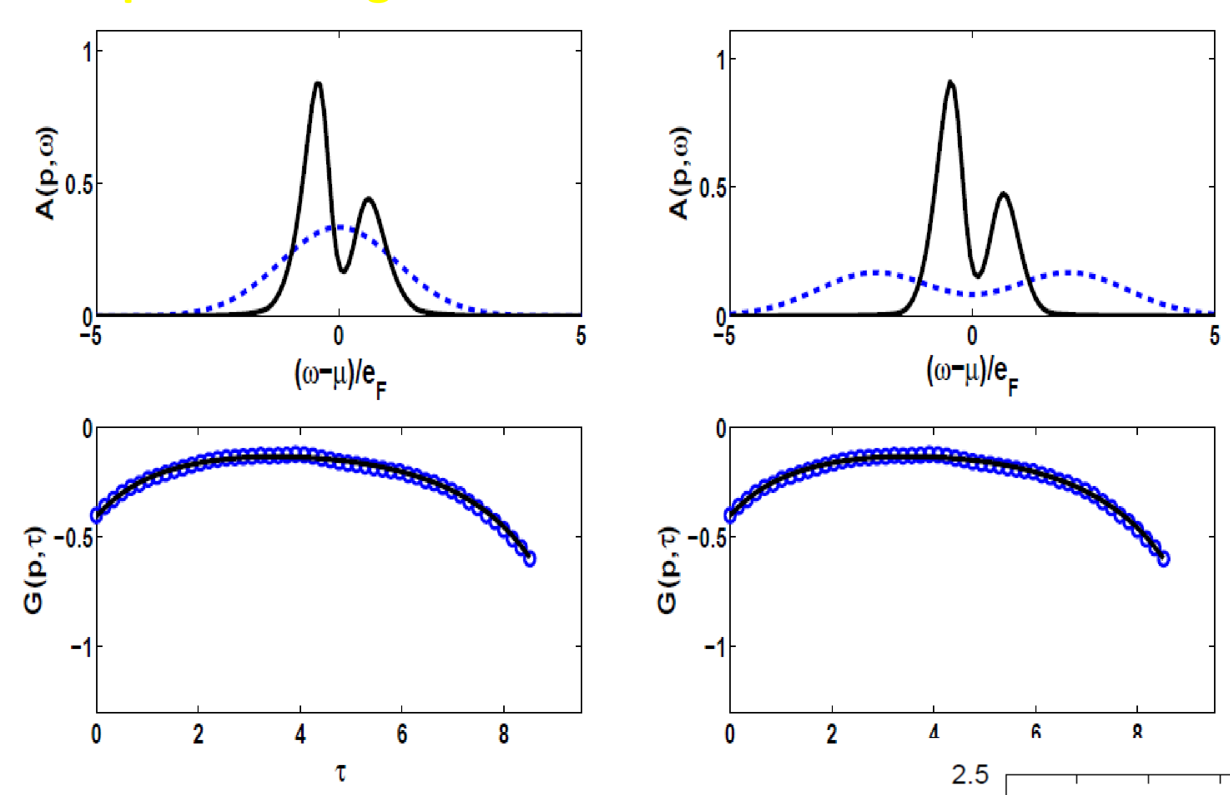
$$\mathcal{G}(\boldsymbol{p}, \tau_i) = (\mathcal{K}A)(\boldsymbol{p}, \tau_i).$$

$$\mathcal{K} u_i = \lambda_i \vec{v}_i, \quad \mathcal{K}^* \vec{v}_i = \lambda_i u_i,$$

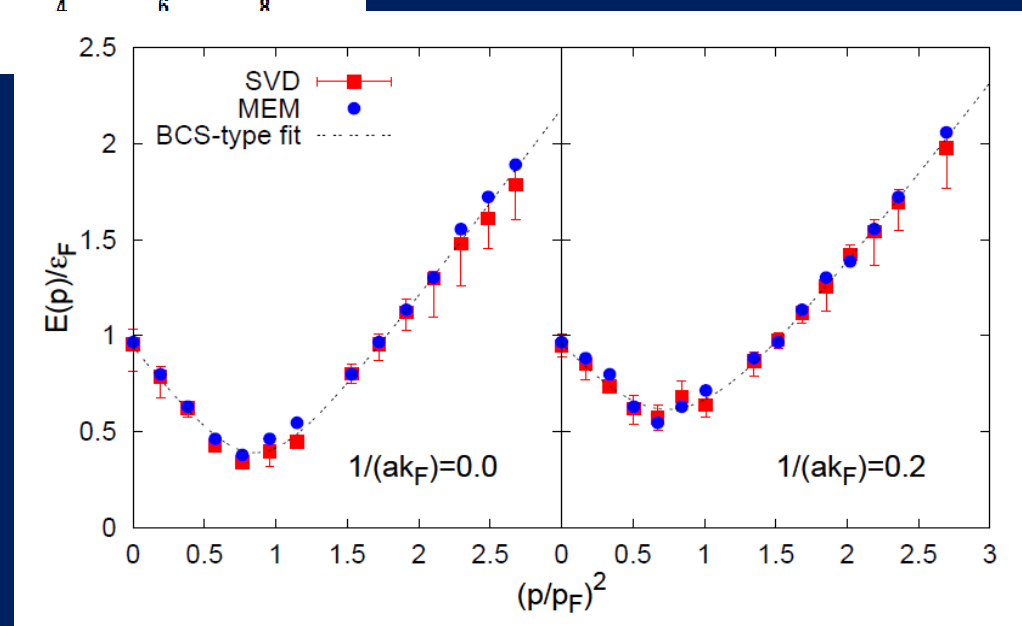
$$u_i(\omega) = \frac{1}{\sigma_i} \sum_{k=1}^{n_\tau} (\vec{v}_i)_k \phi_{\tau_k}(\omega) = -\frac{1}{2\pi\sigma_i} \sum_{k=1}^{n_\tau} (\vec{v}_i)_k \frac{e^{-\omega\tau_k}}{1 + e^{-\omega\beta}}.$$

$$A(\boldsymbol{p}, \omega) = \sum_{i=1}^{r} b_i(\boldsymbol{p}) u_i(\omega), \quad b_i(\boldsymbol{p}) = \frac{1}{\lambda_i} (\vec{\mathcal{G}}(\boldsymbol{p}) \cdot \vec{v}_i),$$

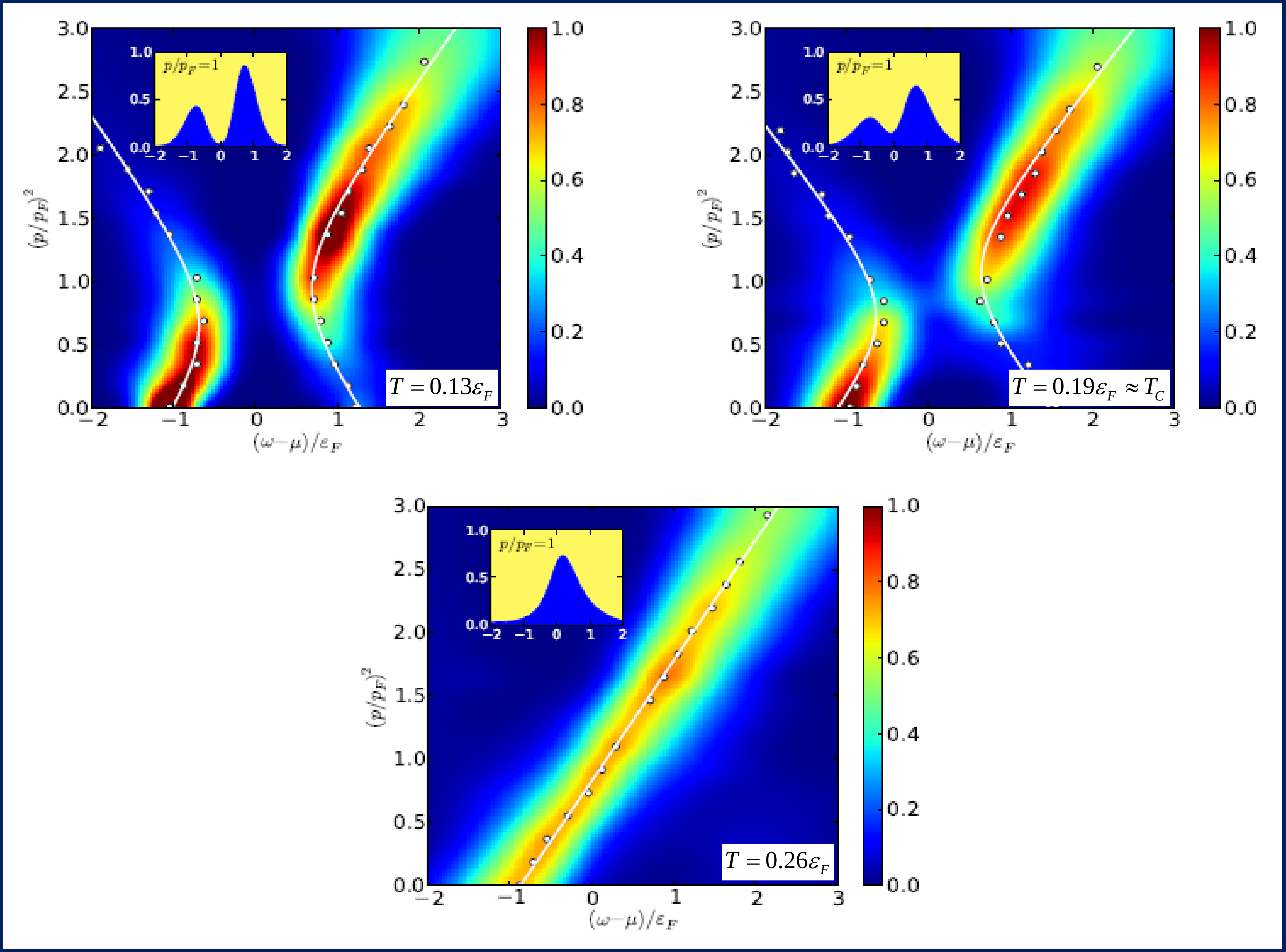
Spectral weight function from MEM



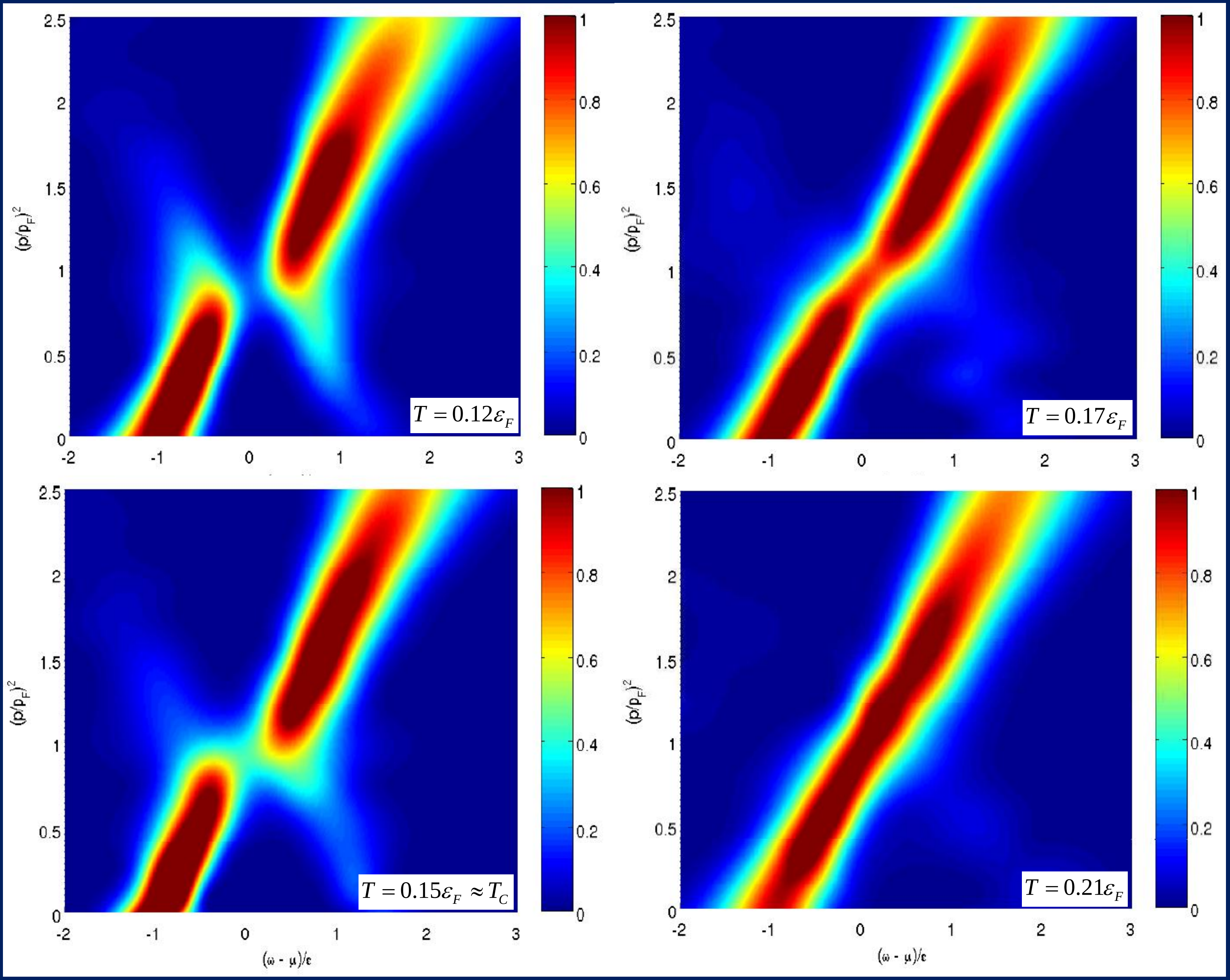
MEM vs SVD



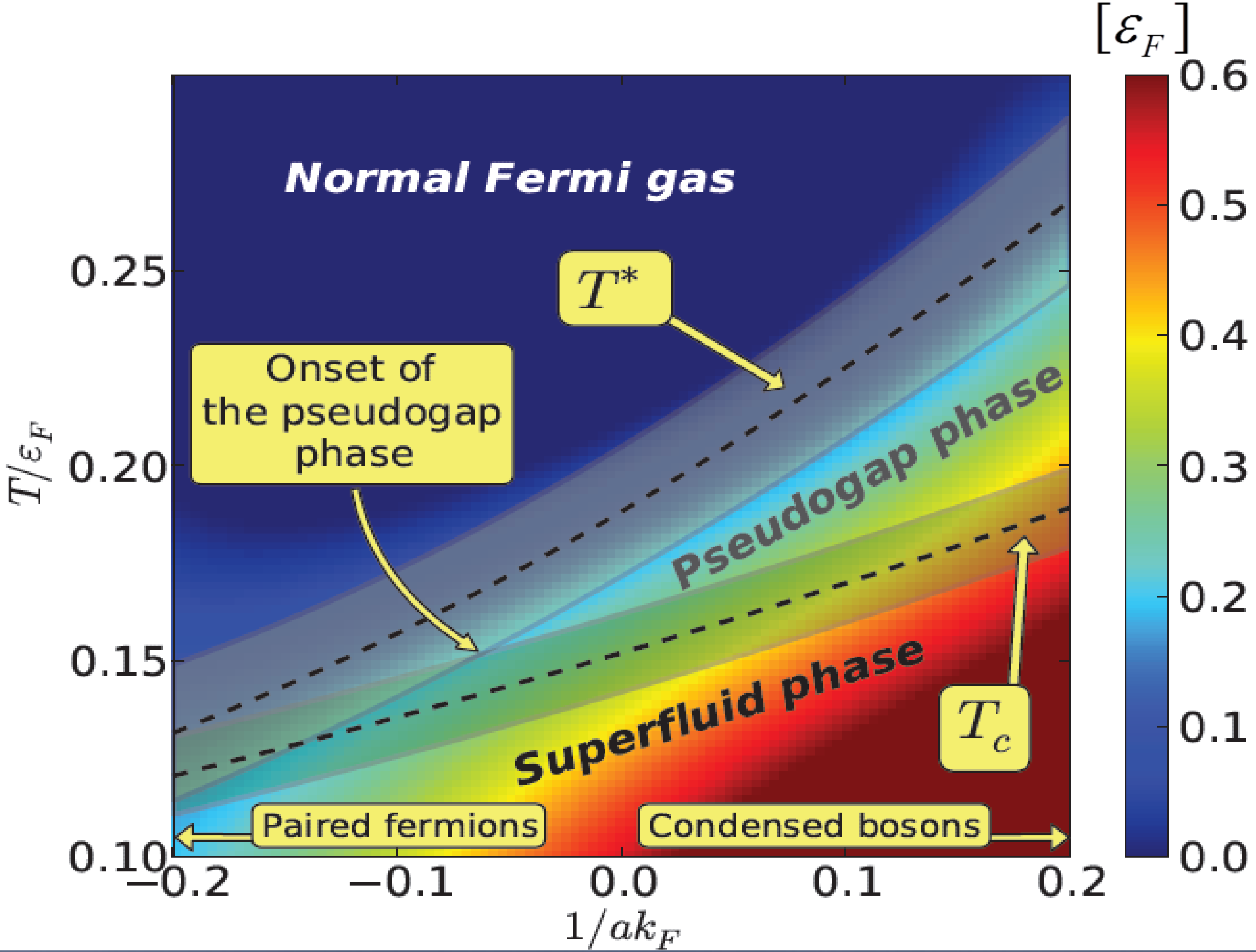
Spectral weight function at the BEC side: $(k_F a)^{-1} = 0.2$



Spectral weight function at unitarity: $(k_F a)^{-1} = 0$



Gap in the single particle fermionic spectrum from MC calcs.

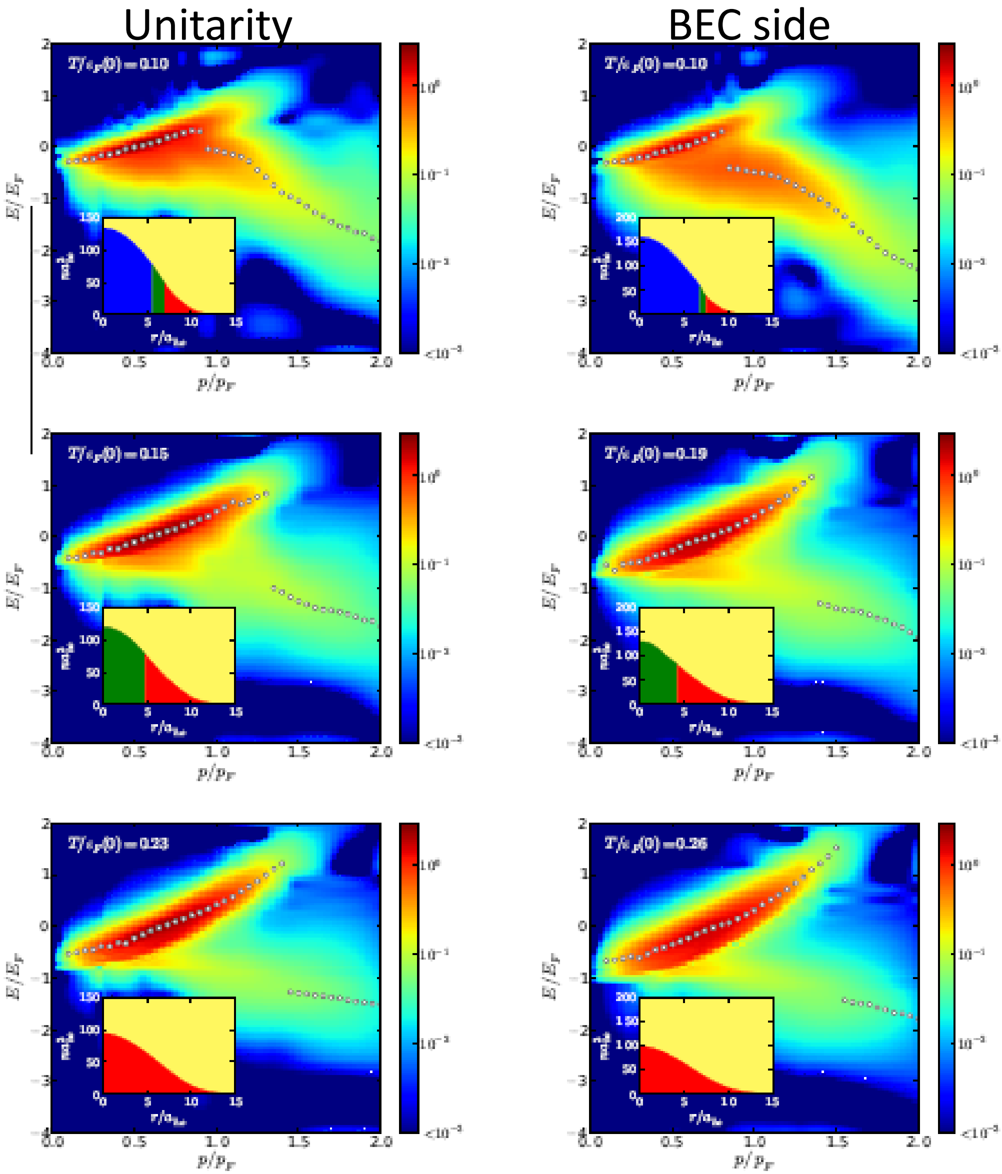


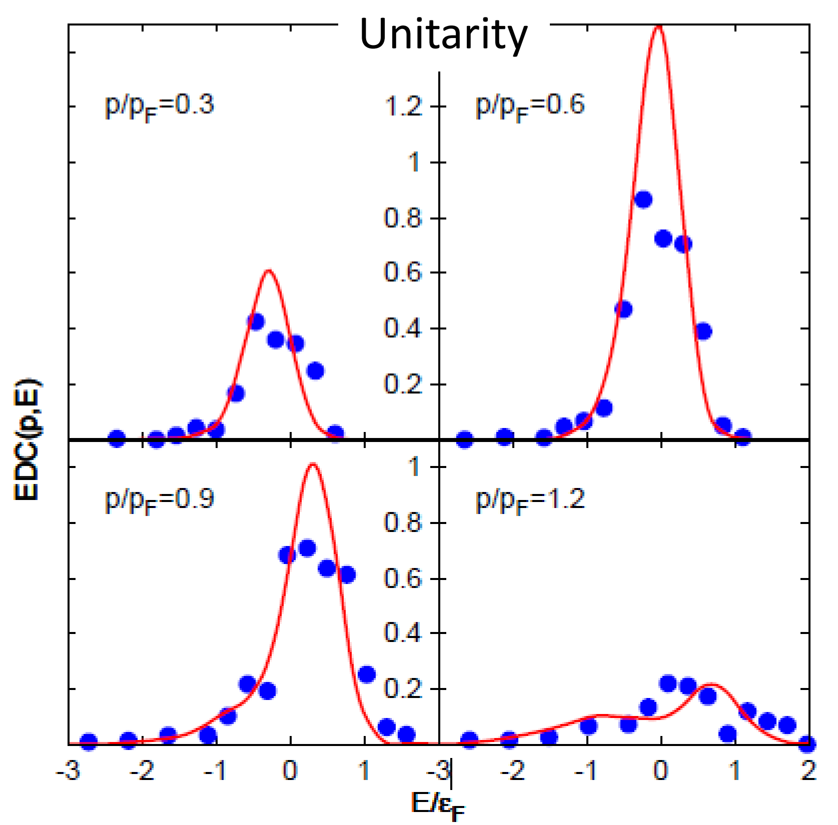
Ab initio result: The onset of pseudogap phase at $1/ak_F \approx -0.05$.

Magierski, Wlazłowski, Bulgac, arXiv1103.4382

Energy distribution curves (EDC) from the spectral weight function

$$\mathrm{EDC}(p,E,T) = \mathcal{C}p^2 \int_0^\infty dr\, r^2 \frac{1}{\varepsilon_F(r)} A\left[\frac{p}{p_F(r)}, \frac{E-\mu(r)}{\varepsilon_F(r)}, \frac{T}{\varepsilon_F(r)}\right] f(E-\mu(r)),$$



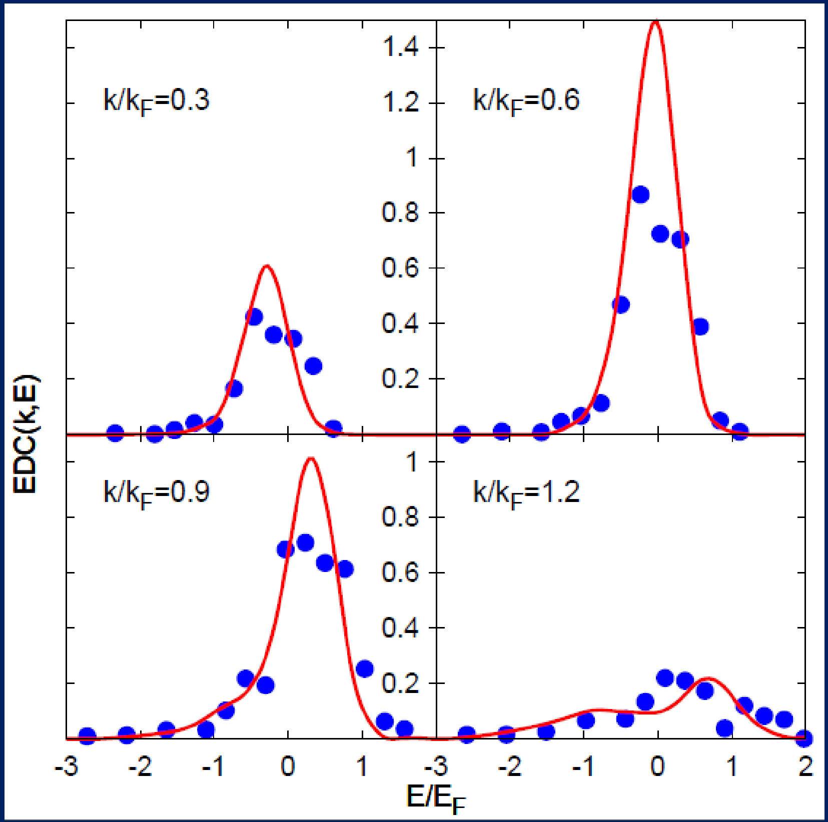


Experiment (blue dots): D. Jin's group
Theory (red line) PIMC:
Magierski, Wlazłowski, Bulgac,
arXiv1103.4382

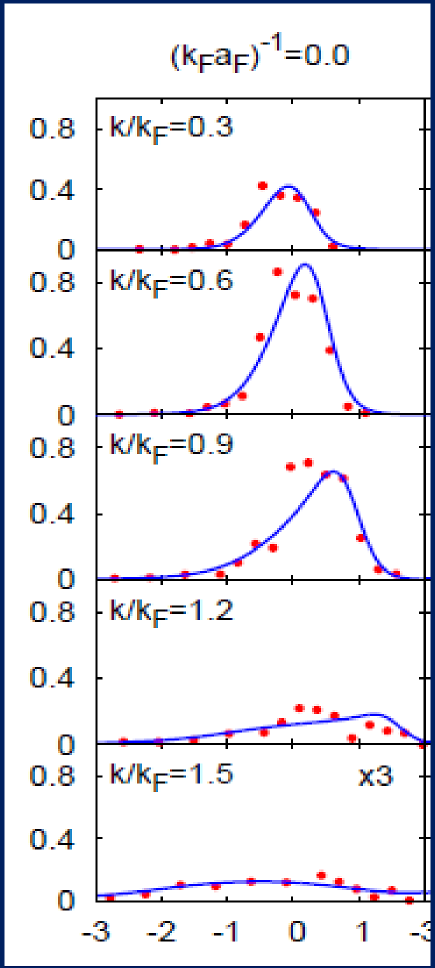
Theory vs Experiment (photoemission spectr.)

$$EDC(k,E) \sim A(k,\omega) f(\omega)$$

PIMC

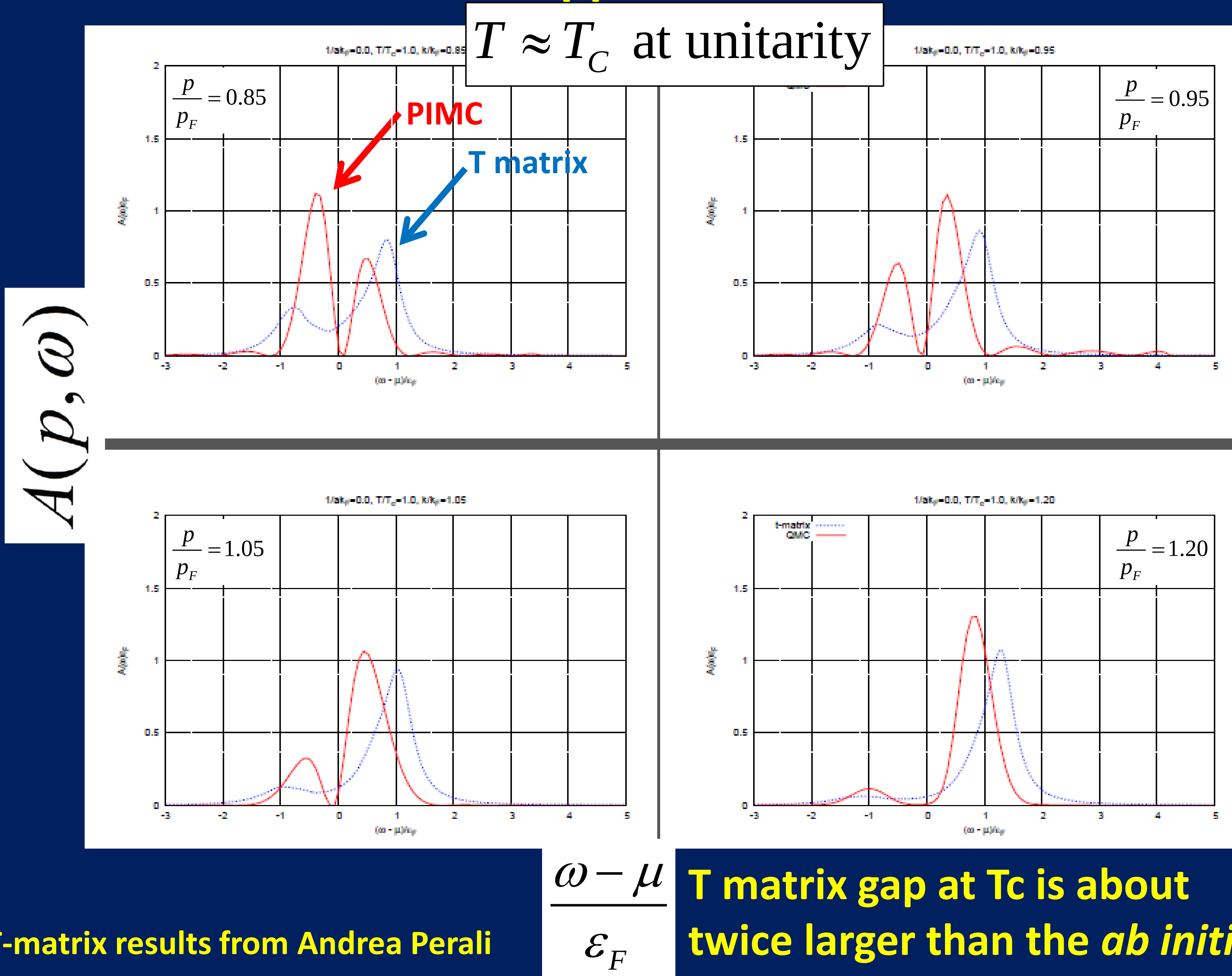


Non selfconsistent t-matrix approx.



Perali, A., Palestini, F., Pieri, P., Strinati, G.C., Stewart, J.T., Gaebler, J.P., Drake, T.E. & Jin, Phys. Rev. Lett. 106, 060402 (2011)

PIMC vs T-matrix approach (preliminary results)



T-matrix results from Andrea Perali

T matrix gap at Tc is about twice larger than the *ab initio* gap!