Quantum simulation of Hubbard Model: Results from DQMC

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Fermi surface for interacting systems

- Fermi surface – locus of low energy single particle excitations, defined by $G^{-1}(k,\omega=0)=0$

- Probing Fermi surface from DQMC-look at single particle Green's function

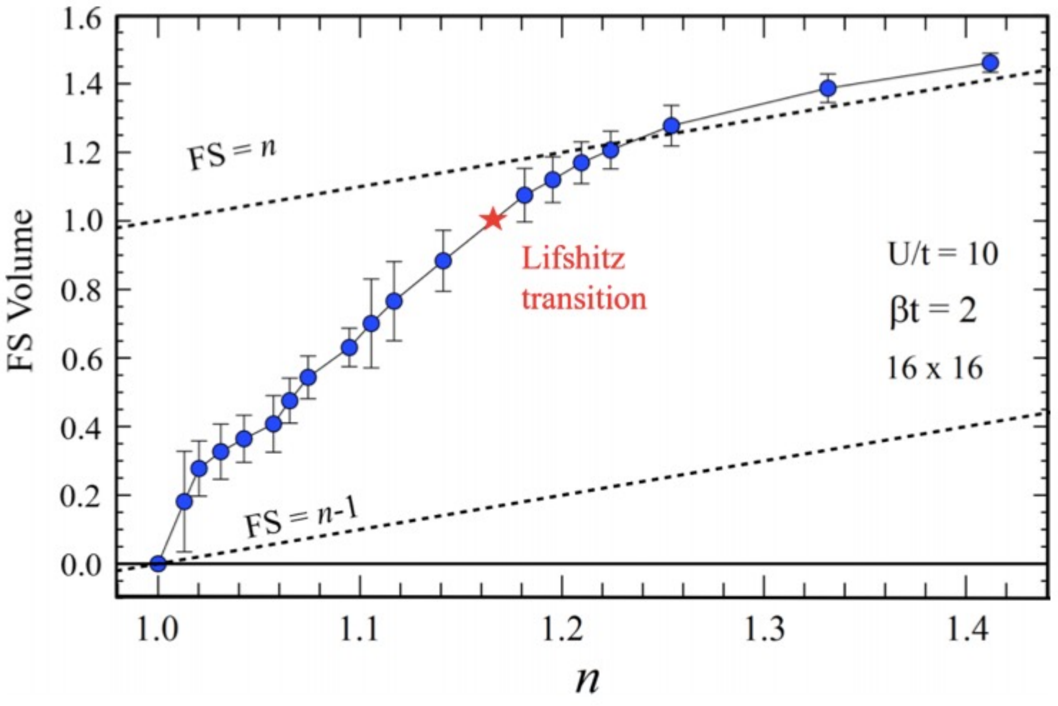
$$G(\mathbf{k},\tau) = -\langle T\hat{c}_{\mathbf{k}\sigma}(\tau)\hat{c}^{\dagger}_{\mathbf{k}\sigma}(0)\rangle$$

- Related to single particle Spectral function via Laplace transform

$$G(\mathbf{k},\tau) = -\int_{-\infty}^{\infty} d\omega \frac{e^{-\omega\tau}}{1+e^{-\beta\omega}}\mathcal{A}(\mathbf{k},\omega)$$

- Provided there is no low energy scale,

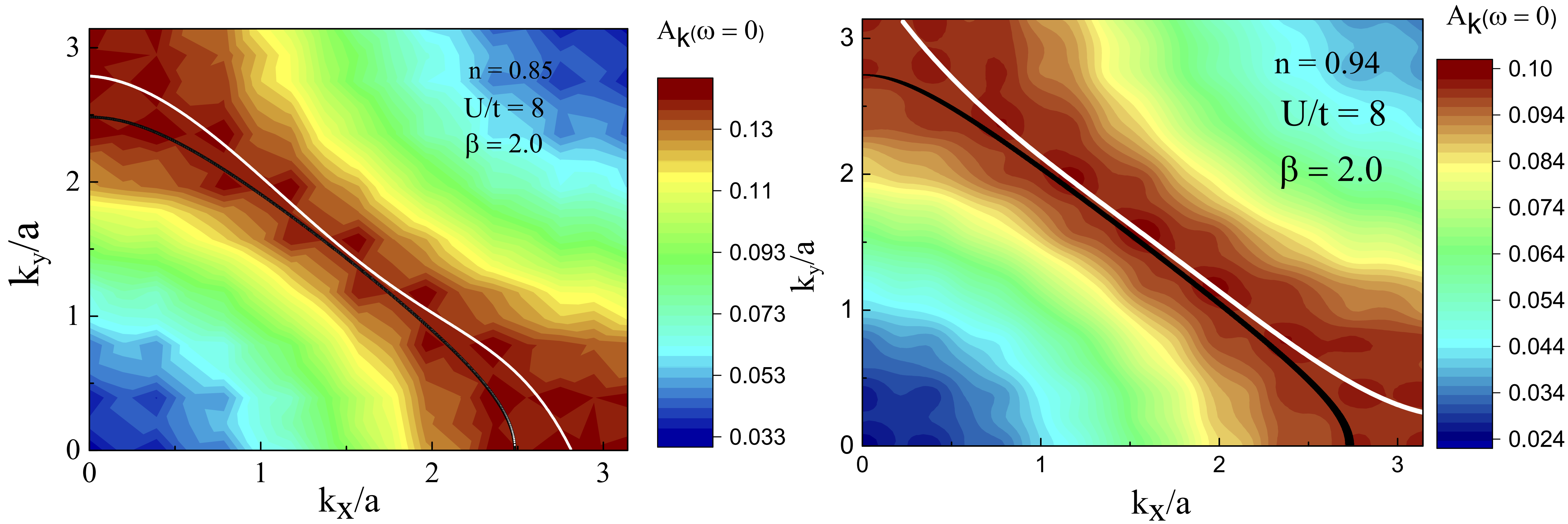
$$G(\mathbf{k},\tau=\beta/2) = -\frac{\pi}{\beta}\mathcal{A}(\mathbf{k},\omega=0)$$



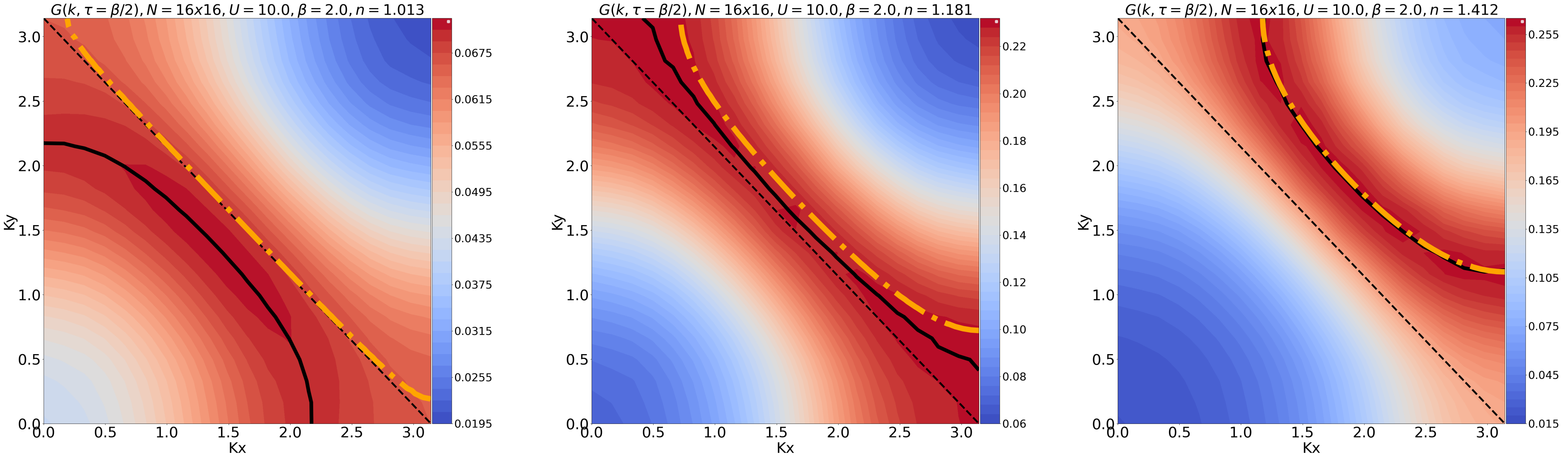
Maximum at $\mathbf{k}=\mathbf{k}_F$, fermi momentum same as noninteracting system → Is this always valid?

– Luttinger's theorem

Fermi surface reconstruction for hole doping



Fermi surface reconstruction for particle doping



Seebeck coefficient of an interacting system

- The thermopower for an interacting system is defined as

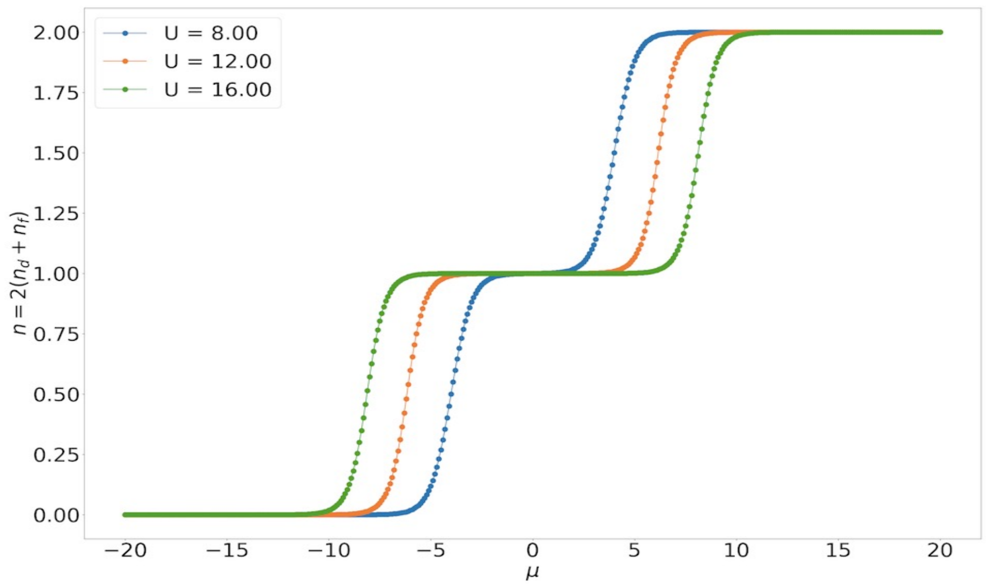
$$S(q_x,\omega)=\frac{\chi_{\rho(q_x),\hat{K}(-q_x)}(\omega)}{T\chi_{\rho(q_x),\rho(-q_x)}(\omega)}$$

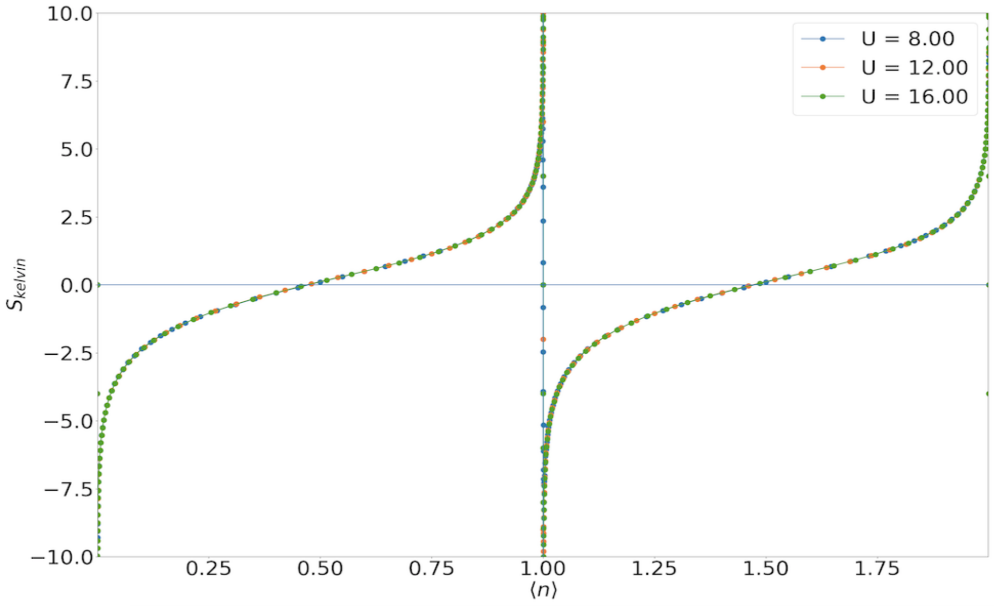
- The Kelvin formula is the slow transport limit of the above formula,

$$S_{\text{Kelvin}}=\lim_{q_x\to 0}\frac{\chi_{\rho(q_x),\hat{K}(-q_x)}(0)}{T\chi_{\rho(q_x),\rho(-q_x)}(0)}=\frac{1}{q_eT}\frac{\frac{d}{d\mu}\langle\hat{H}\rangle-\mu\frac{d}{d\mu}\langle\hat{N}\rangle}{\frac{d}{d\mu}\langle\hat{N}\rangle}$$

- Writing the energy in terms of the grand potential $E=\Omega+T\mathcal{S}+\mu N$,

$$S_{\text{Kelvin}}=\frac{1}{q_e}\frac{\left(\frac{\partial\mathcal{S}}{\partial\mu}\right)_{T,V}}{\left(\frac{\partial N}{\partial\mu}\right)_{T,V}}=\frac{1}{q_e}\left(\frac{\partial\mathcal{S}}{\partial N}\right)_{T,V}$$





Entropy and Seebeck coefficient for the repulsive Hubbard model