PTEROSOR group meeting

DIAGONAL PADÉ APPROXIMANT OF THE ONE-BODY GREEN'S FUNCTION

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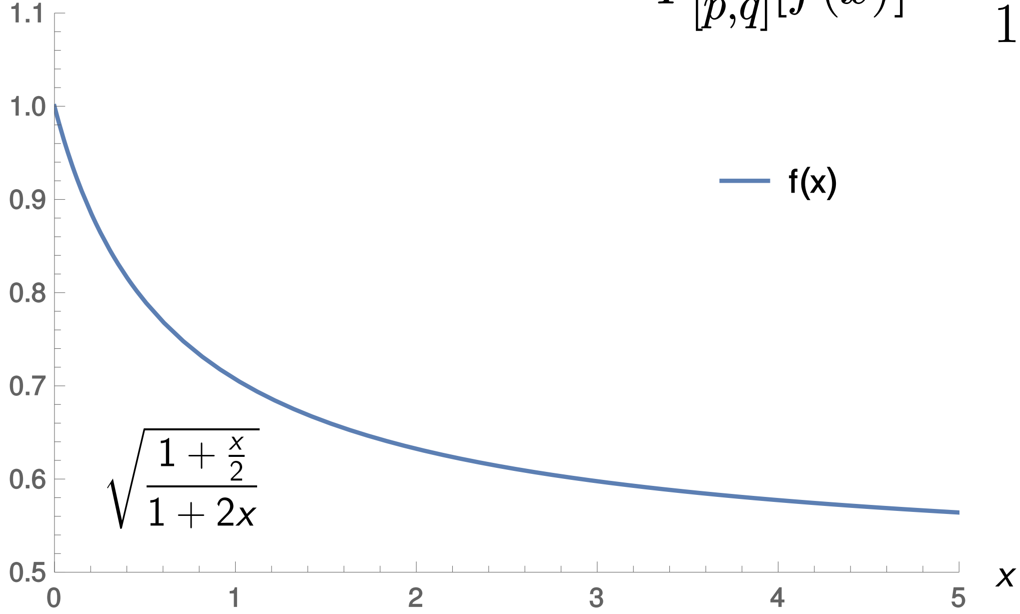
Padé approximant

$$T_n[f(x)] = a_0 + a_1 x + a_2 x^2 + \ldots + a_n x^n$$

$$P_{[p,q]}[f(x)] = \frac{b_0 + b_1 x + \ldots + b_p x^p}{1 + c_1 x + \ldots + c_q x^q}$$



[Baker, Graves-Morris, ***Padé Approximants,*** 2010]

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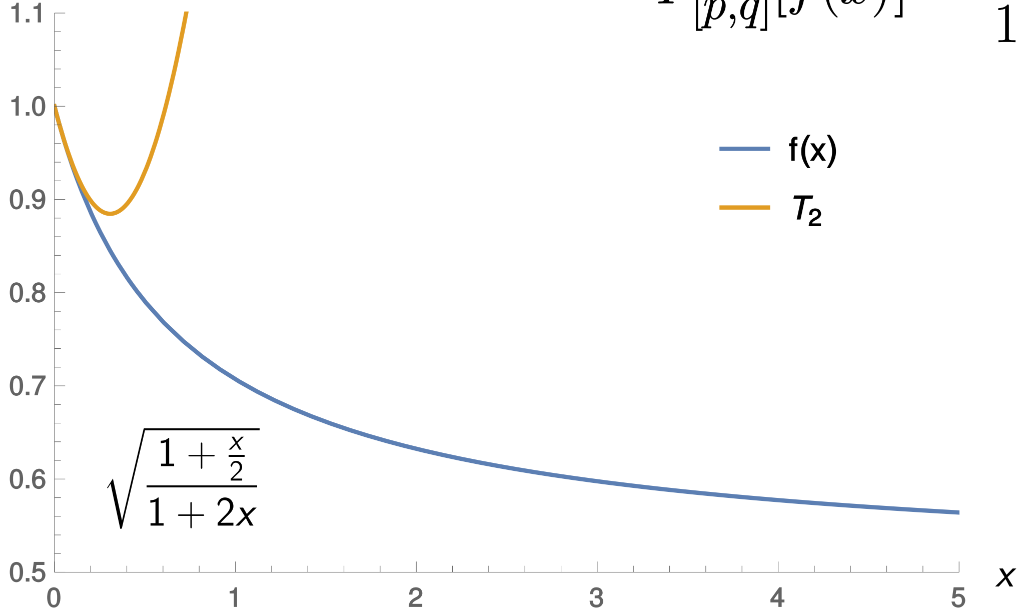

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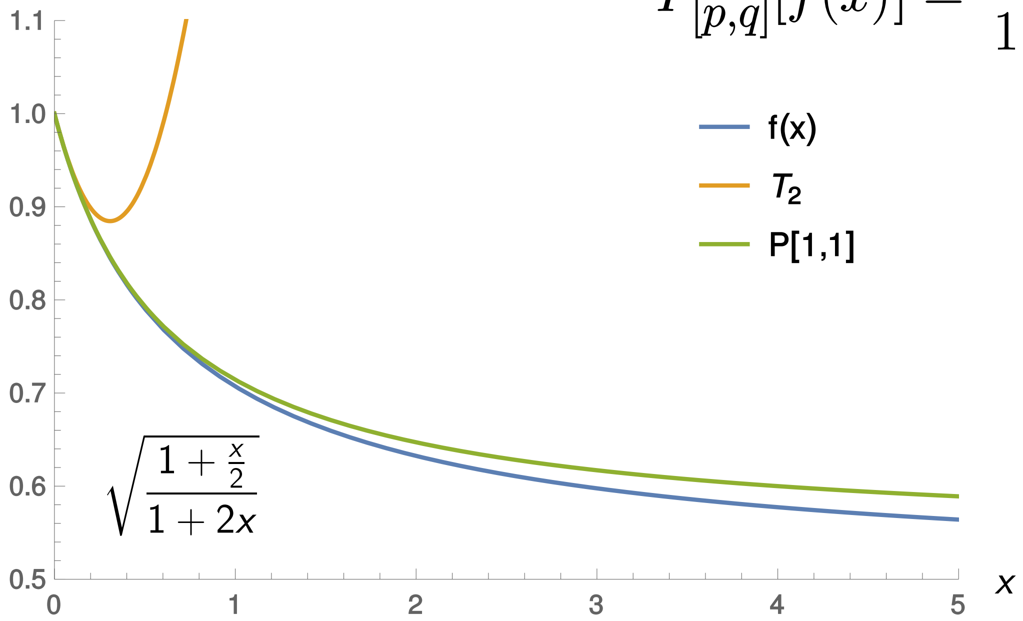

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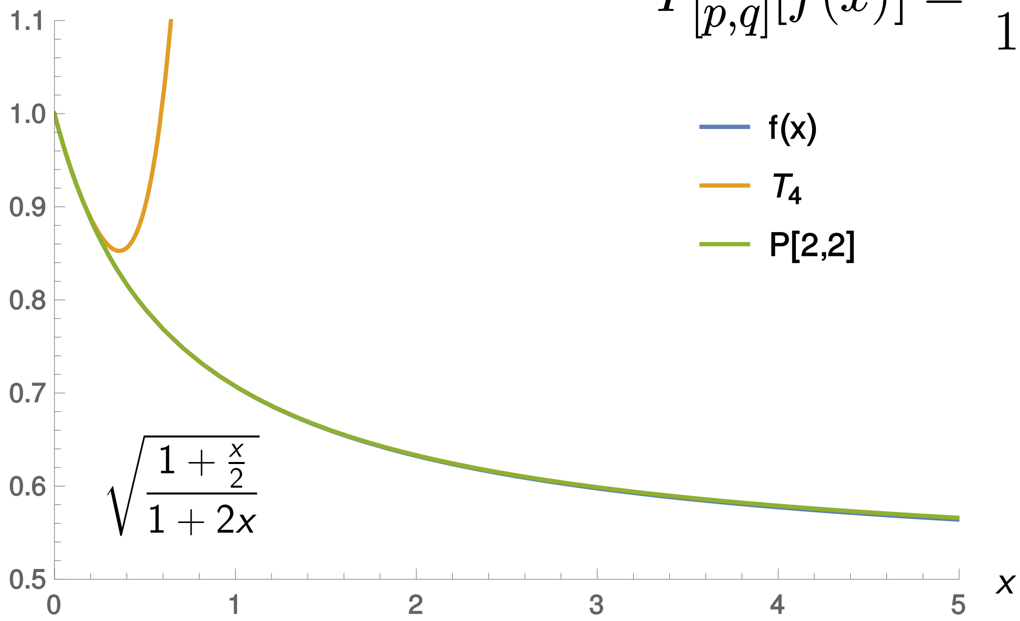

[Baker, Graves-Morris, ***Padé Approximants,*** 2010]

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Diagonal Padé approximant of the one-body Green's function: A study on Hubbard rings

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Padé approximants to the many-body Green's function can be built by rearranging terms of its perturbative expansion. The hypothesis that the best use of a finite number of terms of such an expansion is given by the subclass of *diagonal* Padé approximants is here tested, and largely confirmed, on a solvable model system, namely the Hubbard ring for a variety of site numbers, fillings, and interaction strengths.

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Many Body Perturbation Theory

Perturbation expansion of G

$$G = G_0 + G_0 v G_0 G_0 + G_0 v G_0 G_0 v G_0 G_0 + \ldots$$

Dyson equation

$$G = G_0 + G_0 \Sigma G \qquad\qquad G = [G_0^{-1} - \Sigma]^{-1}$$

Perturbation expansion of Σ

$$\Sigma = v G_0 + v G_0 G_0 v G_0 + \ldots$$

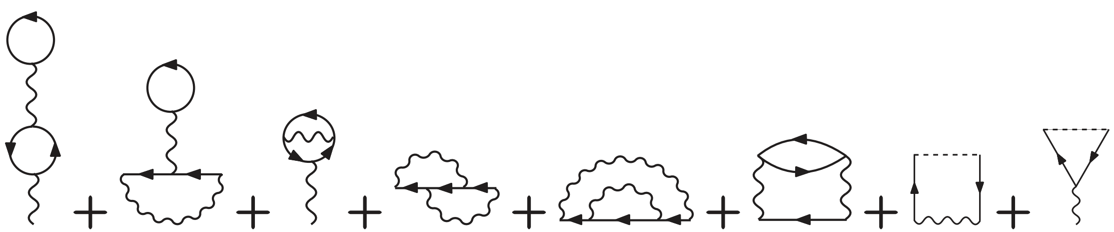
[Fetter, A. L., & Walecka, J. D. (1971). Quantum theory of many-particle systems.]

Many Body Perturbation Theory

$$\Sigma = \Sigma^{(1)} + \Sigma^{(2)} + \ldots$$

$\Sigma^{(1)} =$

$\Sigma^{(2)} =$



Diagonal Padé

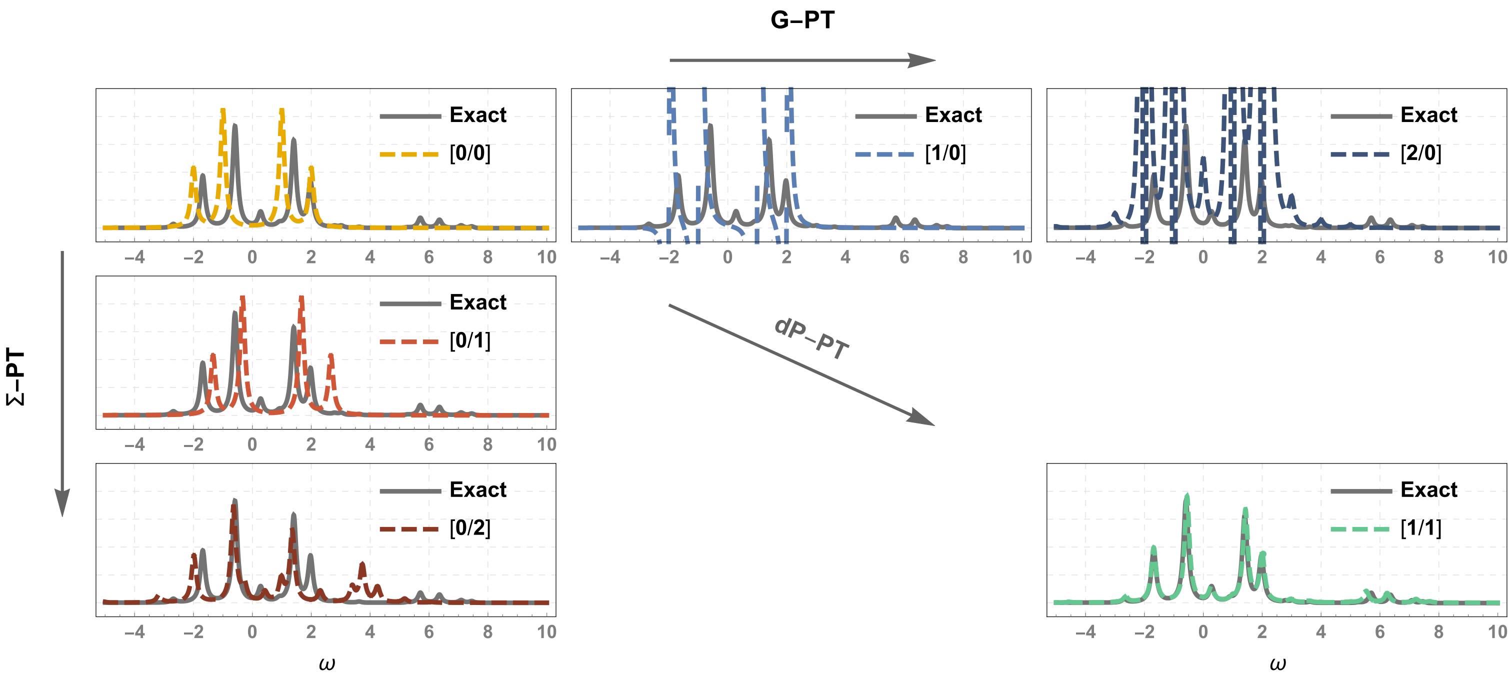
$$\Sigma \approx \Sigma_{[1,1]} = \frac{\left[\Sigma^{(1)}\right]^2}{\Sigma^{(1)} - \Sigma^{(2)}}$$

$$\Sigma^{(1)}_{ij} = \sum_{k\in\mathcal{O}} (v_{ikkj} - v_{ikjk}) - i\delta_{ij} v^{m.f.}_{ii}$$

$$\begin{aligned}\Sigma^{(2)}_{ij}(\omega) = &\sum_{o,q,r} \mathcal{O}_q \left(\frac{\mathcal{O}_o\mathcal{U}_r}{\epsilon_o + \epsilon_r} + \frac{\mathcal{O}_r\mathcal{U}_o}{\epsilon_r + \epsilon_o}\right)(v_{iojr} - v_{iorj})(v_{qroq} - v_{qrqo}) \\ &+ \sum_{nps} v_{isnp}(v_{npjs} - v_{npsj})\left(\frac{\mathcal{O}_s\mathcal{U}_n\mathcal{U}_p}{\omega + i\eta - \epsilon_s - \epsilon_n - \epsilon_p} + \frac{\mathcal{O}_n\mathcal{O}_p\mathcal{U}_s}{\omega - i\eta + \epsilon_p + \epsilon_n + \epsilon_s}\right) \\ &+ \sum_{n,p} (-i)\left(\frac{\mathcal{O}_n\mathcal{U}_p}{\epsilon_n + \epsilon_p} + \frac{\mathcal{O}_p\mathcal{U}_n}{\epsilon_p + \epsilon_n}\right)(v_{injp} - v_{inpj})\, v^{m.f.}_{pn}\end{aligned}$$

Hubbard model

L=6, N=2, U/t=4



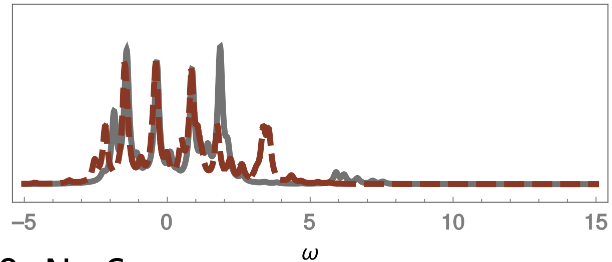
Hubbard model

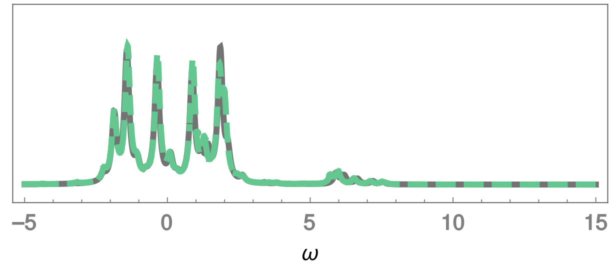
U=4

L=10, N=2

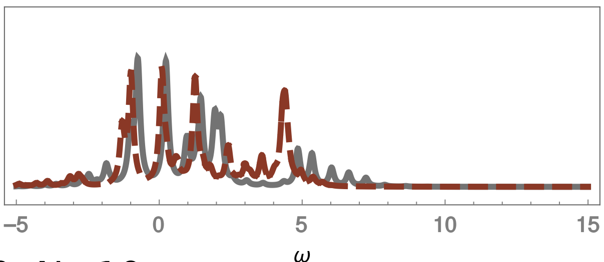
Σ-PT [0/2]

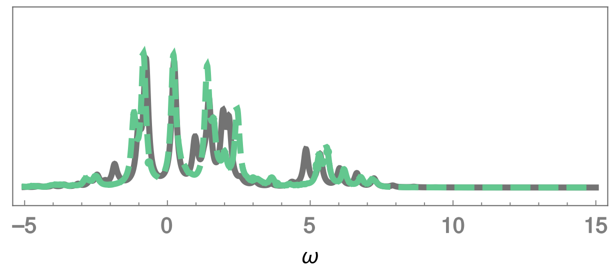
P[1/1]



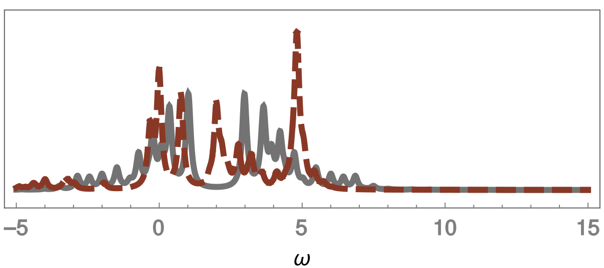


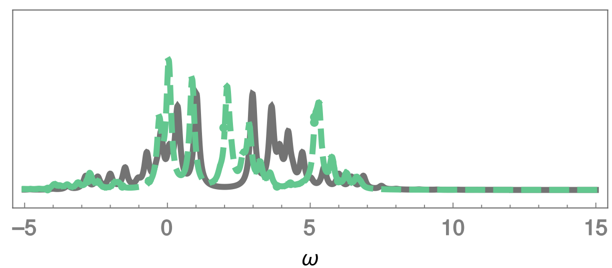
L=10, N=6





L=10, N=10



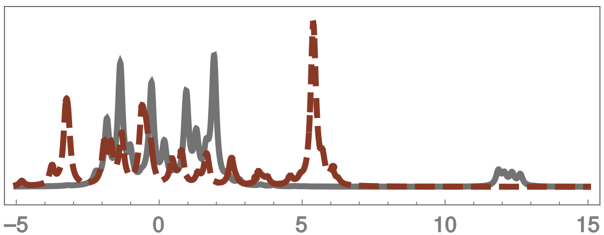


Hubbard model

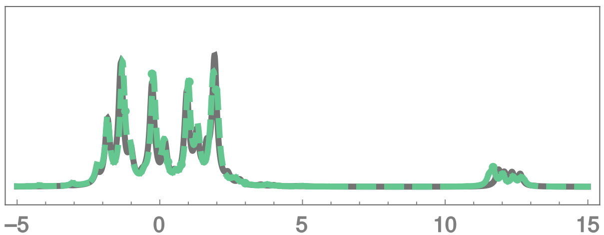
L=10, N=2, U=10

U=10

Σ-PT [0/2]



P[1/1]



Outlooks

- Padé in realistic systems

  Finite or bulk systems?

- Include higher-order diagrams