Multiscale space-time ansatz for correlation functions of quantum systems based on quantics tensor trains arXiv:2210.12984v2 (to appear in PRX) 科研費 PRESTO 埼玉大理1, ウィーン工科大2, 理研CEMS3, 京大理4, フリブール大5 品岡寬¹, Markus Wallerberger², 村上雄太³, 野垣康介⁴, 櫻井理人¹, Philipp Werner⁵, Anna Kauch² What's new Background Desired efficient numerical treatment (\vec{r}'', t'') • Wide range of length scales in space-time $(\vec{r}^{\prime\prime\prime},t^{\prime\prime\prime})$ of space-time dependence of • Systematic control over truncation error $N_t = 10^3, N_r = 100^3 \rightarrow (N_t N_r)^4 = 10^{36}$ correlation functions! Computation in compressed form Quantum embedding, first- (\vec{r},t) (\vec{r}',t') principles calculations Straightforward implementations as computer code Quantics tensor trains (QTT) I. V. Oseledets, Doklady Math. **80**, 653 (2009) If QTT compressible, bond dimension $\ll 2^{R/2}$ B. N. Khoromskij, Constr. Approx. 34, 257 (2011) $(0...0)_2$ $(0\cdots 1)_2$ f(k) $|(1\cdots 1)_{2}|$ k = 0Tensor train/Matrix product state Length-scale separation→Exponential advantage for storage! dimension $\mathbf{2}R-1-b$ R = 16Bond Plateau Bond b Multivariate function Fourier transform Coarse Same length scale f(k, k')Matrix product operator (MPO) for Fourier transform has a small (D < 20). k'_{R-1} K. J. Woolfe *et al.*, Quantum Inf. Comput. **17**, 1 (2017), J. Chen *et al.*, arXiv:2210.08468v1 $r = 0, 1, \dots, 2^R - 1$ Same length scale **Short range** $= (r_1 \cdots r_{R-1} r_R)_2$ Compression Around four-digit accuracy Nonequilibrium system (real-time Green's function) Compression ratio ~ 103 - AF insulator AF insulator $|G_{\text{reconst}} - G_{\text{exact}}|_{\infty} / |G_{\text{exact}}|_{\infty} \times 10^{-5}$ Bond dimension 10^3 in 10^2 10^1 Doped Mott insulator D = 52Impurity model $\underbrace{\mathfrak{F}}_{\mathbf{Q}} 0.4$ $t'/t_{\rm max} = 0.5$ -0.2Impurity model • Sharp peaks can be represented. 0.40.5 $-0.025\,0.000\,0.025$ Larger bond dimension for more features Multipolar susceptibility All QTT compressible! (b) Absolute error $X_{loc}(1,1)$ **2P vertex functions** (c) U = 3.56, m = 10 $|\Gamma_{\text{exact}}|, |\Gamma_{\text{exact}}|_{\infty} = 14.29$ 1P momentum space $|\Gamma_{\rm exact} - \Gamma_{\rm reconst}|$ D = 171 $|G(\mathrm{i} u_1,k_x,k_y)|$ Absolute error 40 -20-0.05 0.10 $2.5 \,\, 5.0 \,\, 7.5$ $\times 10^{-5}$ $X_{\rm loc}(1, 36)$ Absolute error 3 5 7 9 11 13 15 -20--400.0005 0.0010 2.5 5.0 7.5 $0.05\,0.10\,0.15$ 0.000250.00050CeB₆ Computation $C(t,t'') = \int dt' A(t,t') B(t',t'')$ Exponential speed up! Fourier transform Matrix multiplication— $C(t_1, t_1'', \dots, t_R, t_R'') = \sum_{l} A(t_1, t_1', \dots, t_R, t_R') B(t_1', t_1'', \dots, t_R', t_R'')$ Dyson/Bethe-Salpeter equation HS et al., arXiv:2210.12984v2 Quantics tensor cross interpolation M. K. Ritter, Y. N. Fernández, M. Wallerberger, J. von Delft, HS, X. Waintal, arXiv:2303.11819