Barycentric rational approximation made simple: A novel analytic continuation method for quantum Monte Carlo data

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Analytical continuation is a pivotal yet unresolved technical challenge in quantum many-body calculations. It can transform imaginary-time or imaginary-frequency correlation functions into real spectral functions, which can be compared with experiments directly. In this talk, I will try to explain two novel analytical continuation methods that we have developed in recent years: the stochastic pole expansion method (StochPX) and the barycentric rational function approximation method (BaryRFA). The StochPX method is a new variant of the stochastic analytical continuation. Within this method, the Matsubara Green's function is expressed as a pole expansion, and the simulated annealing algorithm is employed to optimize the weights and positions of these poles. With the help of constrained sampling and adaptive sampling algorithms, the StochPX method can successfully reproduce complicated features in the spectral functions, such as large energy gaps and sharp band edges, etc. In the BaryRFA method, initially, the Prony interpolation or Legendre approximation is applied to filter out noise in the Matsubara Green's function, which is then represented in a form of the barycentric rational function. Subsequently, the adaptive Antoulas-Anderson algorithm is utilized to determine the nodes and weights of the rational function. The benchmark results suggest that the BaryRFA method does not require the spectral function to be positive definite, thus offering an exceptionally broad range of applicability. Furthermore, its computational accuracy is comparable to the recently developed Nevanlinna analytical continuation method, while its computational efficiency surpasses that of the classic maximum entropy method.