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Abstract. A new QMC approach for the shell model yielding nearly exact spectroscopy of nuclei is presented. The originality of the formalism lies in the use of a variational symmetry-restored wave function to 'steer' the Brownian motion, and to control the sign/phase problem that generally makes the traditional QMC samplings totally ineffective by causing a prohibitive growth of the statistical errors. Tests of convergence and proof-of-principle results are reported.

1. Introduction

The shell model with configuration mixing is one of the most powerful theoretical frameworks for studying the nuclear structure [1]. In this picture, valence protons and neutrons beyond an inert magic core are confined in one or more active shells and interact through an effective two-body residual interaction. The wave functions of the nucleus are then determined by diagonalizing the Hamiltonian in the set of all the accessible configurations and used to compute physical observables. Unfortunately, the shell model is strongly restricted in its applicability by the combinatorial scaling of the dimension of the many-body basis with the size of the single-particle Hilbert space and the number of valence nucleons.

Quantum Monte-Carlo (QMC) methods represent attractive techniques to overcome such limitations by offering a systematic alternative to the diagonalization of the Hamiltonian. Indeed, *via* a stochastic reformulation of the imaginary-time Schrödinger equation, the many-body problem is reduced to a set of numerically tractable one-body problems describing independent particles that randomly walk in fluctuating external fields. In this way, exact correlated wave functions are reconstructed by averaging independent-particle states called *walkers*.

The shell model Monte Carlo method (SMMC) remains to date the principal QMC approach of the shell model [2], and has enabled to investigate systems out of reach of conventional calculations without severe truncations of the configuration space. It relies on the standard sampling by auxiliary fields of the path integrals resulting from the Hubbard-Stratonovich transformation [3] of the imaginary-time propagator. With schematic residual interactions, the SMMC approach accurately reproduces the properties of even-even or $N = Z$ odd-odd nuclei at zero and finite temperature. However, with realistic effective interactions or for other kind of nuclei, the method is plagued by the so-called fermion sign or phase problem whose signature is an exponential collapse of the signal-to-noise ratio as the temperature is decreased. To circumvent this pathology and guarantee convergent simulations, a class of modified Hamiltonians where interactions causing the problem are artificially reduced is usually

sampled. The physical observables are then recovered by extrapolating these non-physical SMMC results to recover the original Hamiltonian [4].

Besides the phase problem, another limitation of the SMMC approach lies in its incapacity to achieve detailed spectroscopy of nuclei, even though informations on excited states can be extracted from response functions. In contrast, low-lying states can be reconstructed by means of the so-called Monte-Carlo shell model technique [5] that does not utilize the stochastic process to sample eigenstates, but instead to generate a subspace into which the Hamiltonian matrix is diagonalized. Given that such calculations do not suffer from explicit manifestations of sign or phase problems, they may be successfully performed for very large configuration spaces and provides variational estimates of nuclear properties at low excitation energy [6].

In this work, we present a new QMC scheme to obtain yrast states in the shell model framework [7]. The formalism involves a variational symmetry-restored wave function assuming a twofold role. First, it guides the underlying Brownian motion to improve the efficiency of the sampling. Second, it constrains the stochastic paths to control sign or phase problems, in the spirit of the fixed-node approximation, widely applied in *ab initio* QMC calculations [8] where the random walk takes place within the coordinate space.

2. Phaseless quantum Monte-Carlo method
2.1. Guided dynamics
Implementing a QMC approach based on auxiliary fields requires to write the two-body Hamiltonian $\hat{H}$ in a quadratic form of one-body operators $\hat{T}$ and $\{\hat{O}_s\}$:

$$\hat{H} = \hat{T} - \sum_s \omega_s \hat{O}_s^2, \quad \hat{T} = \sum_{i,j} T_{ij} \hat{c}_i^\dagger \hat{c}_j, \quad \hat{O}_s = \sum_{i,j} (O_s)_{ij} \hat{c}_i^\dagger \hat{c}_j, \tag{1}$$

with $\hat{c}_i^\dagger$ ($\hat{c}_i$) the creation (annihilation) operator of a fermion in the single-particle state $|i\rangle$ of a finite-size discrete orthonormal basis. As discussed in Ref. [9], there is substantial freedom in doing so. For the shell model, we choose the isospin density decomposition given in Ref. [9].

Zero-temperature QMC methods rely on the imaginary-time propagation to project an initial wave function $|\Phi_0\rangle$ onto the lowest-energy eigenstate $|\Psi_G\rangle$ of $\hat{H}$ not orthogonal to $|\Phi_0\rangle$:

$$\lim_{\tau \to +\infty} e^{-\tau \hat{H}} |\Phi_0\rangle \propto |\Psi_G\rangle. \tag{2}$$

Thanks to the Trotter-Suzuki breakup [10] and the Hubbard-Stratonovich transformation [3], the propagator for a short step $\Delta\tau$ may then be reformulated stochastically,

$$e^{-\Delta\tau \hat{H}} = \int d\vec{\eta}\, p(\vec{\eta}) \hat{\mathcal{U}}(\vec{\eta}), \tag{3}$$

where $\vec{\eta}$ is a vector of random variables $\{\eta_s\}$, the so-called auxiliary fields (AF), distributed according to a normal Gaussian distribution p. As exponential of one-body operators, the stochastic propagator

$$\hat{\mathcal{U}}(\vec{\eta}) = e^{-\frac{\Delta\tau}{2}\hat{T}} e^{\sum_s \eta_s \sqrt{2\omega_s \Delta\tau} \hat{O}_s} e^{-\frac{\Delta\tau}{2}\hat{T}}, \tag{4}$$

transforms a Slater determinant $|\Phi_\tau\rangle$ at τ to a new one $|\Phi_{\tau+\Delta\tau}\rangle = \hat{\mathcal{U}}|\Phi_\tau\rangle$, used to sample the exact state at $\tau + \Delta\tau$. Consequently, the wave function resulting from the evolution during $\Delta\tau$ of $|\Phi_\tau\rangle$ is reinterpreted as the coherent statistical average $\mathbb{E}[\cdot]$ of independent-fermion states $|\Phi_{\tau+\Delta\tau}\rangle$, i.e. $\exp(-\Delta\tau\hat{H})|\Phi_\tau\rangle = \mathbb{E}[|\Phi_{\tau+\Delta\tau}\rangle]$, and finally the eigenstate of $\hat{H}$ is recovered as follow,

$$|\Psi_G\rangle \underset{\tau \to +\infty}{\propto} \mathbb{E}[|\Phi_\tau\rangle]. \tag{5}$$

In order to improve the efficiency of the standard AFQMC scheme described above, Zhang and Krakauer have proposed to borrow the idea of importance sampling [11], by generating walkers $|\Phi\rangle$ according to their overlap $\langle\Psi_T|\Phi\rangle$ with a trial wave function $|\Psi_T\rangle$ not orthogonal to the ground state. By directly including the complex importance function within the random walk, the exact state at a given τ is therefore reconstructed as

$$\mathrm{e}^{-\tau\hat{H}}|\Phi_0\rangle = \mathbb{E}\left[\Pi_\tau\frac{|\Phi_\tau\rangle}{\langle\Psi_T|\Phi_\tau\rangle}\right], \tag{6}$$

the factor Π being introduced to ensure the exactness of the stochastic scheme. The equations of motion may be derived by the usual Hubbard-Stratonovich procedure provided that the $\hat{O}_s$ operators in Eq. (1) are previously shifted by their local estimates $\langle\hat{O}_s\rangle_{\Psi_T\Phi_\tau} = \langle\Psi_T|\hat{O}_s|\Phi_\tau\rangle/\langle\Psi_T|\Phi_\tau\rangle$:

$$\mathrm{e}^{-\Delta\tau\hat{H}}\Pi_\tau\frac{|\Phi_\tau\rangle}{\langle\Psi_T|\Phi_\tau\rangle} = \int\mathrm{d}\vec{\eta}\,p(\vec{\eta})\,\Pi_\tau\Delta\Pi_\tau\,\frac{\hat{\mathcal{U}}_T(\vec{\eta})|\Phi_\tau\rangle}{\langle\Psi_T|\Phi_{\tau+\Delta\tau}\rangle}. \tag{7}$$

The stochastic propagator $\hat{\mathcal{U}}_T$ that transforms $|\Phi_\tau\rangle$ into $|\Phi_{\tau+\Delta\tau}\rangle$ reads

$$\hat{\mathcal{U}}_T(\vec{\eta}) = \mathrm{e}^{-\frac{\Delta\tau}{2}\hat{T}}\mathrm{e}^{\sum_s\Delta h_{T,s}\hat{O}_s}\mathrm{e}^{-\frac{\Delta\tau}{2}\hat{T}}, \quad \Delta h_{T,s} = 2\Delta\tau\omega_s\langle\hat{O}_s\rangle_{\Psi_T\Phi_\tau} + \eta_s\sqrt{2\omega_s\Delta\tau}. \tag{8}$$

Compared to the standard AFQMC diffusion (4), the trial state $|\Psi_T\rangle$ now takes part in the dynamics *via* the local estimates of the $\hat{O}_s$, and so guides the Brownian motion towards a region of the Slater determinants manifold where the importance of the walker in the sampling is expected to be large. The variation $\Delta\Pi_\tau$ of the weight Π_τ,

$$\Delta\Pi_\tau = \frac{\langle\Psi_T|\hat{\mathcal{U}}_T|\Phi_\tau\rangle}{\langle\Psi_T|\Phi_\tau\rangle}\exp\left(-\Delta\tau\sum_s\omega_s\langle\hat{O}_s\rangle^2_{\Psi_T\Phi_\tau} - \sum_s\eta_s\sqrt{2\omega_s\Delta\tau}\langle\hat{O}_s\rangle_{\Psi_T\Phi_\tau}\right), \tag{9}$$

contains the remaining scalar terms from the rewriting of $\hat{H}$, and may be recast in a more concise form when $\Delta\tau \to 0$. In this limit, the quantities $\eta_s\sqrt{\Delta\tau}$ indeed become infinitesimal increments $\mathrm{d}W_s$ of Wiener processes in the Ito formalism of stochastic calculus [12] that obey $\mathbb{E}[\mathrm{d}W_s] = 0$, $\mathrm{d}W_s\mathrm{d}W_{s'} = \delta_{ss'}\mathrm{d}\tau$. Thus, expanding $\hat{\mathcal{U}}_T$ as well as the exponential scalar term in Eq. (9) yield to the first order

$$\Delta\Pi_\tau = \exp\left(-\Delta\tau\langle\hat{H}\rangle_{\Psi_T\Phi_\tau}\right), \tag{10}$$

for $\Delta\tau$ sufficiently small. Similarly, one may also check that in this context the one-body representation of $\hat{\mathcal{U}}_T$ governing the dynamics of the occupied orbitals transforms into the stochastic differential equations (3) of Ref. [7].

2.2. Phase problem

In general, any QMC sampling is plagued by sign or phase problems as soon as the phase of the overlap $\langle\Psi_G|\Phi\rangle$ varies during the random walk. Indeed, extracting $|\Psi_G\rangle$ is strongly compromised when a large proportion of walkers corresponding to different phases mutually cancel their contributions to the sampling, leading to a mean overlap $\mathbb{E}[\langle\Psi_G|\Phi\rangle] \approx 0$. Hence, such trajectories severely degrade the signal-to-noise ratio: They are useless for reconstructing the ground-state wave function and they only increase the statistical error. In the framework of the QMC scheme (6), the overlap $\langle\Psi_G|\Phi\rangle$ is given by

$$\langle\Psi_G|\Phi\rangle \underset{\tau\to+\infty}{\propto} \langle\Psi_T|\mathrm{e}^{-\tau\hat{H}}|\Phi\rangle \underset{\tau\to+\infty}{=} \mathbb{E}[\Pi_\tau], \tag{11}$$

with $\Pi_0 = \langle \Psi_T | \Phi \rangle$. Managing the phase problem requires to resort to approximations that constrain the random walk through a change $\Pi \to \widetilde{\Pi}$ of the weight of the realizations. First, by taking the real part of the local energy in Eq. (10), we guarantee that the overlaps $\langle \Psi_G | \Phi \rangle$ and $\langle \Psi_T | \Phi \rangle$ have the same phase. Then, we need to prevent the Brownian motion from populating symmetrically the complex $\langle \Psi_T | \Phi \rangle$ plane to avoid the mean overlap merging with the origin. To this end, we apply the *phaseless* approximation [11], in which the constrained weight $\widetilde{\Pi}$ evolves according to the dephasing $\Delta\theta_\tau = \arg\langle \Psi_T | \Phi_{\tau+\Delta\tau} \rangle / \langle \Psi_T | \Phi_\tau \rangle$ of the overlap with the trial state:

$$\Delta\widetilde{\Pi}_\tau = \exp\left(-\Delta\tau \mathrm{Re}\langle \hat{H}\rangle_{\Psi_T \Phi_\tau}\right) \max\left\{0\,;\cos(\Delta\theta_\tau)\right\}. \tag{12}$$

Owing to the factor $\cos(\Delta\theta_\tau)$, the more the phase of the overlap $\langle \Psi_T | \Phi \rangle$ changes during $\Delta\tau$, the more the weight of the associated walker is reduced, and the walker is discarded when $|\Delta\theta_\tau|$ becomes larger than $\pi/2$. As a result, the centroid of the population persists into the half-plane $\mathrm{Re}\langle \Psi_T | \Phi \rangle > 0$ even though some realizations with gradually reduced weights can reach the other half-plane. In this respect, the constraint (12) provides a good compromise between the necessity in controlling the phase problem and the conservation of the initial form for the probability distribution that ensures an exact reproduction of the ground state. Finally, replacing Π by $\widetilde{\Pi}$ in Eq. (6) allows a phase problem-free sampling of an approximate ground state $|\widetilde{\Psi}_G\rangle$. Note that the approximation (12) also removes the risk of infinite variance on the error $|\Psi_G\rangle - |\Phi\rangle$, which would ensue from an accumulation of realizations around $\langle \Psi_T | \Phi \rangle = 0$.

2.3. Trial state: Yrast spectroscopy

The phaseless QMC method has been widely applied in quantum chemistry [11], with a simple mean-field wave function for $|\Psi_T\rangle$. Here, we propose for the shell model a more sophisticated approach allowing to achieve the ground state in each angular-momentum channel J, M, which is now also employed to improve the accuracy of QMC simulations for the ground state of the Hubbard model [13]. Starting from a Slater determinant $|\Phi_0\rangle$, a satisfying trial state $|\Psi_T^{JM}\rangle$ to initiate, guide, and constrain the dynamics may be defined by mixing all the possible values of the spin projection K in the intrinsic frame:

$$|\Psi_T^{JM}\rangle = \sum_{K=-J}^{J} C_K^J \hat{P}_{MK}^J |\Phi_0\rangle, \tag{13}$$

where $\hat{P}_{MK}^J$ are projection operators onto the desired spin [14]. Restricting $|\Phi_0\rangle$ to be factorized into a product of independent-neutron and -proton wave functions, the ansatz (13) also has a good isospin projection. Moreover, when valence spaces containing only one major shell are considered, the parity is a good quantum number and no further restoration is needed. Let us remark that, as a superposition of symmetry-related Slater determinants, $|\Psi_T^{JM}\rangle$ is no longer an independent-particle state so that it can absorb correlations beyond the mean-field level.

The energy E_G^J of the yrast state $|\Psi_G^{JM}\rangle$ can now be determined after a large enough imaginary time as

$$E_G^J \underset{\tau\to+\infty}{=} \frac{\langle \Psi_T^{JM} | \hat{H} e^{-\tau\hat{H}} | \Psi_T^{JM}\rangle}{\langle \Psi_T^{JM} | e^{-\tau\hat{H}} | \Psi_T^{JM}\rangle} \underset{\tau\to+\infty}{=} \frac{\langle \Psi_T^{J} | \hat{H} e^{-\tau\hat{H}} | \Phi_0\rangle}{\langle \Psi_T^{J} | e^{-\tau\hat{H}} | \Phi_0\rangle}, \tag{14}$$

under the proviso that $|\Psi_T^{JM}\rangle$ has a non-zero overlap with the exact state. In Eq. (14), $|\Psi_T^{J}\rangle = \sum_{K,K'} C_K^{J*} C_{K'}^J \hat{P}_{KK'}^J |\Phi_0\rangle$ denotes the state arising from rotational invariance and from the properties $(\hat{P}_{MK}^J)^\dagger = \hat{P}_{KM}^J$ and $\hat{P}_{MK}^J \hat{P}_{K'M'}^{J'} = \delta_{JJ'}\delta_{KK'}\hat{P}_{MM'}^J$. This wave function thus appears as a natural candidate to apply the QMC formalism (6, 8) with the biased weight (12)

to constrain stochastic paths. Finally, an approximate yrast state $|\widetilde{\Psi}_G^{JM}\rangle$ is obtained with energy

$$
\widetilde{E}_G^J \underset{\tau \to +\infty}{=} \frac{\mathbb{E}\left[\widetilde{\Pi}_\tau \mathrm{Re}\langle \hat{H}\rangle_{\Psi_T^J \Phi_\tau}\right]}{\mathbb{E}\left[\widetilde{\Pi}_\tau\right]}, \tag{15}
$$

deduced from Eqs. (6) and (14). Note that a similar expression also holds for any scalar observable that commutes with $\hat{H}$. In other cases, the well-known mixed and extrapolated estimators can be utilized to approximate ground-state expectation values of any operator [8].

The quality of the trial wave function obviously affects the efficiency of the phaseless QMC approach: The better the state $|\Psi_T^{JM}\rangle$, the more reduced the artificial bias due to the constraint. In addition, the imaginary time needed to converge depends on the quality of the state used to initiate the propagation. Both these arguments have naturally led us to adopt as trial wave function the symmetry-restored variational solution obtained by energy minimization in the subspace of Slater determinants after quantum number projection, i.e. by a variation-after-projection (VAP) approach [7]. For the shell model, such a method is similar to the so-called VAMPIR (Variation After Mean-field Projection In Realistic model spaces) approach [15].

2.4. Numerical issues
Let us now focus on the simulation of the probability distribution and the computation of observables, especially the energy. A direct evaluation of Eq. (15) turns out generally very ineffective owing to the exponential spread of the weights $\widetilde{\Pi}_\tau$ with τ. This problem may however be circumvented by sampling the realizations $\{|\Phi_\tau\rangle\}$ according to their weight *via* stochastic reconfiguration schemes developed in the framework of Green's-function Monte-Carlo methods. They are based on a birth/death mechanism, applied regularly during the Brownian motion every step $\Delta\tau_r$ before the variance of the probability distribution becomes too large. The walkers being cloned or killed depending on their weight, those causing phase problems are automatically filtered ($\widetilde{\Pi} = 0$ in this case). Therefore, the number N_w of realizations is variable, which introduces a bias in the calculated averages. Nevertheless, a stochastic reconfiguration scheme that eliminates this bias by maintaining a fixed number of walkers has been proposed in Ref. [16], and we implement it in our QMC simulations. When the size N_w of the population is large enough, it does not affect the averages, but artificial statistical correlations between the walkers are induced by the birth/death process and have to be taken into account. Instead, we consider an alternative approach that consists in performing several independent simulations with N_w Slater determinants. In this way, the energy (resp. estimator of an observable) is deduced by averaging the energies (resp. estimators) reconstructed for each population, and the associated error bars are determined on the basis of the central limit theorem.

3. Application: proof-of-principle results
The implementation described above of the phaseless QMC scheme for the shell model thus contains three tunable parameters: The imaginary-time step $\Delta\tau$, the number N_w of walkers that compose the populations, and the period of stochastic reconfiguration $\Delta\tau_r$. In order to assess the sensitivity of the results with respect to these variables, the QMC energies of the $J = 0$ ground state of ^{28}Mg as obtained with different sets of values $(\Delta\tau, \Delta\tau_r, N_w)$ and the USD effective interaction [17] are reported in Fig. 1. They are compared to the exact energies from direct diagonalization carried out by the code ANTOINE [1]. First, we notice that the phase problem is well managed since no explosion of error bars is observed during the imaginary-time evolution. Furthermore, the upper panel shows that a systematic deviation emerges for a time step $\Delta\tau = 0.1$ MeV^{-1}. It is explained by the Trotter-Suzuki breakup [10] whose validity is limited to second order in $\Delta\tau$. In the central panel, the energies for $N_w = 100$ and $N_w = 200$ walkers are in
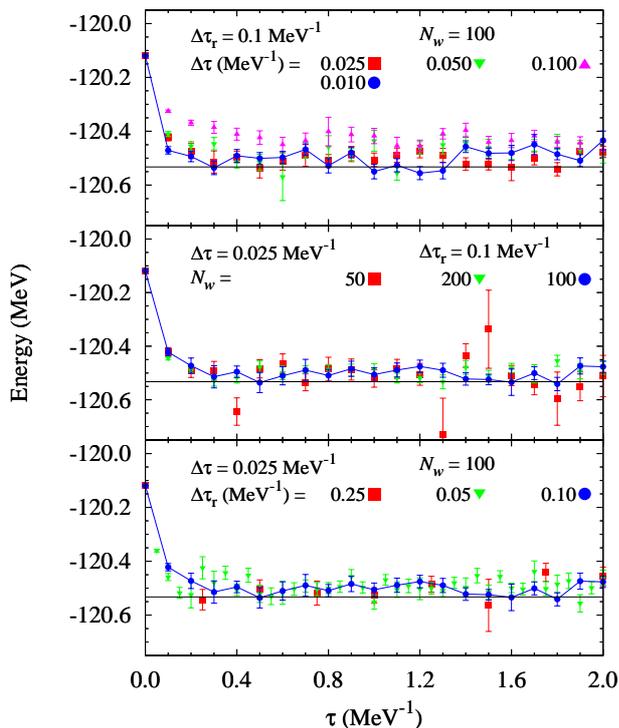
Figure 1. Influence of the simulation parameters: ground-state QMC energies of ^{28}Mg versus imaginary time for different steps $\Delta\tau$ (upper panel), sizes N_w of the populations (central panel), periods of reconfiguration $\Delta\tau_r$ (bottom panel), compared to the exact one (black line).

agreement within statistical errors, while significant fluctuations appear for $N_w = 50$. This ensues from the stochastic reconfiguration scheme that roughly samples the distribution of the weights and entails a bias when the number of realizations is too small. Finally, we see on the bottom panel that the time step of reconfiguration hardly affects the results, even though the error bars are larger for a longer period $\Delta\tau_r = 0.25$ Mev^{-1} as a consequence of a larger dispersion of the weights that exponentially spread with τ. In view of these observations, all the calculations reported here and in Ref. [7] have systematically been performed with the following set of parameters: $\Delta\tau = 0.01$ Mev^{-1}, $\Delta\tau_r = 0.1$ Mev^{-1}, and populations of $N_w = 100$ walkers.

Let us now report proof-of-principle results by addressing a system for which exact results are available. Figure 2 displays the VAP, QMC, and exact yrast spectra of ^{27}Na with the USD interaction. First, we observe that the VAP method offers a good approximation: Yrast energies differ from the exact values by less than about 1 MeV. Then, the phaseless energies agree remarkably well with the values from exact diagonalization: For any angular momentum, the relative errors do not exceed 0.3%, with statistical error bars of about 40-50 keV. The case of ^{27}Na provides a particularly good evidence of the efficiency of the method in controlling the phase problem. Indeed, it represents the most pathological systems for QMC simulations because it combines two sources of phase problems that are an odd number of particles, and a 'bad-sign' interaction [9]. Accordingly, this example clearly shows the ability of the method to provide nearly exact yrast energies, irrespective of the interaction or the kind of nuclei.

4. Conclusions and perspectives

In summary, we have presented a new QMC formalism for the shell model able to almost exactly reproduce the spectroscopy of any type of nucleus with realistic effective interactions. The formalism relies on a trial wave function whose roles are (i) to initiate and guide the underlying Brownian motion in order to improve the efficiency of the sampling (ii) to constrain the stochastic paths in order to control the phase problem thanks to the phaseless approximation.

Recent developments have aimed to extend the approach for computing excited states of a
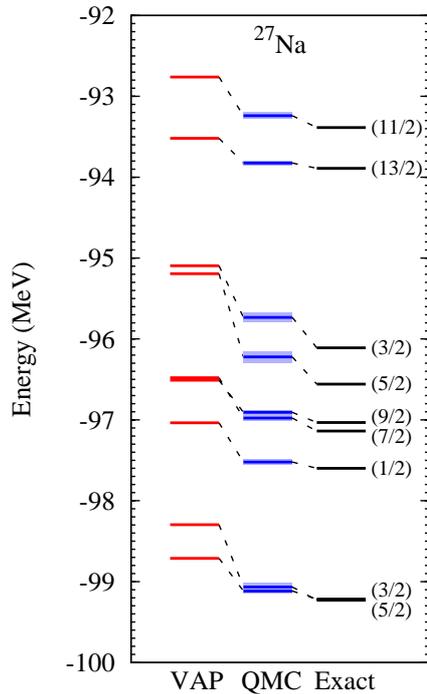
Figure 2. Yrast spectra of ^{27}Na as obtained with the VAP and phaseless QMC methods compared to the exact energy levels. The lighter areas indicate the QMC statistical errors. Preliminary results on non-yrast states are also shown (see section 4).

given angular momentum, achieving thus a complete spectrum of nuclei. To fulfil this objective, the main task is the determination of VAP wave functions orthogonal to the one previously computed for the ground state: For instance, the first excited state of spin J is obtained by minimizing the energy with the wave function $\hat{Q}|\Psi^{JM1}\rangle$, where $|\Psi^{JM1}\rangle$ is a projected Slater determinant of form (13) and $\hat{Q}$ the projector onto the subspace orthogonal to the VAP ground state. This ansatz can easily be generalized for sequentially searching the n-th excited state. In this way, by using such VAP solutions to initiate, guide, and constrain the Brownian motion, the phaseless QMC approach is no longer restricted to yrast spectroscopy. Preliminary results of this extended formalism are shown in figure 2, where the energies of the first excited $5/2^-$ and $3/2^-$ states are reproduced with the same accuracy than the yrast states.

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