

Effective hamiltonian approach and the lattice fixed node approximation

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Abstract. We define a numerical scheme that allows to approximate a given Hamiltonian by an effective one, by requiring several constraints determined by exact properties of generic "short range" Hamiltonians. In this way the standard lattice fixed node is also improved as far as the variational energy is concerned. The effective Hamiltonian is defined in terms of a guiding function ψ_G and can be solved exactly by Quantum Monte Carlo methods. We argue that, for reasonable ψ_G and away from phase transitions, the long distance, low energy properties are rather independent on the chosen guiding function, thus allowing to remove the well known problem of standard variational Monte Carlo schemes based only on total energy minimizations, and therefore insensitive to long distance low energy properties.

INTRODUCTION

After many years of intense numerical and theoretical efforts the problem of strong correlation in 2d or higher dimensional systems is still open. The main difficulty is to calculate the ground state of a many-body strongly correlated Hamiltonian with a technique which is systematically convergent to the exact solution with a reasonable computational effort. Quite generally all the known approximate techniques rely on the variational principle. The many-electron wavefunction is determined by an appropriate minimization of the energy within a particular class of wavefunctions. The Hartree-Fock method is the first clear example: here the many-electron wavefunction is approximated by a single Slater determinant. Indeed also a very recent technique like the Density-Matrix Renormalization Group (DMRG)[1] falls in this class, being certainly a variational approach, based on a particularly smart iteration scheme to define a variational wavefunction very good for low dimensional systems. However, within the variational approach, one faces the following problem: By increasing the system size the gap to the first excited state scales generally to zero quite rapidly. Thus between the ground state energy and the variational energy there may be a very large number of states with completely different correlation functions. In this way one can generally obtain different variational wavefunctions with almost similar energy, but with completely different correlation functions and therefore compelling physical meaning. By the above consideration it is easily understood that, within a straightforward variational technique and limited accuracy in energy -say 1%, there is no hope to obtain sensible results for large system size, unless for model Hamiltonians with a finite gap to all excitations, such as the simplest band insulators. The most striking example of this limitation of the variational approach is given by the Heisenberg model $H = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j$ where it was shown in[2] that two

wavefunctions with completely different long-distance properties, with or without anti-ferromagnetic long range order, provide almost similar (and very accurate within 0.1% accuracy) energy per site in the thermodynamic limit.

In the following we will consider a possibility to overcome the above limitation by means of the "effective Hamiltonian" approach. The main task is not to approximate a wavefunction as in the variational approach, but more conveniently our effort is to approximate the Hamiltonian H as closely as possible by means of a correlated Hamiltonian H^{eff} that can be solved numerically by Quantum Monte Carlo schemes. The important point is that, within this construction, some important properties of physical short range Hamiltonians are preserved, providing in this way a much better control of correlation functions.

HAMILTONIAN AS MATRIX ELEMENTS: BACK TO HEISENBERG

Let us consider the configuration basis $\{x\}$, where all the N electrons have definite spin (\uparrow or \downarrow) and positions on a lattice with L number of sites. The matrix elements of an Hamiltonian \tilde{H} in this physical basis will be indicated by $\tilde{H}_{x,x'}$. Obviously the chosen basis is crucial to define the concept of locality, a property of the hamiltonian. A physical short range Hamiltonian \tilde{H} has non zero off-diagonal matrix elements $\tilde{H}_{x,x'}$ only for configurations x and x' differing one another by local short-range moves of electrons, more precisely:

$$\tilde{H}_{x',x} \neq 0 \quad \text{if} \quad |x - x'| \leq \Lambda \quad (1)$$

where $|x - x'|$ indicates the distance in the $d \times N$ dimensional space, and $\Lambda \ll L$ is a suitable constant denoting the short-range character of the Hamiltonian \tilde{H} . In this definition the diagonal matrix elements do not play any role, so not only conventional Hubbard-Heisenberg-t-J model are short range Hamiltonian (with $\Lambda = 1$), but also models with long range interactions, provided these interactions-like the Coulomb one-are defined in the basis of configurations x , thus representing classical interactions in absence of the kinetic term. We believe that within this definition, essentially all physical Hamiltonian can be considered to belong to this class.

The $J_1 - J_2$ model

The simplest model that describes frustration of antiferromagnetism is the Heisenberg model with superexchange couplings extended up to nearest (J_1) and next nearest neighbor (J_2) couplings:

$$H = J_1 \sum_{\langle i,j \rangle_{n.n.}} \vec{S}_i \cdot \vec{S}_j + J_2 \sum_{\langle i,j \rangle_{n.n.n.}} \vec{S}_i \cdot \vec{S}_j \quad (2)$$

where summations $\langle i, j \rangle_{n.n.}$ ($\langle i, j \rangle_{n.n.n.}$) are over the nearest neighbor (next nearest neighbor) lattice sites R_i, R_j and periodic boundary conditions (PBC) are assumed.

Whenever the next-nearest neighbor exchange J_2 is large enough compared to the nearest neighbor one J_1 , it is widely believed that the antiferromagnetic phase is destabilized, until a second order transition takes place and a phase with a spin gap and a finite correlation length appears for J_2 large enough.

THE EFFECTIVE HAMILTONIAN

We will define here a simpler effective Hamiltonian matrix H^{eff} closely related to H , by means of the matrix elements $H_{x',x}^{eff}$ in the basis $\{x\}$ of configurations where all electrons have a definite spin \uparrow or \downarrow in all lattice sites R_i . Such an extension of the Hamiltonian H , whose matrix elements are analogously denoted by $H_{x',x}$, is obtained by means of the so called guiding function $\psi_G(x)$. This wavefunction is required to be non zero for all configurations x . Once the guiding function is defined for given $\{J_i\}$ the model H^{eff} can be solved exactly and, as we will show in some simple case, the low energy properties are independent of the low energy properties of ψ_G . The effective Hamiltonian approach allows to obtain ground state (GS) wavefunctions with non trivial signs (the one of ψ_G), in this sense representing a more generic GS of strongly correlated models. For instance the spin Hamiltonians that can be solved exactly by QMC methods are the ones for which:

$$s_{x',x} = \psi_G(x') H_{x',x} \psi_G(x) \leq 0 \quad (3)$$

for particularly simple $\psi_G(x)$ satisfying the Marshall sign rule

$$\psi_G(x) \propto (-1)^{\text{Number of spin down in one sublattice}}.$$

This is the case for the Heisenberg model 1d (gapless), 2chains (gapped but not spin liquid), 2d (gapless antiferromagnet), where it is also clear that with the same sign of the wavefunction different low energy properties can be obtained by solving exactly H or $H^{eff} = H$ being an exact equality in these simple cases.

Though there are particular models where the Marshall sign and (3) are satisfied even in presence of strong frustration[3, 4], it is clear that these are just particular and not generic models, since Eq.(3) is generally violated even when the GS of H is used in Eq.(3). The reason is that for generic frustrated Hamiltonian (with sign problem) there are off diagonal matrix elements with $s_{x,x'} > 0$, namely some matrix elements do not decrease the expectation value of the energy: they are "unhappy" even in the ground state as can be simply tested in the $J_1 - J_2$ model for $J_2 \neq 0$ or in even simpler model.

In this case the effective Hamiltonian H^{eff} is defined in terms of the matrix elements of H , in order to generate a dynamic as close as possible to the exact one. An obvious condition to require, is that if ψ_G is exact the ground state of H^{eff} has to coincide with the one of H . In order to fulfill this condition the so called lattice fixed node was proposed[5], $H^{eff} = H^{FN}$, and H^{eff} was obtained by strict analogy with the continuous fixed node scheme. In the following we will argue that there is a better way to choose the effective Hamiltonian, which not only provides better variational energies, but also allows a better accuracy of low energy long distance properties of the ground state. In the standard fixed node approach all the matrix elements that satisfy Eq.(3) are unchanged, whereas the remaining off-diagonal matrix elements are dealt semiclassically

and traced to the diagonal term of $H_{x,x}^{eff}$. The FN-effective hamiltonian can be obtained by modifying the diagonal term $H_{x,x}^{eff}$, in order to have the same local energy of the exact Hamiltonian for any configuration x , namely: $e_H(x) = e_{H^{eff}}(x)$, where the local energy is defined in terms of the guiding function ψ_G and an Hamiltonian \bar{H} by:

$$e_{\bar{H}}(x) = \sum_{x'} \psi_G(x') \bar{H}_{x',x} / \psi_G(x) \quad (4)$$

This approach was inspired from the similarity of the fixed node on continuous systems, and indeed is a well established approach giving also variational upper bounds of the ground state energy[5]. However in the lattice case there is an important difference.

Even for the fixed node ground state the number of matrix elements that do not satisfy the condition (3) may be a relevant fraction of the total number of matrix elements, whereas in the continuous case the so called nodal surface (the analogous of this frustrating matrix elements) represents just an irrelevant "surface" of the phase space.

In order to compensate for this bias in the dynamic, here we propose to modify slightly the fixed node scheme on a lattice, by compensating this error in the diffusion of the electrons:

$$H^{eff} = \begin{cases} KH_{x',x} & \text{if } x' \neq x \text{ and } s_{x',x} < 0 \\ 0 & \text{if } x' \neq x \text{ and } s_{x',x} > 0 \end{cases} \quad (5)$$

where K is a constant that can be determined in a way that the ground state of H^{eff} has the lowest possible expectation value of the energy on the exact Hamiltonian H . This procedure has been attempted previously but is very computer and time demanding, so its practical implementation is difficult[6].

The diffusion constant K and the Lieb-Schultz-Mattis theorem

In order to determine efficiently the value of the constant K we use a relation which is well known in the continuous fixed node[7] and was used to correct efficiently the error due to the finite time slice discretization of the diffusion process.[7] The method uses that, for small imaginary time ($\Delta\tau$), the electron positions change by means of the exact Hamiltonian propagation $\psi_G \rightarrow \exp(-H\Delta t)\psi_G$, with a diffusion coefficient determined only by the free Kinetic operator (the analogous of the off-diagonal matrix elements of a lattice Hamiltonian). It is possible then to correct the approximate finite Δt dynamic, by requiring that it satisfies exactly this short time condition, that mathematically can be simply written as:

$$[\vec{x}, [H, \vec{x}]] = D \quad (6)$$

where $D = 3\hbar^2/m$ is the diffusion coefficient, \vec{x} is the electron position operator, and m the electron mass.

In a lattice case, or more generally for a system with periodic boundary conditions, the lattice position operator \vec{x} is not well defined, as it cannot be matched with the boundary conditions, namely the same lattice point with (x, y) and $(x + L, y)$ coordinates, related by PBC in a $L \times L$ lattice, have different values for \vec{x} . Analogously to the Berry's phase

calculation[8] the spin and charge position operators are more appropriately defined in the exponential form:

$$O_{\rho,\mu}(x) = \exp(i \sum_R (\tau_\mu \cdot R) n_R) \quad (7)$$

$$O_{\sigma,\mu}(x) = \exp(i \sum_R (\tau_\mu \cdot R) S_R^z) \quad (8)$$

where $\mu = x, y, \dots$ labels the spatial coordinates, e.g. $\tau_x = (2\pi/L, 0)$, $\tau_y = (0, 2\pi/L)$ for a $L \times L$ square lattice. Both operators are defined in the basis of configurations x , as the analogous \vec{x} does in the continuous case.

Remarkably the spin position operator $O_{\sigma,\mu}$ is exactly equivalent to the well known Lieb-Schultz-Mattis operator, used to show a well known properties on the low energy spectrum of spin one-half Heisenberg Hamiltonians.[9] For a generic spin- $\frac{1}{2}$ Hamiltonian there may be two independent coupling constants K_ρ, K_σ that can be used to rescale the off-diagonal matrix elements and correct the spin and charge lattice diffusion constants independently. For instance in the $t - J$ model the charge diffusion is determined by the hopping matrix elements proportional to t and the spin-diffusion is set by the J matrix elements.

After simple inspection the following relation holds both for $O_{\mu,\sigma}$ and $O_{\rho,\sigma}$ (thus we omit σ, ρ labels):

$$\begin{aligned} \langle \psi_G | \left[O_\mu^\dagger, [\bar{H}, O_\mu] \right] | \psi_G \rangle = \\ - \sum_{x \neq x'} \psi_G(x) \psi_G(x') \bar{H}_{x,x'} | O_\mu(x) - O_\mu(x') |^2 \end{aligned} \quad (9)$$

This quantity can be very simply calculated by standard variational Monte Carlo both for $\bar{H} = H$ and $\bar{H} = H^{eff}$, at fixed guiding function ψ_G . In this way the value of the undetermined constant K_σ (K_ρ) is very well determined with high degree of statistical accuracy by imposing that both the effective Hamiltonian and the exact one have the same expectation value for the above quantity.

The final scheme

The constant K and therefore the effective model H^{eff} (5) are *uniquely* defined in terms of ψ_G and the exact Hamiltonian H . The ground state ψ_0^{eff} and low energy excitations of H^{eff} can be computed without sign problem. For a spin Hamiltonian, only the value of $K_\sigma < 1$ is required, whereas for the Hubbard model only $K_\rho < 1$ is important.

In order to compute the expectation value of the energy $\langle \psi_0^{eff} | H | \psi_0^{eff} \rangle$ over this approximate ground state for H (or at least an upper bound as in the standard lattice FN), one can use the method described in[6], which typically sizably improves the standard FN upper bound even in the standard case with $K_\sigma = K_\rho = 1$. As remarked in[6], it is not true (as in the continuous case) that in the lattice the lowest variational energy value correspond to $K = 1$.

The clear advantage of the effective Hamiltonian H^{eff} is that it remains in the same physical Hilbert space of H (compare for instance with large N or infinite dimension schemes) and, if universal low energy properties for generic model Hamiltonians are concerned, *it is just irrelevant* that H^{eff} is slightly different from H . In fact when we write down a model Hamiltonian in order to understand low energy properties (such as order, spin gap etc.) the underlying assumption is that between similar Hamiltonians (with similar matrix elements) the low energy properties cannot be too much different. If this is not the case, it is not even justified to write down H itself, rather the complete solution of the *all* electron problem with electron-electron and electron-ion Coulomb interaction should be fully considered: a clearly prohibitive task so far.

In a lattice case the effective Hamiltonian H^{eff} does not even imply a restriction of the Hilbert space (as in the continuous case where fixing the nodes determines a boundary condition that may not be satisfied by the excitations) and therefore it represents also a meaningful approximation to study the properties of its excitation spectrum.

RESULTS AND CONCLUSIONS

We have shown in a previous work[10] that, with the simple variational method, it is possible to obtain an almost exact representation of the GS wavefunction on small sizes, up to 6x6 sites, where exact diagonalization is possible. This remains true even in the strongly frustrated regime where also the Marshall sign rule is violated. That the correct signs of the wavefunction can be obtained with a BCS wavefunction (an uncorrelated one) is one of the most important facts that comes out from exact diagonalization on small sizes.

We present here preliminary results on the $J_1 - J_2$ model, by comparing the variational approach (VMC) the standard Fixed node method (FN) and the proposed one (FNSR) with $K_\sigma \neq 1$. As it is seen from Tab.(1) the value of K_σ is sizably different from zero in the spin liquid region and allows a remarkable improvement in the variational energy, significantly closer to the exact results available on this small clusters. The value of K_σ can reach values as small as 0.5, much different from the standard approach.

The reason of such a difference from the continuous case is easily understood. In the lattice case the number of matrix elements that can provide a sign change to a given configuration x , may be a considerable fraction of all the possible ones. For instance if we take for ψ_G a guiding function with the Marshall sign and consider $J_2 > 0$, all the spin-flip matrix elements determined by J_2 -namely almost half of all possible spin-flips-, are removed by the fixed node scheme (5). In the continuous case instead only the configurations that are on the so called nodal surface (where $\psi_G(x) = 0$) may be considered in an analogous situation, implying that the short time diffusion (6) is exactly satisfied for almost all configurations x , implying $K = 1$ in the limit when the fixed node is implemented exactly, namely with vanishing small Δt time step error.

As far as correlation functions are concerned we present in Tab. (2) the estimate of the static spin structure factor obtained with standard forward walking technique[11]:

$$S(\pi, \pi) = \sum_R e^{i(\pi, \pi)R} \langle \psi_0^{eff} | S_0^z S_R^z | \psi_0^{eff} \rangle \quad (10)$$

TABLE 1. Comparison of energies between standard fixed node (FN) and the present improved one (FNSR) as a function of J_2/J_1

J_2/J_1	VMC	FN	K_σ^{-1}	FNSR	Exact
0.00	-0.65112(5)	-0.6752(5)	1	-0.6752(5)	-0.6789
0.10	-0.61869(6)	-0.6326(1)	1.1093(1)	-0.6342(2)	-0.6381
0.20	-0.58700(4)	-0.5942(1)	1.2365(3)	-0.5962(1)	-0.5990
0.30	-0.55646(4)	-0.55937(3)	1.3831(5)	-0.56063(4)	-0.5625
0.40	-0.52732(1)	-0.52832(2)	1.5406(8)	-0.52891(2)	-0.5297
0.45	-0.51372(2)	-0.51441(2)	1.6146(9)	-0.51490(2)	-0.5157
0.50	-0.50117(2)	-0.50203(2)	1.677(1)	-0.50265(2)	-0.5038
0.55	-0.49024(2)	-0.49144(2)	1.732(1)	-0.49241(2)	-0.4952

TABLE 2. Comparison of the static magnetic structure factor $S(\pi, \pi)$ between standard fixed node (FN) and the present improved one (FNSR) as a function of J_2/J_1 . The values of K_σ are the ones of the previous table.

J_2/J_1	VMC	FN	FNSR	Exact
0.00	1.903(4)	3.06(13)	3.06(13)	2.518
0.10	1.840(8)	3.27(2)	2.94(9)	
0.20	1.733(7)	2.86(1)	2.94(2)	2.2295
0.30	1.645(7)	2.26(1)	2.47(1)	2.0132
0.40	1.505(7)	1.687(7)	1.766(7)	1.6604
0.45	1.394(6)	1.430(5)	1.439(7)	1.4309
0.50	1.258(5)	1.214(5)	1.167(5)	1.1695
0.55	1.124(5)	1.012(4)	0.927(5)	0.8946

and using as guiding function the variational wavefunction obtained in [10].

From the table we see that the value at $J_2 = 0$ slightly departs from the exact value both for the *FN* and the *FNSR* technique, which in this case should be the same and exact. The problem is that the guiding function ψ_G vanishes on a small size for a considerable fraction of configurations, preventing us to obtain the exact result. The large number of zero's for ψ_G affects also the small J_2 region, where indeed the FNSR does not improve the FN technique. However the situation drastically changes in the strongly frustrated regime, where the number of zero's is vanishingly small, the wavefunction being much more accurate, and the FNSR provides essentially exact results, by considerably improving both the standard VMC and FN approaches.

It is clear however that further and more systematic work is necessary to clarify the relevance of the proposed method compared with the conventional ones. Certainly it greatly simplifies -being equivalent in spirit- the standard SR technique[6], as the latter one may also provide even better variational energies, but very similar correlation functions, which should represent our main task in the study of strongly correlated systems.

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REFERENCES

1. S.R. White and D. Scalapino, Phys. Rev. Lett. **80** 1272 (1998); *ibidem* Phys. Rev. B **60**, 753 (1999).
2. S. Liang, B. Doucot, and P. W. Anderson, Phys. Rev. Lett. **61**, 365 (1988).
3. G. Santoro, S. Sorella, L. Guidoni, A. Parola, and E. Tosatti, Phys. Rev. Lett. **83**, 3065 (1999).
4. A. W. Sandvick, S. Daul, R. R. P. Singh, and D. J. Scalapino, Phys. Rev. Lett. **89**, 24720 (2002).
5. D. F. B. ten Haaf, J. M.J. van Leeuwen, W. van Saarloos, and D. M. Ceperley, Phys. Rev. B **51**, 13039 (1995).
6. S. Sorella cond-mat/0201388, lecture notes for the Euro-Winter School Kerkade-NL (2002); see also S. Sorella, Phys. Rev. B **64**, 024512 (2001).
7. P. J. Reynolds, D. M. Ceperley, B. J. Alder, and W. A. Lester, J. Chem. Phys. **77**, 5593 (1982).
8. R. Resta and S. Sorella, Phys. Rev. Lett. **74**, 4738 (1995).
9. E.H. Lieb, T.D. Schultz, D.C. Mattis, Ann. Phys. (N.Y.) **16**, 407 (1961); I. Affleck and E.H. Lieb, Lett. Math. Phys. **12**, 57 (1986).
10. L. Capriotti, F. Becca, A. Parola, and S. Sorella, Phys. Rev. Lett. **87**, 097201 (2001).
11. M. Calandra and S. Sorella, Phys. Rev. B **57**, 11446 (1998).