A Quantum Monte Carlo formulation for non-local interactions

Francesco Pederiva

Physics Department, University of Trento, Italy
and
INFN-TIFPA (Trento Institute for Fundamental Physics and Applications)
pederiva@science.unitn.it

October 14, 2015

Collaborators

- Abhishek Mukherjee (ClusterVision B.V. - Amsterdam)
- Alessandro Roggero (INT - Seattle)
- Lorenzo Contessi, Paolo Mori (Trento)

Overview

Some Motivations...

- In many cases of interes, it might be useful to have a stochastic projection algorithm *a la* Quantum Monte Carlo defined in a generic representation of the Hilbert space (e.g. momentum space). For certain Hamiltonians, this is not just useful, but necessary.
- There are very efficient variational methods, like CI, CI, NCSM, providing very accurate wavefunctions, but hard to manage in coordinate space, hence useless in standard QMC. *An accurate wavefunction is an essential ingredient in projection MC calculations.*
- Momentum distribution (and other momentum related observables) in QMC, or response functions from the inversion of general kernels, not just Laplace:
  "difficult" in standard coordinate-space MC.

Some references...

- Projection Monte Carlo in Fock space (from Quantum chemistry...):
  G. H. Booth, A. J. W. Thom, and A. Alavi, *J. Chem. Phys.* **131**, 054106 (2009); D. Cleland, G. H. Booth, and A. Alavi, *ibid.* **132**, 041103 (2010).
- Importance sampling:
  M. Kolodrubetz and B. K. Clark, *Phys. Rev. B* **86**, 075109 (2012).
- CIMC for cold fermion gases:
  A. Mukherjee and Y. Alhassid, *Phys. Rev. A* **88**, 053622 (2013).
- This work:
  A. Roggero, A. Mukherjee, and FP *Phys. Rev. B* **88**, 115138 (2013); A. Roggero, A. Mukherjee, and FP *Phys. Rev. Lett.* **112**, 221103 (2014).

Configuration Interaction Monte Carlo

We start considering a generic Hamiltonian including up to two–body interactions (generalization to three-body, when needed, is easy).

$$H \equiv \sum_{\alpha \in \mathcal{S}} \epsilon_\alpha a^\dagger_\alpha a_\alpha + \sum_{nmpq \in S} V_{\alpha\beta\gamma\delta} a^\dagger_\alpha a^\dagger_\beta a_\gamma a_\delta$$

Here S is he set of single particle states labeled by the index α. Such set is assumed to be finite and of size $\mathcal{N}_\mathcal{S}$ (in general this is a *model* Hilbert space).

Notice that no assumption is made on the local or non-local nature of the Hamiltonian.

Configuration Interaction Monte Carlo

The idea is to project the ground state of the Hamiltonian *restricted to the model Hilbert space chosen* by means of a stochastic implementation of the *power method*.

Consider a matrix $\mathbf{A}$ and assume it has a dominant eigenvalue $\lambda_0 > \lambda_1 > \lambda_2 \cdots$, and a corresponding dominant eigenvector $\mathbf{x}_0$. Start from a generic vector $\mathbf{x}$ not orthogonal to $\mathbf{x}_0$, and apply M times to it the matrix A:

$$\mathbf{A}^M \mathbf{x} = \mathbf{A}^M \sum_n c_n \mathbf{x}_n = \sum_n \lambda_n^M \mathbf{x}_n$$

Clearly the component along the dominant eigenvector takes over al the other components exponentially with M.

Configuration Interaction Monte Carlo

Define now a *projection operator*:

$$\mathcal{P}_{\Delta\tau} = 1 - \Delta\tau(H - E_T)$$

Clearly $\mathcal{P}_{\Delta\tau}$ has the same eigenvectors as H, but given the minus sign we will pick up the dominant egenvector will correspond to the lowest eigenvalue E_0. If $E_T = E_0$ the normalization of the dominant eigenvector is preserved, since the dominant eigenvalue is 1.
Given the finiteness of the space, if we choose $\Delta\tau$ such that

$$\Delta\tau < \frac{2}{E_{max} - E_T}$$

where E_{max} is the highest eigenvalue of H in the model Hilbert space, all the eigenvalues of $\mathcal{P}$ are *guaranteed to be positive*.

Configuration Interaction Monte Carlo

The propagation of a generic state $|\Psi\rangle$ for an imaginary time interval $\Delta\tau$ is defined as:

$$|\Psi(\tau + \Delta\tau)\rangle = \mathcal{P}_{\Delta\tau}|\Psi(\tau)\rangle.$$

A repeated application of the propagator yelds the projection on the ground state:

$$|\Psi_0\rangle = \lim_{\tau\to\infty} |\Psi(\tau)\rangle$$

provided that the projection is started from a state that is non-orthogonal to the ground state.

Configuration Interaction Monte Carlo

For a N-Fermion system we label the Slater determinants constituting the Hilbert space with a label $\mathbf{n} \equiv \{n_1 \dots n_N\}$ where $n_\alpha = 0, 1$, and α labels a set of quantum numbers determining the single particle state (any other way is just as good).
In configuration representation the imaginary time step can be written as:

$$\langle \mathbf{n}|\Psi(\tau + \Delta\tau)\rangle = \sum_{\mathbf{m}} \langle \mathbf{n}|\mathcal{P}|\mathbf{m}\rangle\langle \mathbf{m}|\Psi(\tau)\rangle.$$

As it is commonly done also in standard coordinate space DMC, we rewrite the matrix elements of the propagator as:

$$\langle \mathbf{n}|\mathcal{P}|\mathbf{m}\rangle = g(\mathbf{m})p(\mathbf{n},\mathbf{m})$$

where

$$g(\mathbf{m}) = \sum_{\mathbf{n}} \langle \mathbf{n}|\mathcal{P}|\mathbf{m}\rangle \qquad p(\mathbf{n},\mathbf{m}) = \frac{\langle \mathbf{n}|\mathcal{P}|\mathbf{m}\rangle}{g(\mathbf{m})}.$$

Configuration Interaction Monte Carlo

If all the matrix elements of $\mathcal{P}$ are non- negative, then we can interpret $p(\mathbf{n},\mathbf{m})$ as a transition probability between the states $\mathbf{n}$ and $\mathbf{m}$, while $g(\mathbf{m})$ is a "weight" of the configuration (relative change in normalization).

From this point on, the algorithm might seem trivial. Transitions are sampled according to the magnitude of the matrix elements and walkers in the Hilbert space are replicated in the usual way.

PROBLEMS!

1. As the number of states and/or particles increases, the upper bound for $\Delta\tau$ gets smaller and smaller, introducing huge autocorrelations $\rightarrow$ VERY INEFFICIENT ALGORITHM
2. For a generic Hamiltonian, for which the matrix elements $\langle\mathbf{n}|H|\mathbf{m}\rangle$ have arbitrary sign, we can have $p(\mathbf{n},\mathbf{m}) < 0$, and the algorithm breaks down.

Exponential propagator

We cope with the first problem by using the algorithm introduced by Trivedi and Ceperley (PRB **41**, 4552 (1990)) which has some analogies with the Domain's Green's Function Monte Carlo of Kalos Verlet and Levesque.

We start from the state $|\mathbf{m}\rangle$. A time-step $\Delta\tau$ is set after which the state is declared not to change (i.e. the "$\delta_{\mathbf{n},\mathbf{m}}$" part of P is used). The initial weight is $g = 1$. Then, a time $\Delta\tau_{od}$ is sampled with probability:

$$e^{-\Delta\tau_{od}\sum_{\mathbf{n}\neq\mathbf{m}}\langle\mathbf{n}|H-E_T|\mathbf{m}\rangle}$$

If $\Delta\tau_{od} > \Delta\tau$ then the state is propagated unchanged with weight $\exp[-\Delta\tau\sum_{\mathbf{n}\neq\mathbf{m}}\langle\mathbf{n}|H-E_T|\mathbf{m}\rangle]$.

Exponential propagator

If we have instead $\Delta\tau_{od} < \Delta\tau$, a transition to a new state $|\mathbf{n}'\rangle$ is sampled with probability:

$$\frac{\langle \mathbf{n}'|H - E_T|\mathbf{m}\rangle}{\sum_{\mathbf{n}\neq\mathbf{m}}\langle \mathbf{n}|H - E_T|\mathbf{m}\rangle}$$

The time step $\Delta\tau$ is then reduced so that $\Delta\tau \to \Delta\tau - \Delta\tau_{od}$, and the weight of the walker is multiplied by $\exp\left[-\Delta\tau_{od}\sum_{\mathbf{n}\neq\mathbf{m}}\langle \mathbf{n}|H - E_T|\mathbf{m}\rangle\right]$. This process is repeated until $\Delta\tau_{od} > \Delta\tau$. This procedure exactly samples

$$\langle \mathbf{n}|\mathcal{P}|\mathbf{m}\rangle = \langle \mathbf{n}|e^{-\Delta\tau(H-E_T)}|\mathbf{m}\rangle$$

without any time-step error.

(For an extended discussion see e.g. Schmidt, Niyaz, Vaught, Lee, PRE **71**, *016707 (2005))*

Importance sampling

The sign problem cannot be circumvented for a Hamiltonian that is not purely attractive.
However, it is possible to come up with an algorithm similar to constrained algorithms (such as the fixed-node or fixed-phase approximations) in standard DMC. The difference is that the constraint is now implemented as a transformation of H (see Shell Model MC calculations).

At this point we might want to introduce an importance function $\Phi_G(\mathbf{n}) \equiv \langle \mathbf{n}|\Phi_G\rangle$ which in general includes dynamic correlations.
Let's then define a "sign" function:

$$\mathfrak{s}(\mathbf{n},\mathbf{m}) = \mathrm{sgn}\{\mathfrak{Re}\left[\langle\Phi_G|\mathbf{n}\rangle\langle\mathbf{n}|H|\mathbf{m}\rangle\langle\mathbf{m}|\Phi_G\rangle\right]\}$$

Importance sampling

Now we can build a family of parametrized Hamiltonians $\mathcal{H}_\gamma$ defined as:

$$\langle \mathbf{m}|\mathcal{H}_\gamma|\mathbf{n}\rangle = \begin{cases} -\gamma\langle \mathbf{n}|H|\mathbf{m}\rangle & \mathfrak{s}(\mathbf{n},\mathbf{m}) > 0 \\ \langle \mathbf{n}|H|\mathbf{m}\rangle & \text{otherwise} \end{cases}$$

when $\mathbf{n} \neq \mathbf{m}$, and the diagonal elements are given by:

$$\langle \mathbf{m}|\mathcal{H}_\gamma|\mathbf{m}\rangle = \langle \mathbf{m}|H|\mathbf{m}\rangle + (1+\gamma) \sum_{\substack{\mathbf{n}\neq\mathbf{m} \\ \mathfrak{s}(\mathbf{n},\mathbf{m})>0}} \langle \mathbf{n}|H|\mathbf{m}\rangle$$

Clearly for $\gamma = -1$ we obtain the original Hamiltonian.

Importance sampling

For any $\gamma \geq 0$ the *importance sampled* propagator:

$$\langle \mathbf{m}|\mathcal{P}_\gamma|\mathbf{n}\rangle = \delta_{\mathbf{m},\mathbf{n}} - \Delta\tau \frac{\Re e[\langle \Phi_G|\mathbf{n}\rangle\langle \mathbf{n}|\mathcal{H}_\gamma - E_T|\mathbf{m}\rangle\langle \mathbf{m}|\Phi_G\rangle]}{|\langle \mathbf{m}|\Phi_G\rangle|^2}$$

is free from the sign problem, and the ground state of $\mathcal{H}_\gamma$ is an upper bound of the exact ground state energy of H. Moreover, the ground state is better than the expctation of the original Hamiltonian over $|\Phi_G\rangle$.

This procedure is somewhat equivalent to the standard way of constraining calculations in QMC.

(For the upper bound proof see e.g.ten Haaf et al, PRB **51**, 13039 (1995), and Sorella et al. PRB **61**, 2599 (2000))

Energy evaluation

Energies can be easily estimated for any positive value of γ via the usual "mixed" estimate

$$E_\gamma \simeq \frac{\sum_{\mathbf{n_i}} \mathcal{E}_\gamma^L(\mathbf{n_i}) g(n_i)}{\sum_{\mathbf{n_i}} g(n_i)}$$

where $\mathcal{E}_\gamma^L$ is the local energy defined by:

$$\mathcal{E}_\gamma^L = \frac{\langle \Phi_G | \mathcal{H}_\gamma | \mathbf{n} \rangle}{\langle \Phi_G | \mathbf{n} \rangle}$$

The energy E_γ can then be extrapolated to $\gamma = -1$ to obtain an even tighter upper bound, and assuming that the extrapolation is linear:

$$E_{CIMC} = 2E_{\gamma=0} - E_{\gamma=1}$$

Use of Coupled-Cluster wavefunctions

An excellent importance function is given by the CC wavefunction

$$|CC\rangle = e^{\hat{T}}|HF\rangle$$

where $|HF\rangle$ is the Hartree-Fock solution of the problem. The operator $\hat{T}$ is hierarchically divided in $\hat{T} = \hat{T}_1 + \hat{T}_2 + \hat{T}_3 + \cdots$, where:

$$\hat{T}_1 = \sum_{ia} t_i^a a_a^\dagger a_i \quad \hat{T}_2 = \frac{1}{4} \sum_{ijab} t_{ij}^{ab} a_a^\dagger a_b^\dagger a_i a_j \quad \cdots$$

What we need in our calculation is an efficient evaluation of the overlap of the CC wavefunction with an arbitrary Slater determinant describing an M-particle–M-hole state

$$|\mathbf{m}\rangle \equiv a_{p_1}^\dagger, \ldots, a_{p_M}^\dagger, a_{h_1}, \ldots, a_{h_M}|HF\rangle.$$

Use of Coupled-Cluster wavefunctions

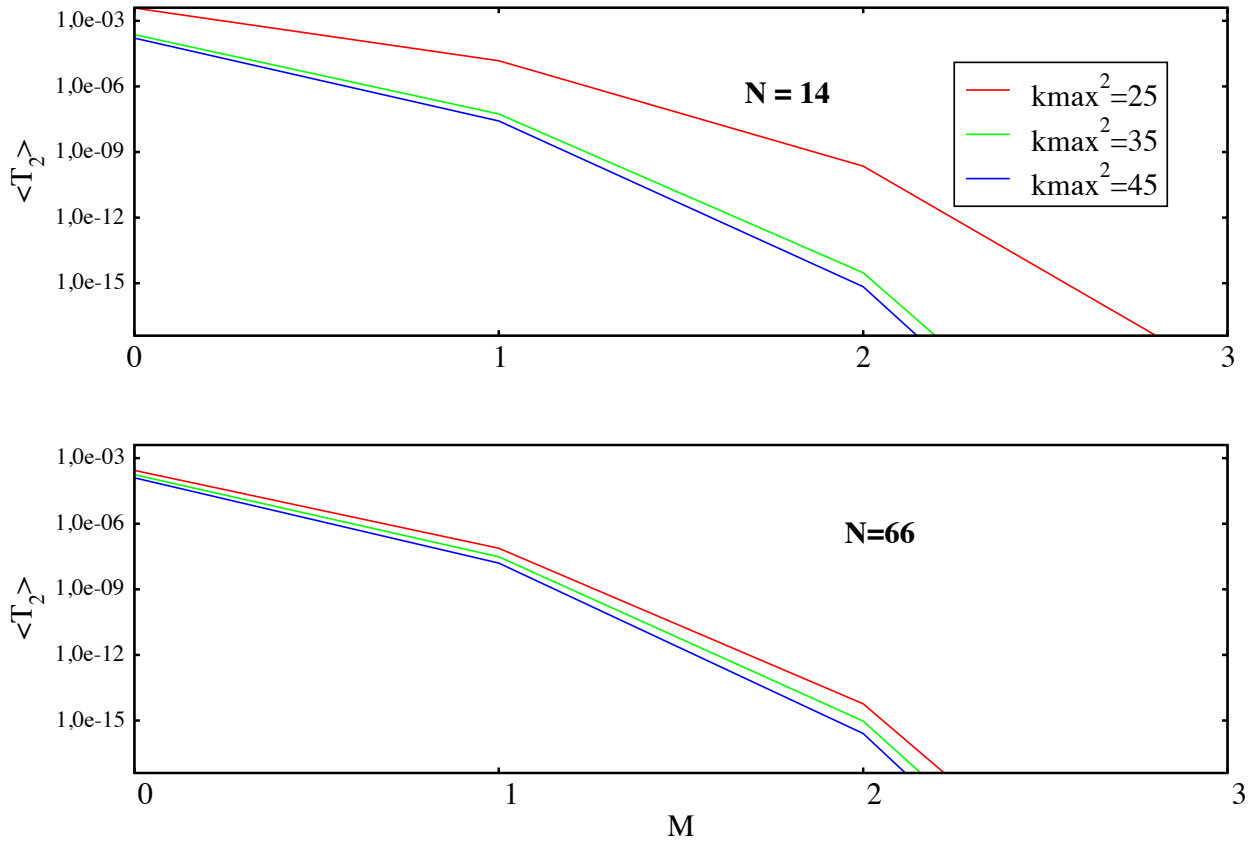
Let us consider e.g. the wavefunction for a homogeneous system (for which the lowest order is CCD because of the request of translational invariance). The required amplitude can be expressed in turn as a superposition of $M-2$ particle/hole states that can be generated from $\mathbf{m}$. Eventually (the proof is lengthy) one obtains:

$$\langle \mathbf{m} | \Phi_{CCD} \rangle = \sum_{\gamma=2}^{M} \sum_{\mu<\nu}^{M} (-1)^{\gamma+\mu+\nu} t_{h_1,h_\gamma}^{p_\mu p_\nu} \Phi_{CCD}^{M-2} \begin{pmatrix} p_1,p_2,\ldots,p_{\mu-1},p_{\mu+1},\ldots,p_{\nu-1},p_{\nu+1},\ldots,p_M \\ h_2\ldots,h_{\gamma-1},h_{\gamma+1},\ldots,h_M \end{pmatrix}$$

assuming $p_1 < p_2 < \cdots < p_M$ and $h_1 < h_2 < \cdots < h_M$.
The extension to singlets (ph states) and triplets (3p-3h states) is straightforward.

Use of Coupled-Cluster wavefunctions

Average T_2 coefficients



CIMC vs. standard GFMC/DMC

A FEW PROS:

- CIMC has the same propagator for any Hamiltonian. One just needs to compute matrix elements between basis states. Standard GFMC/DMC can in principle deal with non-local interactions in some cases, but propagators are highly non-trivial and expensive to compute.
- CIMC can be proved to provide an upper bound for the ground state energy also when using complex wavefucntions. At present some versions of the standard DMC method (like AFDMC) do not provide upper bounds.

CIMC vs. standard GFMC/DMC

A FEW CONS:

- CIMC suffers of a bias coming from the truncation of a the basis, while DMC virtually makes use of an *infinite* basis set, and does not have such bias (but in CIMC cutoffs in momentum space are defined in a more natural way...)
- The evaluation of wavefunctions for CIMC may become costly with the system size, while in DMC the evaluation of the function always has a well defined scaling.

Electron gas results

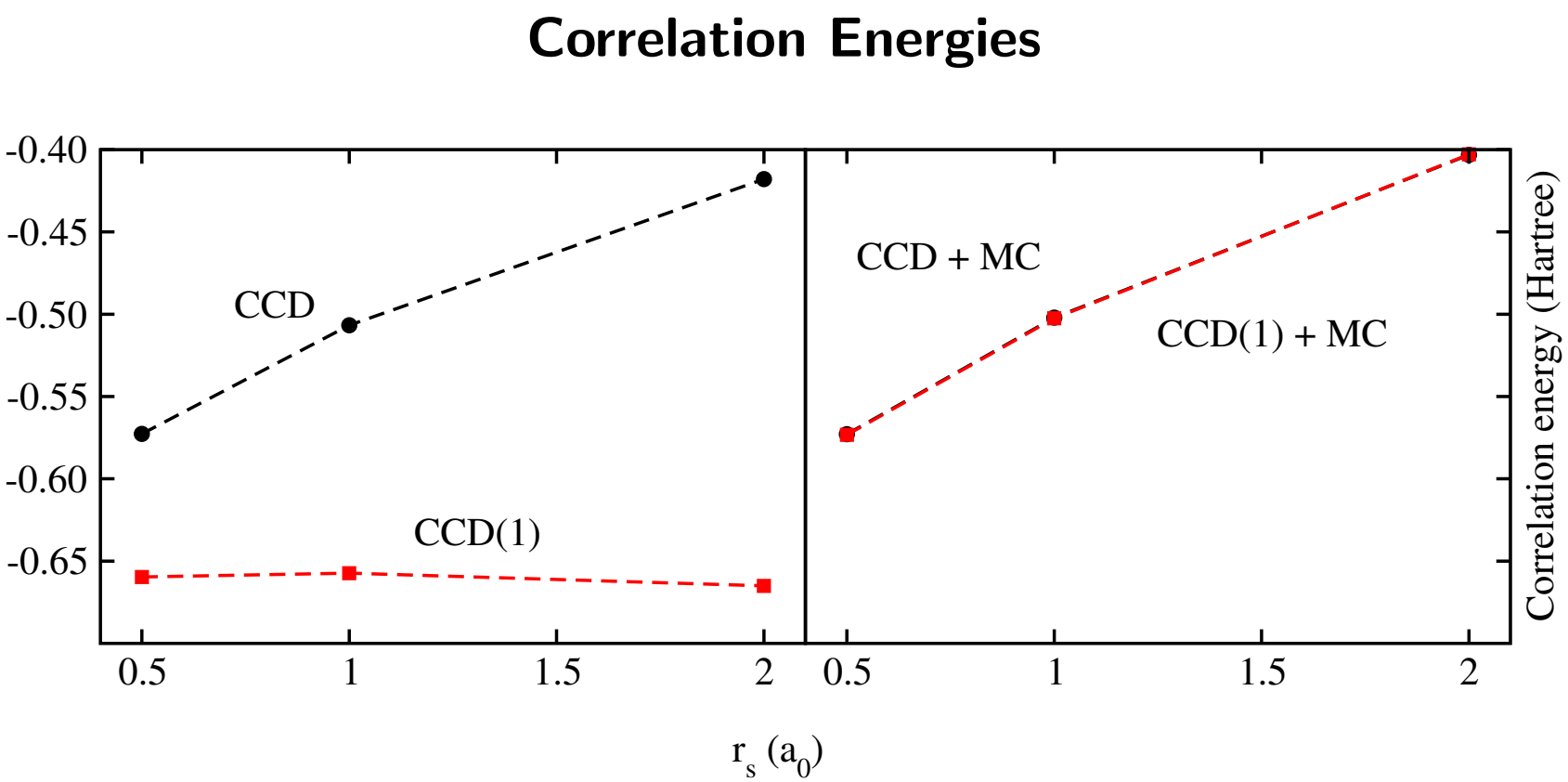
$$V(q) = \frac{4\pi}{q^2}, \quad \text{periodic b. c.}, \quad r_s = \left(\frac{3}{4\pi\rho}\right)^{\frac{1}{3}}$$

Charge neutrality is imposed by a uniform background of positive charge at density ρ.

In the table we show the CCD correlation energies, calculated using conventional CC theory, along with the corresponding Monte Carlo energies of an 3D electron gas system with $N = 14$ and $\mathcal{N}_s = 342$, for $r_s = 0.5, 1.0$ and 2.0.

	Correlation energy (a.u.)			
r_s	CCD	+ CIMC	CCD(1)	+ CIMC
0.5	-0.572682	-0.5729(3)	-0.659641	-0.5733(2)
1.0	-0.506701	-0.5021(3)	-0.657347	-0.5025(2)
2.0	-0.417946	-0.40317(2)	-0.665071	-0.4029(3)

Electron gas results



Electron gas results

- The results labeled with CCD(1) have been obtained by second order order perturbation theory (Moeller-Plesset approximation).
- It is extremely interesting to notice that the constrained projection gives essentially the same results both for the full CCD wavefunction and for CCD(1)!.
- This means that the prominent features of the nodal structure of the functions are recovered very soon in the perturbative expansion.
- → possible strong reduction of the computational cost with respect to a full CC calculation.

Electron gas results

Correlation energy (a.u)

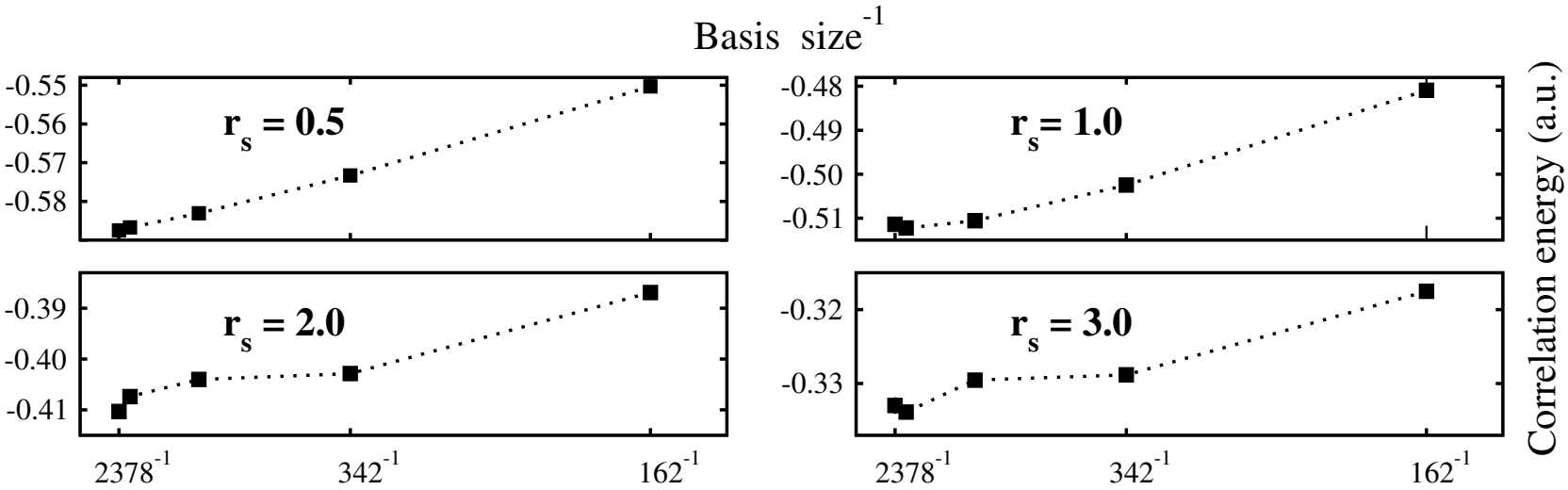
r_s	N	CIMC	Other
0.5	14	-0.5875(6)	-0.5959(7) [1]
	38	-1.809(4)	-1.849(1) [1]
	54	-2.354(2)	-2.435(7) [1]
			-2.387(2) [2]
1.0	14	-0.5114(5)	-0.5316(4) [1]
	38	-1.521(4)	-1.590(1) [1]
	54	-2.053(4)	-2.124(3) [1]
			-2.125(2) [2]
2.0	14	-0.4103(6)	-0.444(1) [1]
	38	-1.134(7)	-1.225(2) [1]
3.0	14	-0.333(1)	

Correlation energies obtained from CIMC calculations with the wavefunction evaluated at second order perturbation theory (MP2).
For these calculations we use $\mathcal{N}_{\mathcal{S}} = 2378$

[1] *J. J. Shepherd, G. H. Booth, and A. Alavi, J. Chem. Phys.* **136**, *244101 (2012).*
[2] *P.Lopez Rios, A.Ma, N.D.Drummond, M.D.Towler, and R. J. Needs, Phys. Rev.* **E** *74, 066701 (2006).*

Electron gas results

Extrapolation in Basis Size

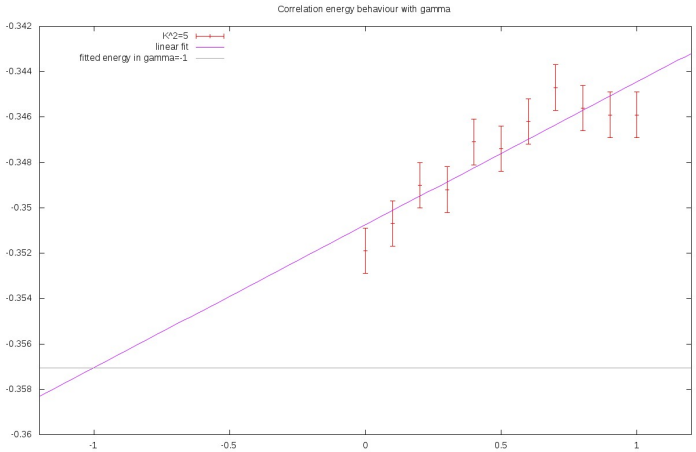


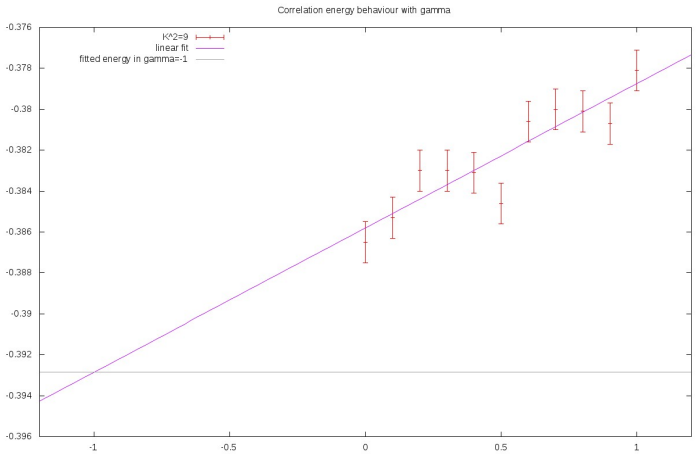
- No clear linear extrapolation for large values of $\mathcal{N}_S$.
- The situation is similar for calculations we performed with $N = 32$ and 54. Thus, at least up to our largest basis size $\mathcal{N}_s = 2378$, we cannot safely do an extrapolation to $\mathcal{N}_s \to \infty$ with a reasonably low χ^2.

Electron gas results

CCDT(1) Results (Preliminary)

CCDT(1)		
	Energy	Error
K^2=5	-0.3570	0.0016
K^2=9	-0.3865	0.0018
CCD		
	Energy	Error
K^2=5	-0.3538	0.0009
$K^2 = 9$	-0.3851	0.0020





Electron gas results

Computational gain

			Computational time (cpu hours)	
r_s	N	$\mathcal{N}_s$	CIMC	i-FCIQMC
0.5	14	1850	384	200
1.0	14	1850	768	2500
2.0	14	1850	768	2500
2.0	38	922	4608	16000

Computational cost of our method CIMC compared with the i-FCIQMC method (Sheperd et al.) for different r_s, N and $\mathcal{N}_s$.

CIMC for finite systems: Atoms

The algorithm was recently extended to finite systems, in particular to a subset of first row atoms (Be, C, O, Ne).

This calculation is not performed in momentum space, but in a space of determinants spanned by some Gaussian basis set. This is more convenient for the computation of the matrix elements and to benchmark the results.

Several different basis sets can be used. Here we report results for cc-pVDZ and a subset of aug-cc-pVDZ not including contractions with the *d* orbital.

CC and MP2 amplitudes in atoms

amplitude	MP2 value	CC value
t_1^9	-0.000419584968505	-0.000401806290974
t_1^{13}	0.000726032756716	0.000733616388008
t_2^{10}	-0.000419584968505	-0.000507490573453
t_2^{14}	0.000726032756716	0.000769255545851
t_{13}^{78}	-0.000933006312113	-0.000424639373447
t_{13}^{1112}	-0.000023957069557	0.000049419081067

Amplitudes for Carbon atom wave function in a MP2 and CCSD calculation using the cc-pVDZ basis. CC amplitudes have been taken after 10 iterations, when full convergence has not been reached yet.

Results for first row atoms (Preliminary)

cc-pVDZ

atom	MP2	CIMC	CCSD	CIMC
Be	-0.0217	-0.040(1)	-0.04073	-0.04090(1)
C	-0.03458	-0.0625(5)	-0.06474	-0.0628(3)
O	-0.00456	-0.06741(2)	-0.06107	-0.0714(1)
Ne	0.0895	-0.0589(2)	-0.0095	-0.0589(1)

aug-cc-pVDZ*

atom	MP2	CIMC	CCSD	CIMC
Be	-0.0228	-0.0437(3)	-0.0395	-0.0436(1)
C	-0.0455	-0.0860(1)	-0.0712	-0.0791(3)
O	-0.0393	-0.1300(3)	-0.1001	-0.1287(2)
Ne	0.0179	-0.1900(4)	-0.0103	-0.1839(6)

Non local effective interactions in neutron matter

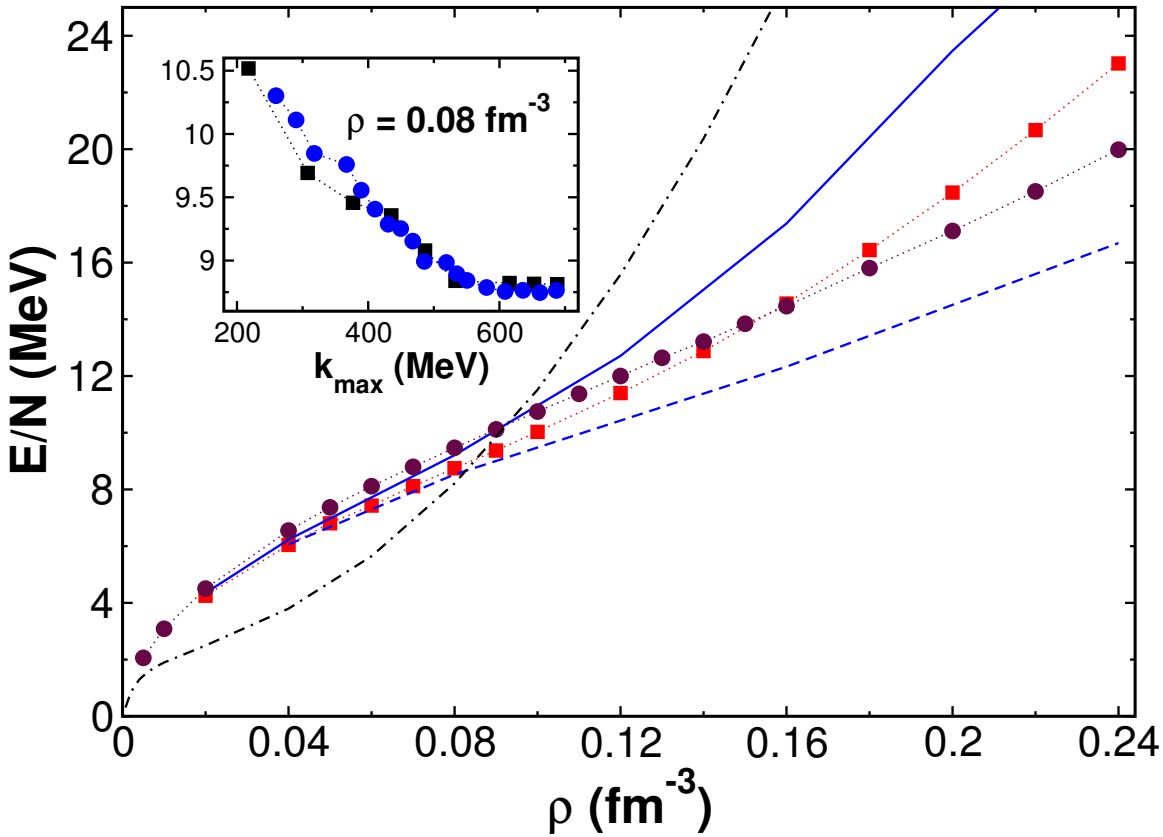
As previously mentioned, one of the advantages of CIMC is the the possibility of directly using non-local interactions.
In nuclear physics this means the possibility of using χ-EFT potentials with no need of a regularization in coordinate space.

Application: PNM with $NNLO_{opt}$ interactions (A Ekström *et. al*, PRL **110**, 192502 (2013)), fitting scattering data with $\chi^2 \sim 1$ at laboratory energies < 125MeV, but with a reduced contribucion of the TNF.

Non local effective interactions in neutron matter

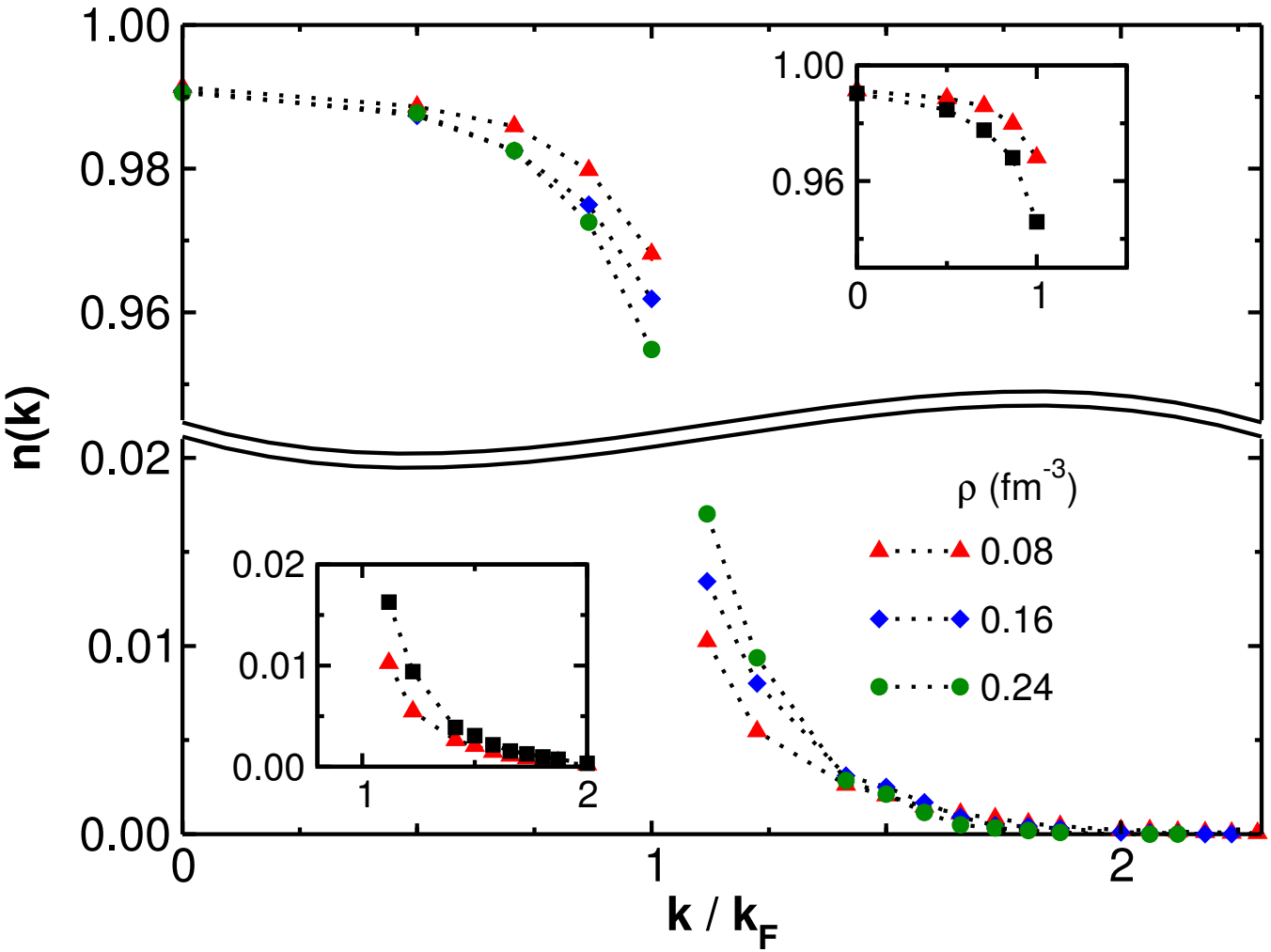
- Calculations performed at given density ρ for a periodic box containing A nucleons. Size of the box $L = (A/\rho)^{1/3}$.
- sp states on a lattice of size $l = 2\pi/L$, therefore the sp states are labelled by momentum $l(n_x, n_y, n_z)$, with $n_{\alpha=x,y,z}$ integers.
- We use a *spherical cutoff*, i.e. we include only momenta such that $\mathbf{k}^2 \leq k_{cut}^2$.
- As previously stated we do not include three-body forces in this calculation.

Non local effective interactions in neutron matter



Red squares - our results (66 neutrons), brown circles - AFDMC EoS with the 2b AV8, blue dashed line - APR EoS with the 2b AV18, blue solid line - APR EoS with the 2b AV18 + 3b UIX, black dashed dotted line - NL3 EoS (Shen, Horowitz et al.). The inset shows the convergence of our energies as a function of kmax at = 0.08 fm3 for 14 (black squares) and 66 (blue circles) particles. The dotted lines are a guide to the eye.

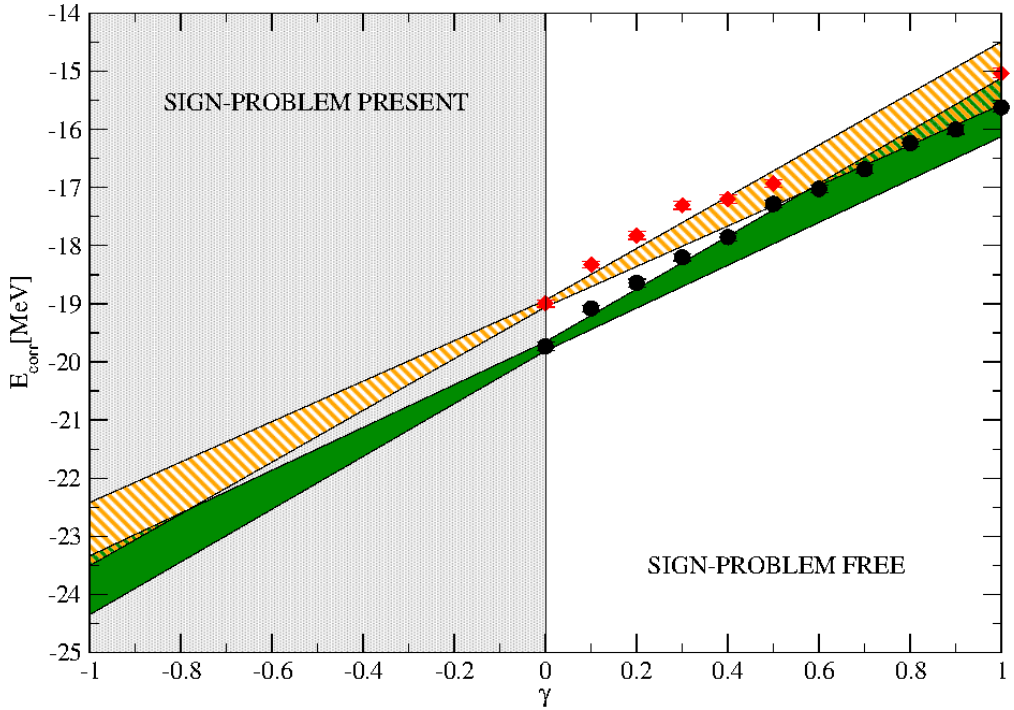
Momentum Distribution (66 neutrons, $NNLO_{opt}$)



Roubustness

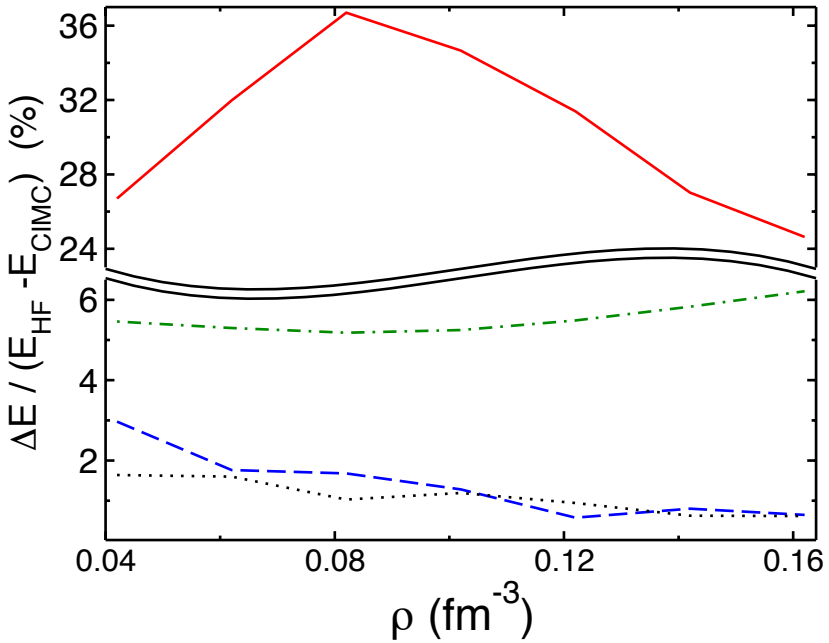
The results are quite robust with respect to the variation of the coefficients of the CC calculations. In this plot black dots are results obtained from MP2 and red dots are obtained varying the MP2 coefficients of a random amount with a Gaussian distribution (50% width).

Nucleon-Nucleon potential $NNLO_{opt}$, 66 neutrons



Extrapolation to $\gamma = 0$ is still overlapping within errorbars.

Analysis of uncertainties



- Red line: difference (in %) between PT-2 and QMC (effect of projection)
- Dashed blue line: Difference between CCD (thanky you Gaute and Thomas!) and QMC
- Black dotted line: Statistical error
- Green dashed line: Estimate of the fixed-phase bias

Spin/isospin impurities in polarized nuclear matter

Another interesting application of the method was the accurate determination of the energy of a spin/isospin impurity (the analog of a "polaron" in a polarized electron gas) in nuclear matter.

Calculations of the spin and isospin polaron are useful to constrain the "time-odd" components of density functionals.

Calculations are analogous to those made for the EoS of neutron matter, but for the fact that we in an elementary box we take A nucleons with spin (isospin) up (down) and one with spin (isospin) up (down). **Polaron energies at low ρ are essentially independent of the choice of the potential**.

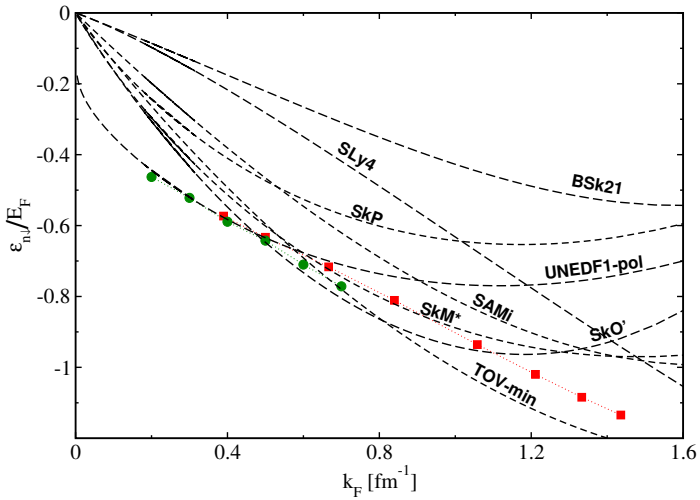
Spin/isospin impurities in polarized nuclear matter

Problem

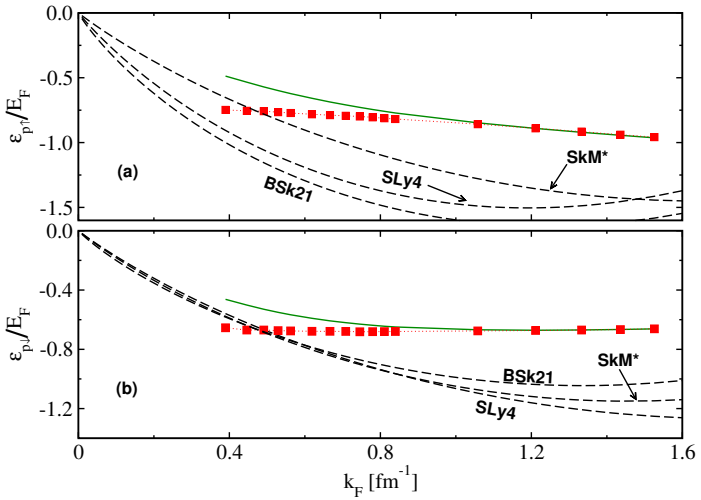
The energy difference we want to extract is order $1/A$. We might have to compromise between accuracy in the determination of the difference and reduction of finite size effects!

Actually we have verified that differences are quite small. For example at $\rho = 0.06\text{fm}^{-3}$ (the largest density considered) the polaron energy in NM is $\epsilon_{n\downarrow}/E_F = -0.6617 \pm 0.0003$ for $A = 7$ and -0.647 ± 0.004 for $A = 33$, i.e. $\sim 2\%$. Moreover the box size at this density is ~ 4.9fm, more than three times the π Compton wavelength.

Spin/isospin impurities in polarized nuclear matter

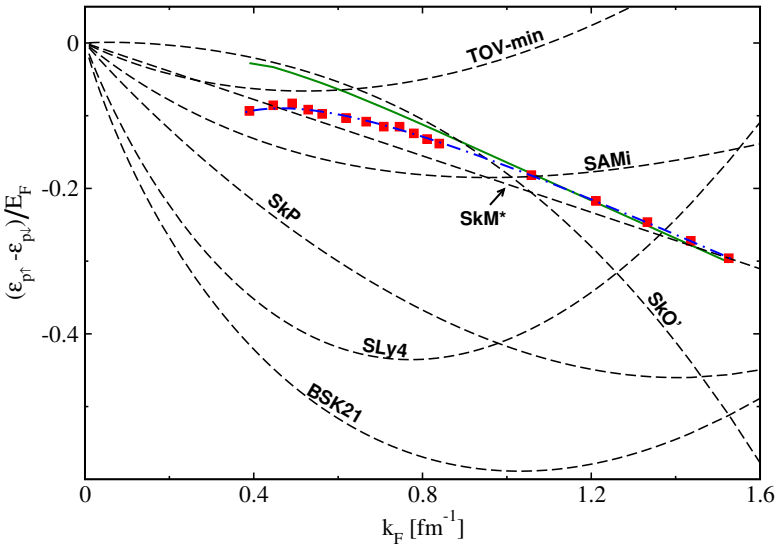


Neutron polaron energy



Proton-up and proton-down polaron energy

Spin/isospin impurities in polarized nuclear matter



The weak dependence of $\Delta\epsilon$ on ρ does not match any of the results given by existing DFT EoS.

This a quantity that only depends on the *time-odd* components in the density functionals. It can be well fitted by an expression such as:

$$A - \frac{B}{k_F|a_s|} - Ck_F r_e$$

with $a_s = -23.75$fm and $r_e = 2.75$fm (n-p scattering length and effective range)

Difference in the proton polaron energies

$$\Delta\epsilon[\rho] = \frac{\epsilon_{p\uparrow} - \epsilon_{\downarrow}}{E_F}$$

REMINISCENT OF DILUTE UNITARY FERMI GASES

Conclusions

- We developed a protocol to perform efficient QMC calculations in a generic representation of the Hilbert space (e.g. momentum space, Gaussian basis sets etc.)
- Important ingredients: Continuous time propagator, importance sampling.
- Thanks to an efficient recursive algorithm it is now possible to use CC wavefunctions as importance functions.
- Applications can be very diverse: infinite and finite systems, local and non local potentials.

Perspectives

- Extend calculations to nuclei and hypernuclei using χ-EFT interaction and other kinds of soft-core interactions.
- Implementation of the algorithm for spin Hamiltonians (Hubbard model, topological insulators, but also spin propagation for nuclear Hamiltonians)