Static response of neutron-rich matter

Matthew Buraczynski & Alexandros Gezerlis

University of Guelph

Outline

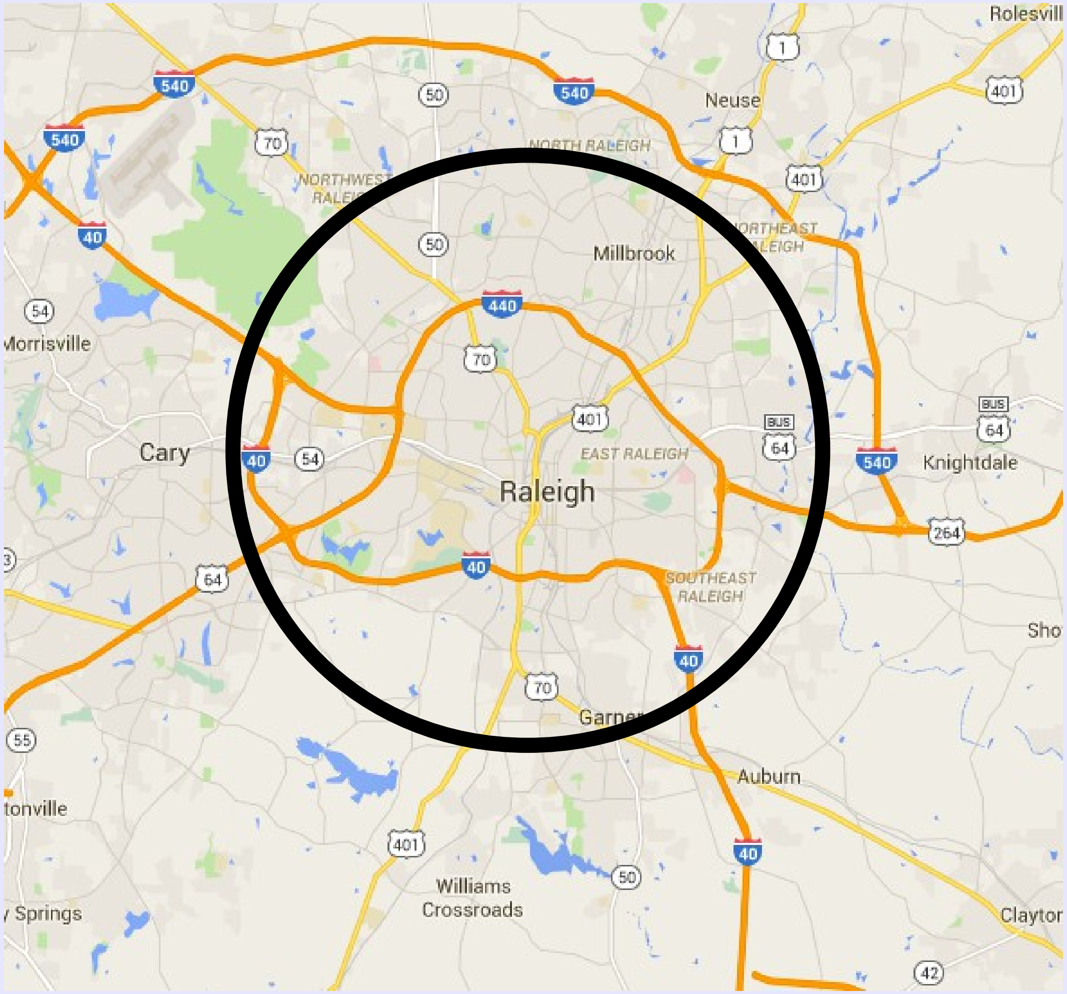
- Motivation
- Quantum Monte Carlo
- Local density approximation
- Linear density-density static response function
- Conclusion

Motivation

- Neutron matter is relevant to neutron-star crusts and neutron-rich nuclei.
- We perform ab-initio calculations of the response of neutron matter and use these as constraints on energy density functionals.

Motivation:
neutron stars

- Incredibly dense
- Mass ~ 1.4 - 2 solar masses
- Radius ~ 10 km



Hamiltonian

- We study the response of the system to an external periodic modulation.

$$H = -\frac{\hbar^2}{2\mathrm{m}} \sum_i \nabla^2 + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} + \sum_i v_0 \cos\left(A z_i\right)$$

- Interactions in microscopic calculations given by AV8' and UIX.

Quantum Monte Carlo

- We use Variational Monte Carlo (VMC) and Auxiliary Field Diffusion Monte Carlo (AFDMC) in our calculations.
- Simulate 66 particles.
- VMC optimizes the trial wave function.

Quantum Monte Carlo:
Trial wavefunction

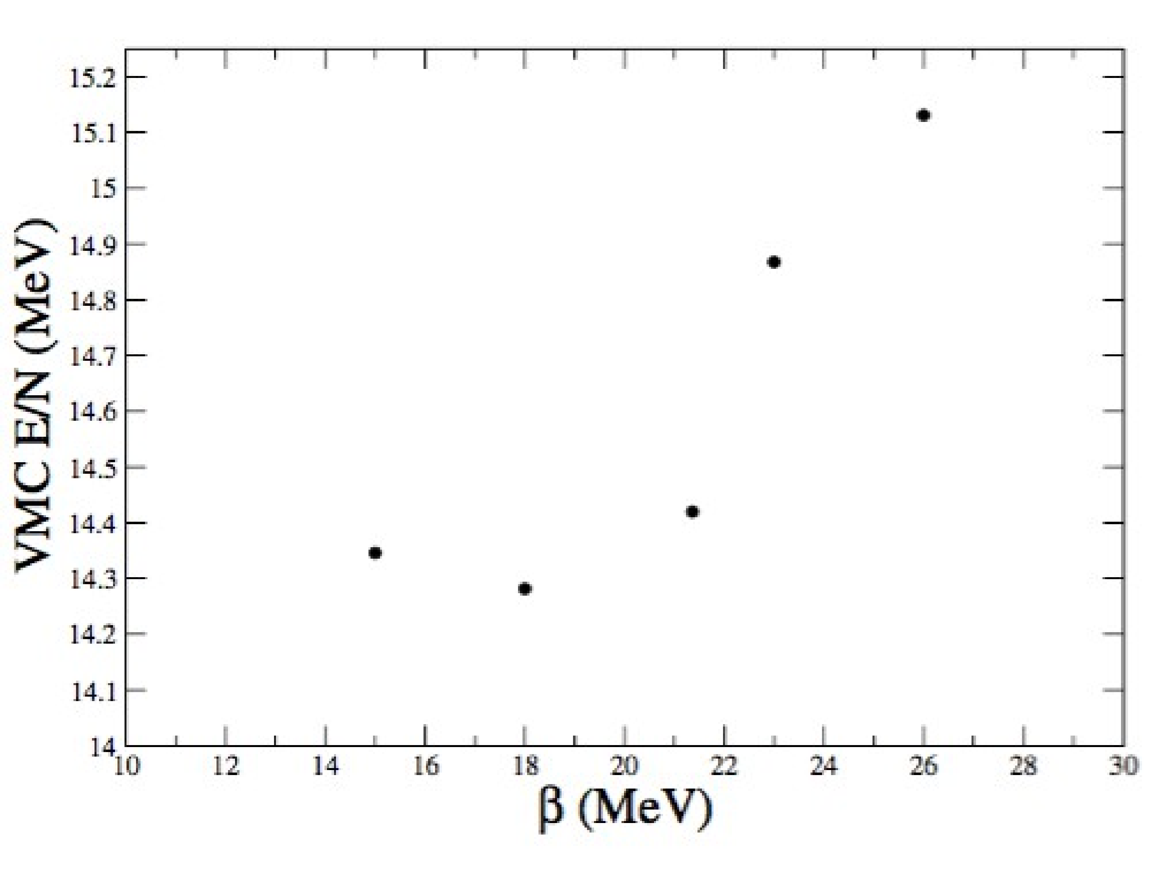
- Trial wave function is a product of a Jastrow factor and Slater determinant.

- Slater determinant of orbitals satisfying:

$$\frac{d^2\psi}{dx^2} + [a - 2\mathrm{q}\cos(2\mathrm{x})]\psi = 0$$

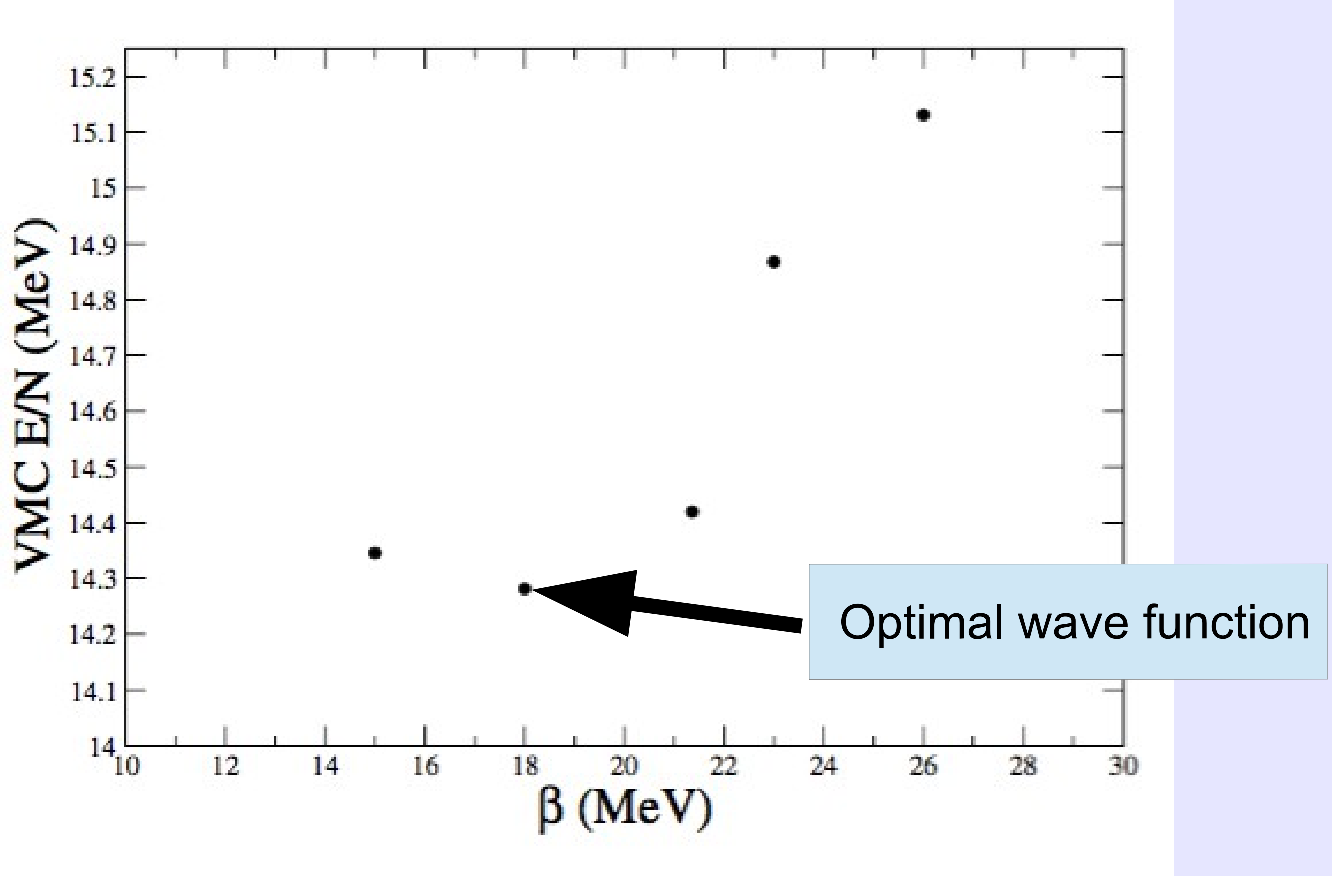
Quantum Monte Carlo:
VMC results

- VMC optimization using q as a variational parameter:



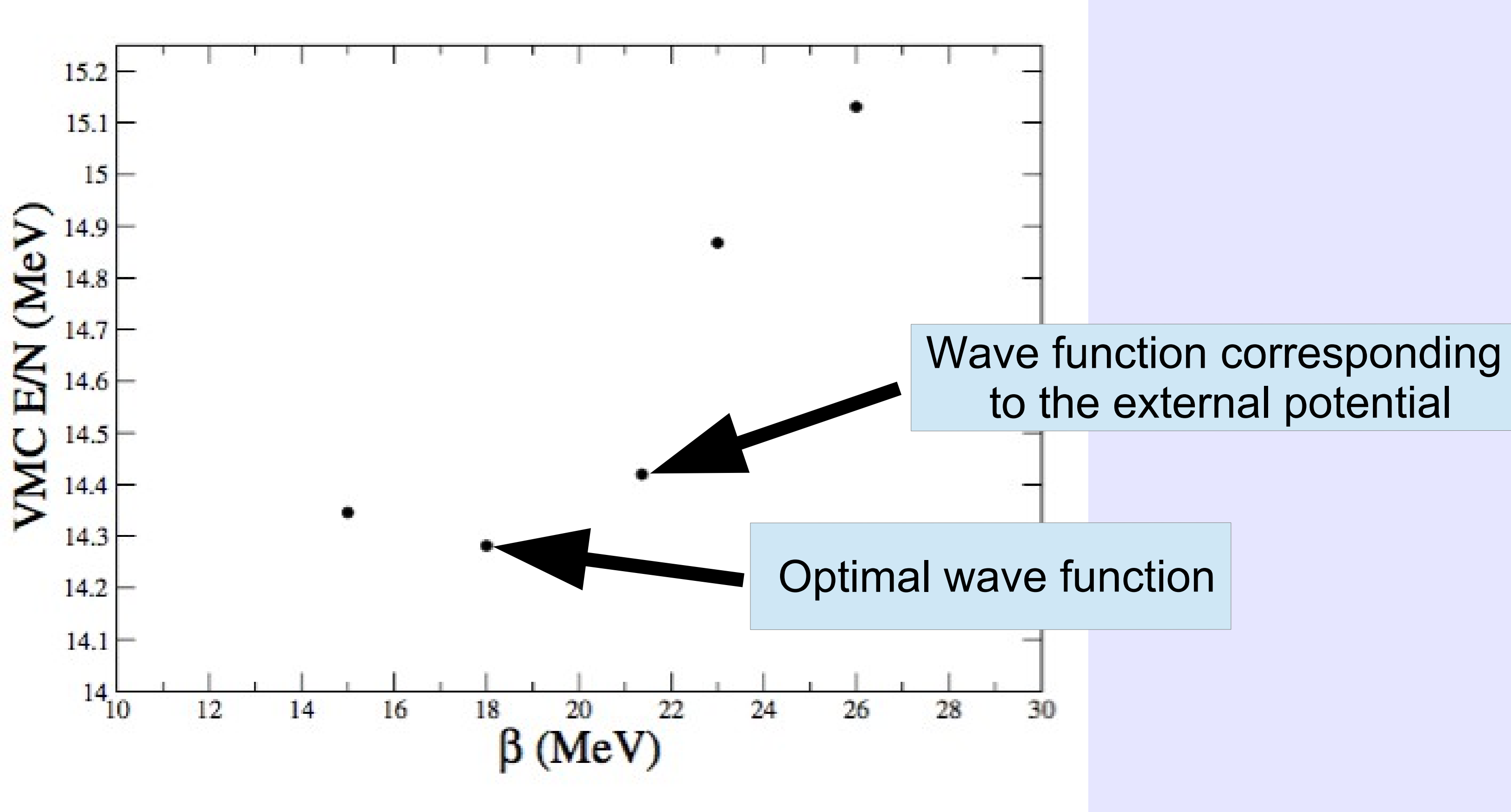
Quantum Monte Carlo:
VMC results

- VMC optimization using q as a variational parameter:



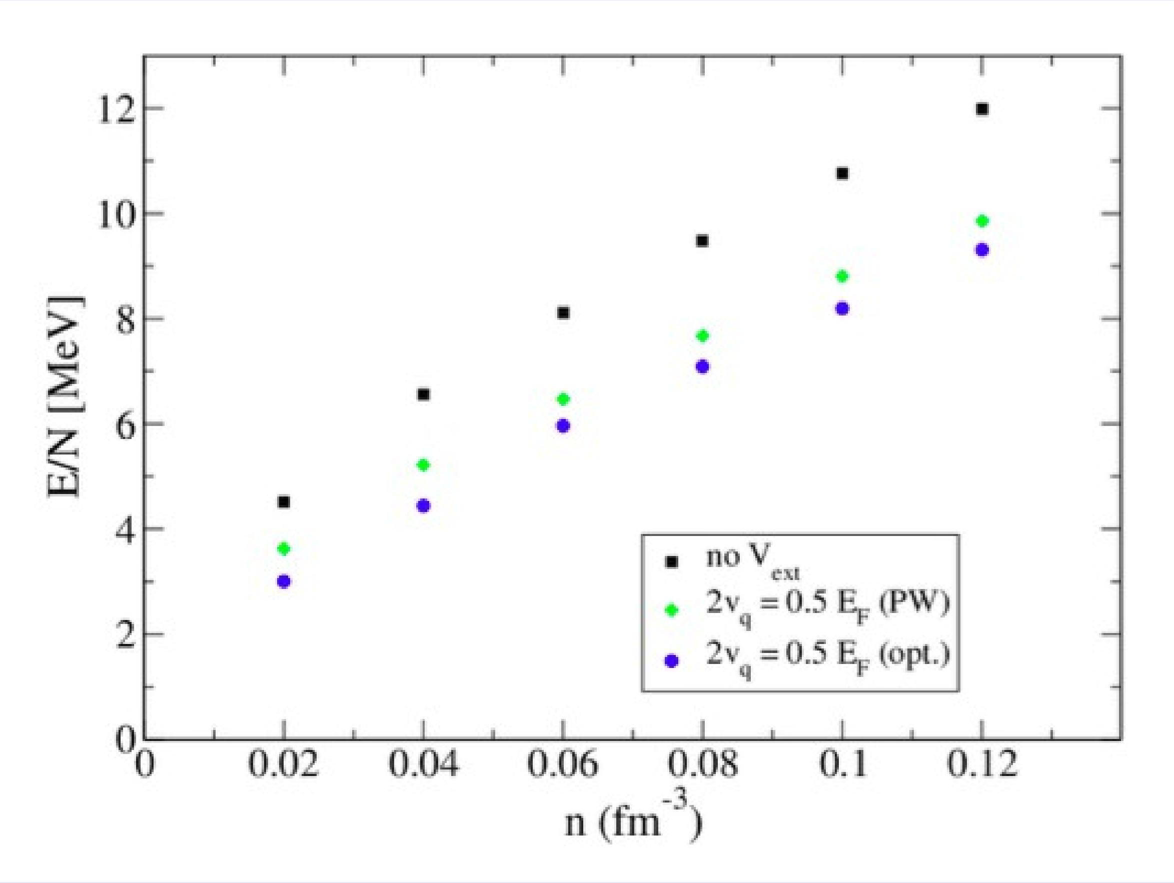
Quantum Monte Carlo:
VMC results

- VMC optimization using q as a variational parameter:



Quantum Monte Carlo:
AFDMC results

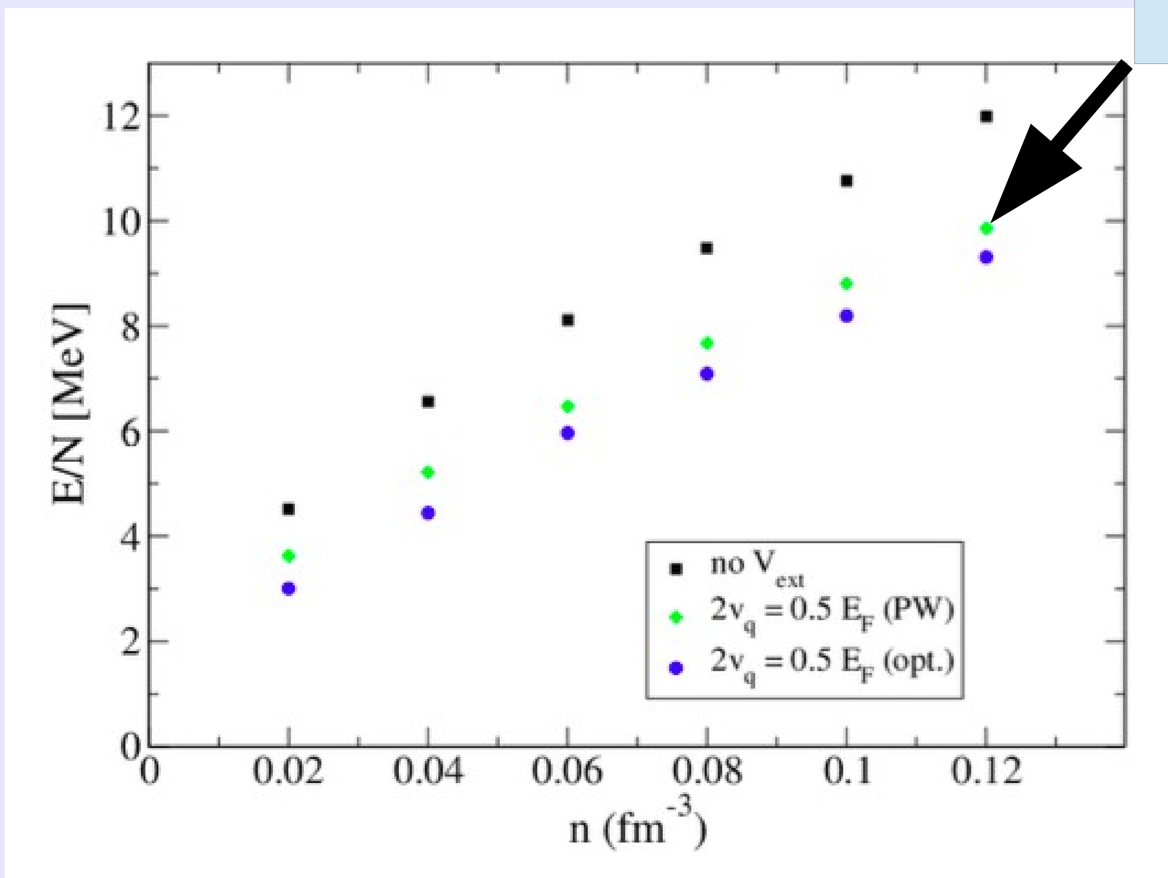
- AFDMC energy versus density both with and without the external potential.



Quantum Monte Carlo:
AFDMC results

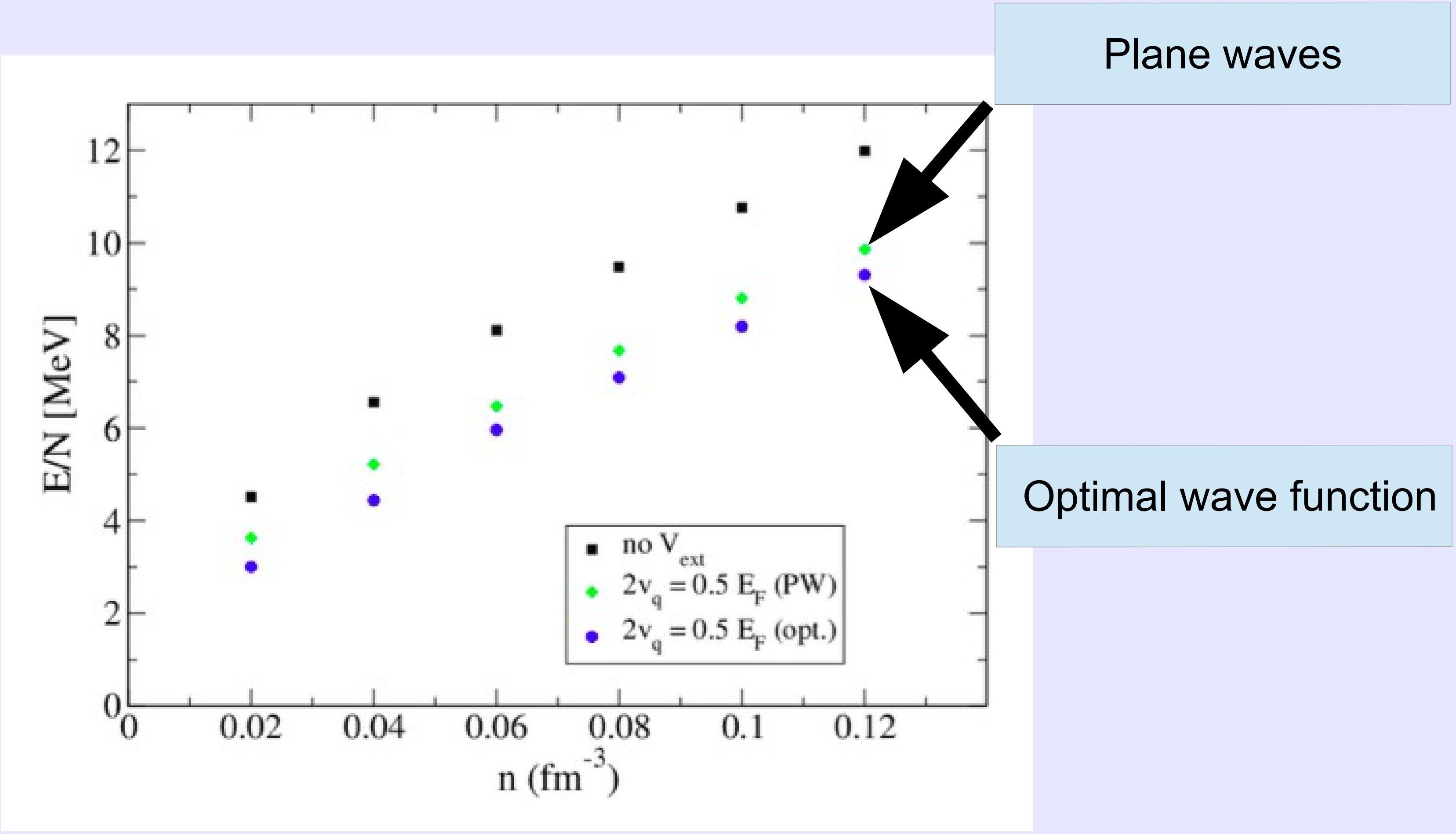
- AFDMC energy versus density both with and without the external potential.

Plane waves



Quantum Monte Carlo:
AFDMC results

- AFDMC energy versus density both with and without the external potential.



Local Density Approximation
Energy density functional

For neutron matter:

$$\mathcal{H}(\boldsymbol{r}) = \frac{\hbar^2}{2\mathrm{m}}\tau + \frac{1}{4}t_0(1-x_0)\rho^2 + \frac{1}{8}(t_1+3\mathrm{t}_2)\rho\tau + \frac{3}{32}(t_1-t_2)(\nabla\rho)^2,$$

where:

$$\rho(\boldsymbol{r}) = \sum_i |\psi_i(\boldsymbol{r})|^2$$

$$\tau(\boldsymbol{r}) = \sum_i |\nabla\psi_i(\boldsymbol{r})|^2$$

The energy is the minimum of:

$$\langle\Psi|H|\Psi\rangle = \int\mathcal{H}(\boldsymbol{r})\,d^3r$$

Local Density Approximation

Energy density functional

For neutron matter:

parameters

$$\mathcal{H}(\boldsymbol{r}) = \frac{\hbar^2}{2\mathrm{m}}\tau + \frac{1}{4}t_0(1-x_0)\rho^2 + \frac{1}{8}(t_1+3\mathrm{t}_2)\rho\tau + \frac{3}{32}(t_1-t_2)(\nabla\rho)^2,$$

where:

$$\rho(\boldsymbol{r}) = \sum_i |\psi_i(\boldsymbol{r})|^2$$

$$\tau(\boldsymbol{r}) = \sum_i |\nabla\psi_i(\boldsymbol{r})|^2$$

The energy is the minimum of:

$$\langle\Psi|H|\Psi\rangle = \int \mathcal{H}(\boldsymbol{r})\, d^3 r$$

Local Density Approximation
Energy density functional

For neutron matter:

parameters

Gradient term

$$\mathcal{H}(\boldsymbol{r}) = \frac{\hbar^2}{2m}\tau + \frac{1}{4}t_0(1-x_0)\rho^2 + \frac{1}{8}(t_1+3t_2)\rho\tau + \frac{3}{32}(t_1-t_2)(\nabla\rho)^2,$$

where:

$$\rho(\boldsymbol{r}) = \sum_i |\psi_i(\boldsymbol{r})|^2$$

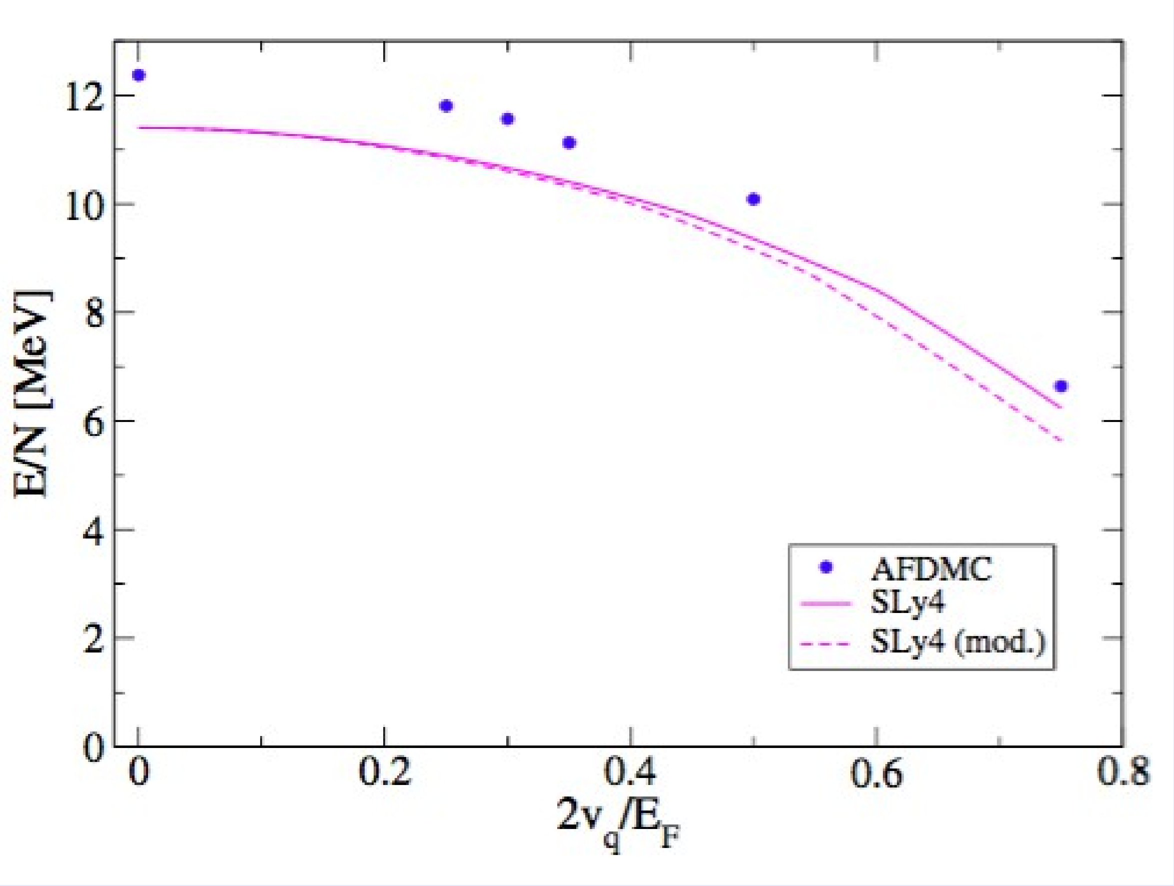
$$\tau(\boldsymbol{r}) = \sum_i |\nabla\psi_i(\boldsymbol{r})|^2$$

The energy is the minimum of:

$$\langle\Psi|H|\Psi\rangle = \int \mathcal{H}(\boldsymbol{r})\, d^3r$$

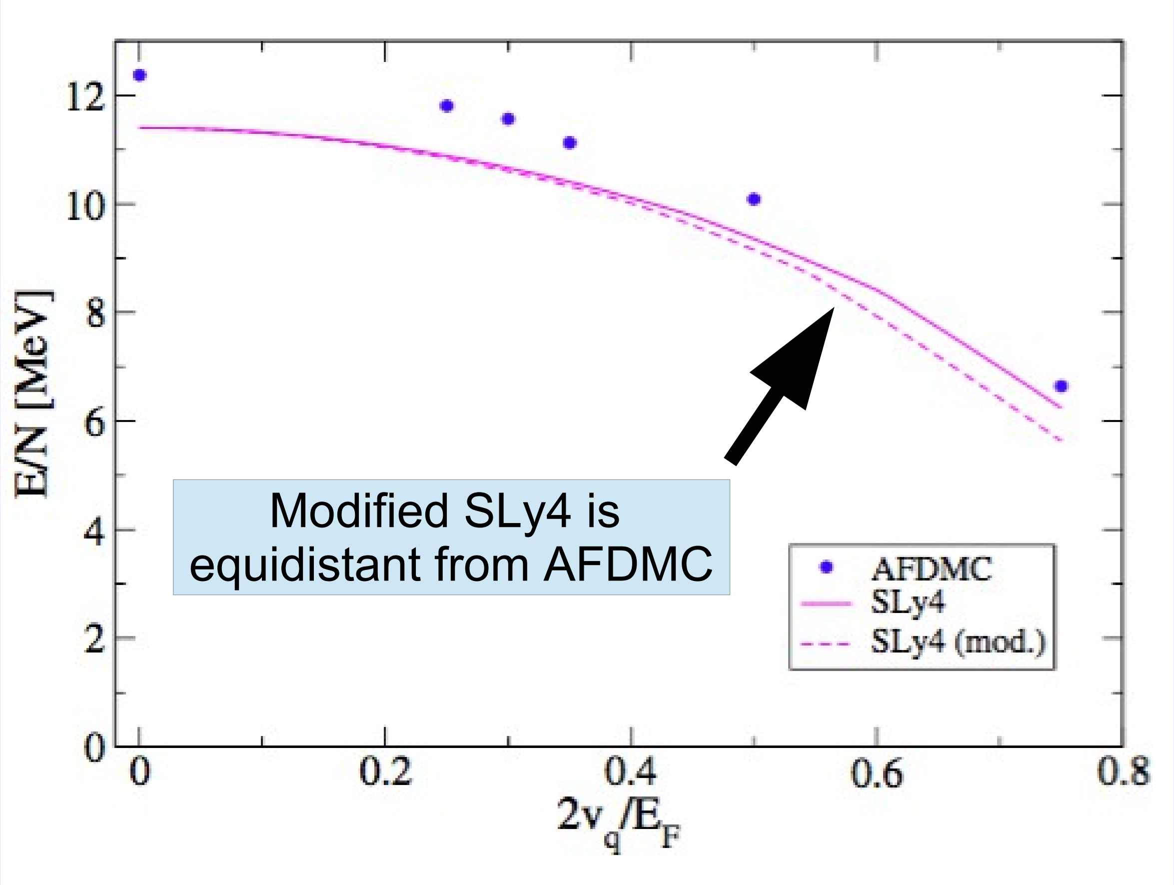
Local Density Approximation:
$n = 0.1\ \mathrm{fm}^{-3}$

- QMC and DFT energy versus strength of the potential.



Local Density Approximation:
$n = 0.1\ \text{fm}^{-3}$

- QMC and DFT energy versus strength of the potential.



Response functions

- Describe how a system responds to perturbations:

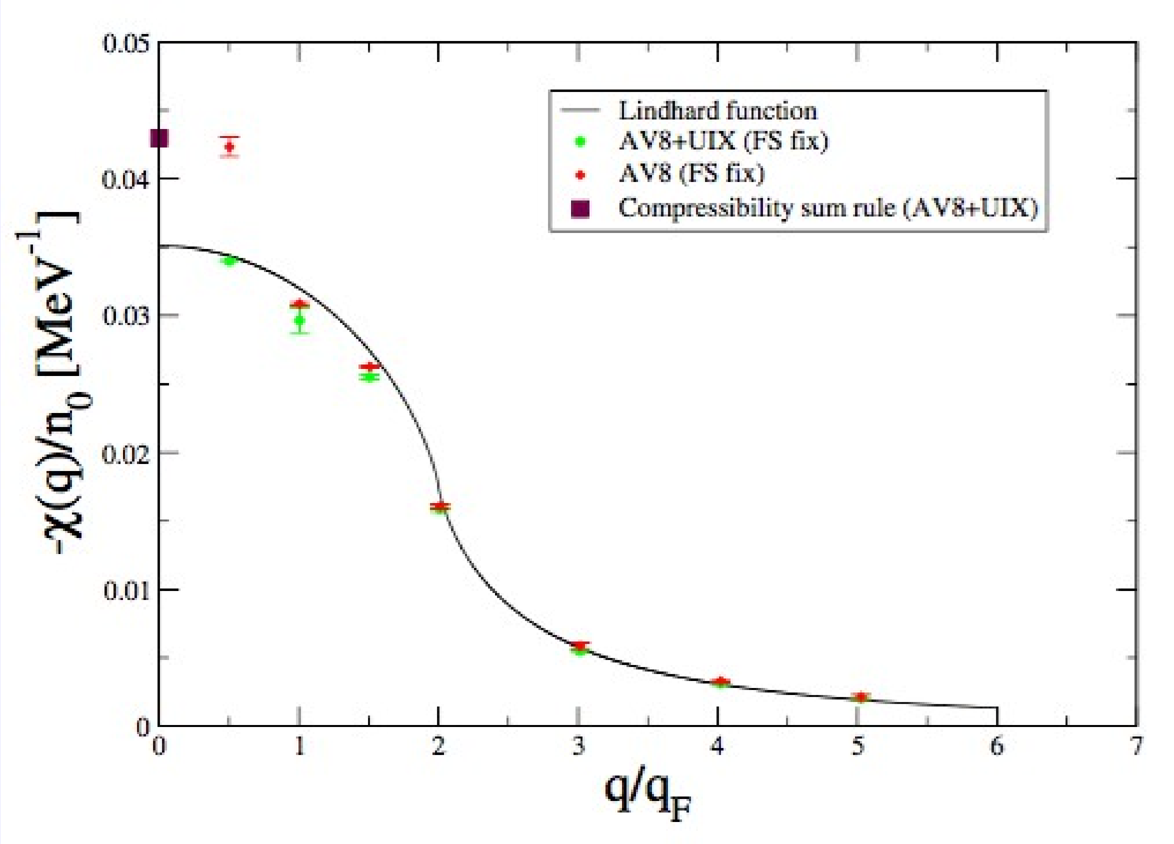
$$n_v(\boldsymbol{r}) = n_0 + \sum_{k=1}^{\infty} \frac{1}{k!} \int d\boldsymbol{r}_1 \dots d\boldsymbol{r}_k \, \chi^{(k)}(\boldsymbol{r}_1 - \boldsymbol{r}, \dots, \boldsymbol{r}_k - \boldsymbol{r}) \, v(\boldsymbol{r}_1) \dots v(\boldsymbol{r}_k)$$

- For the one-body potential $v = 2\mathrm{v}_q \cos(\boldsymbol{q}\cdot\boldsymbol{r})$ the energy is given by:

$$\frac{E_v}{N} = \frac{E_0}{N} + \frac{\chi^1(q)}{n_0} v_q^2 + \frac{\chi^3(\boldsymbol{q}, \boldsymbol{q}, -\boldsymbol{q})}{4\mathrm{n}_0} v_q^4 + \dots$$

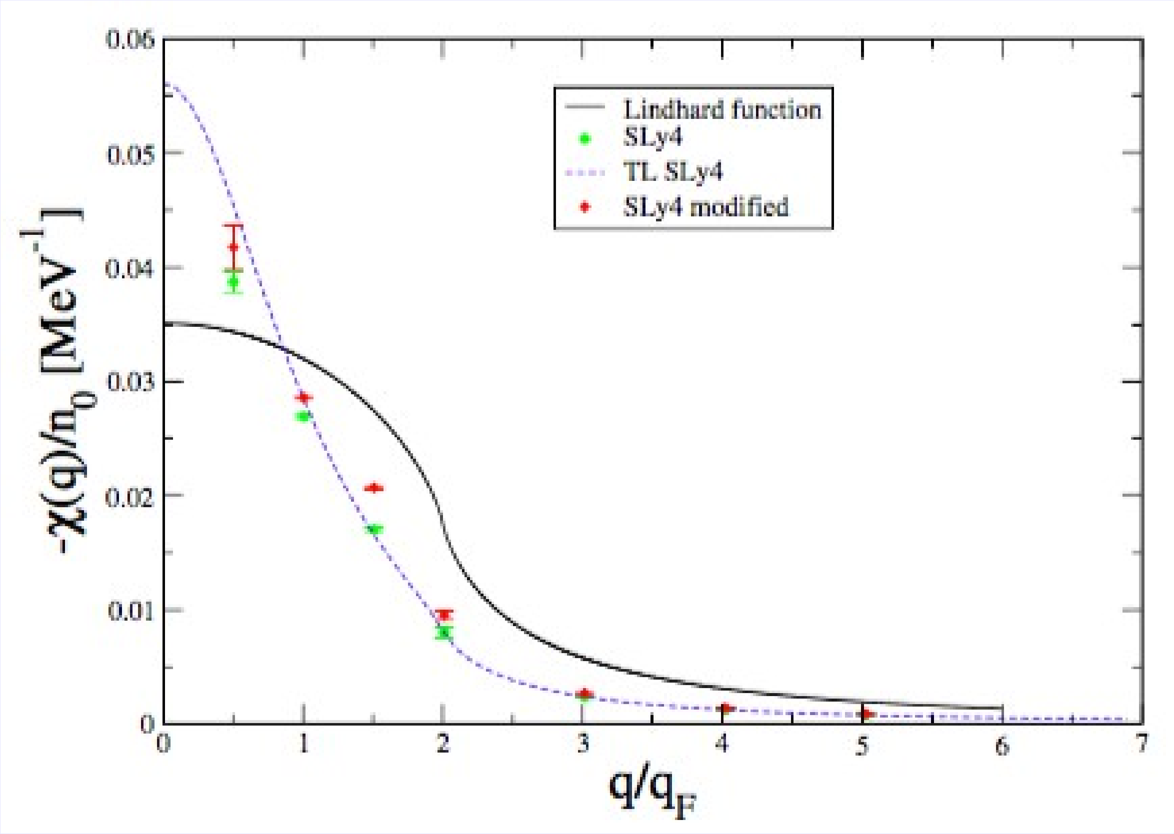
Response function
$n_0 = 0.1\ \mathrm{fm}^{-3}$

- Linear density-density response functions obtained from AFDMC results:



Response function $n_0 = 0.1\ \mathrm{fm}^{-3}$

- Linear density-density response functions obtained from DFT results:



Conclusions

- We can describe neutron-star crusts by microscopic simulations of periodically modulated neutron matter.
- QMC energy calculations may be used to constrain phenomenological theories of neutron-rich nuclei.

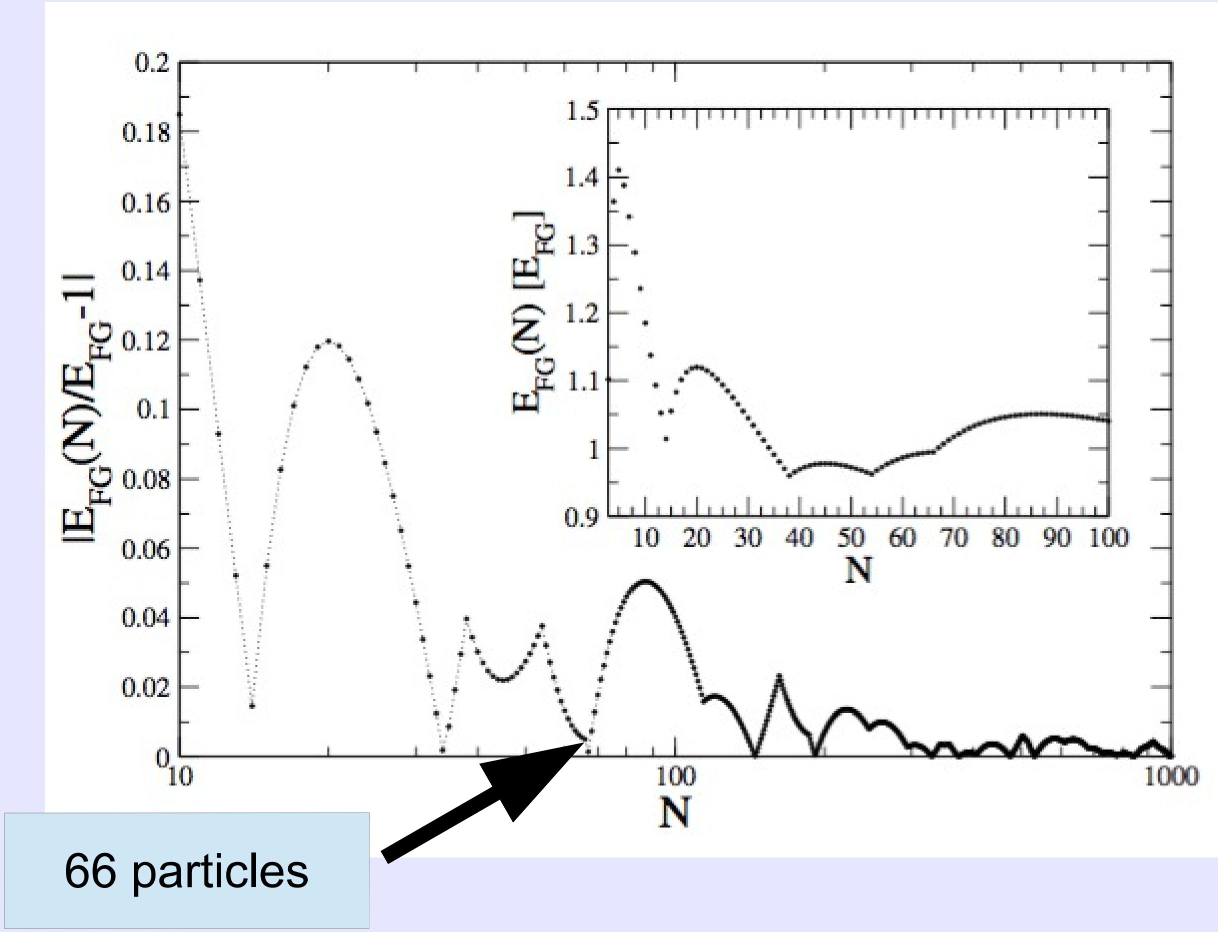
Finite-size effects

- Our microscopic calculations are limited to a small number of particles.
- Extrapolations must be made to study neutron matter:

$$E_I(\infty) = E_I(N) - E_{NI}(N) + E_{NI}(\infty)$$

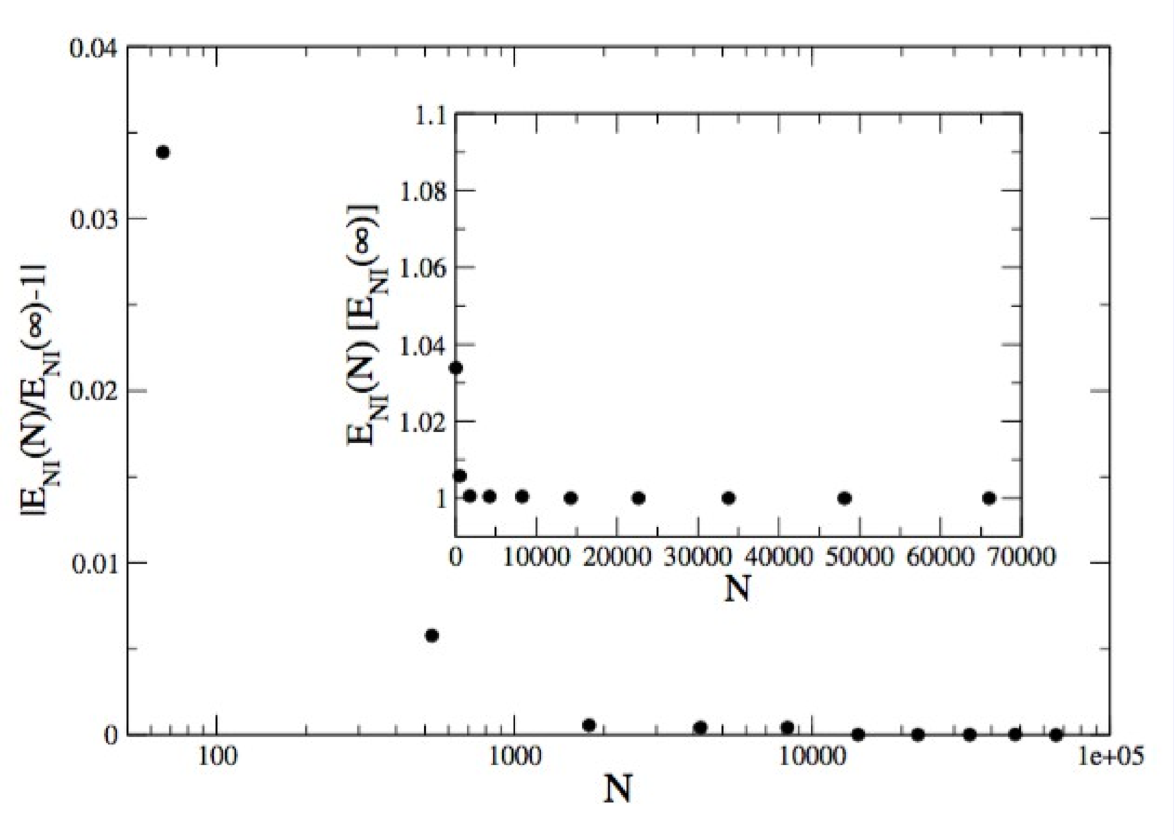
Finite-size effects

- Finite-size effects for the 3D non-interacting Fermi gas



Finite-size effects

- Finite-size effects for the non-interacting gas with external potential



Finite-size effects

- Response function for the non-interacting Fermi gas