Quantum Monte Carlo Studies of Neutron Matter

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Outline

What is Nuclear Matter

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- Symmetric nuclear matter, $N = Z$
- Neutron matter, $Z = 0, A = N$
- Volume and particle numbers are infinite but ratios are finite

Why do we care?

- Who cares?

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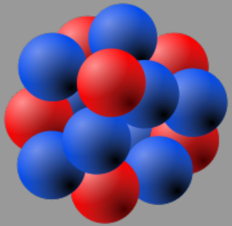
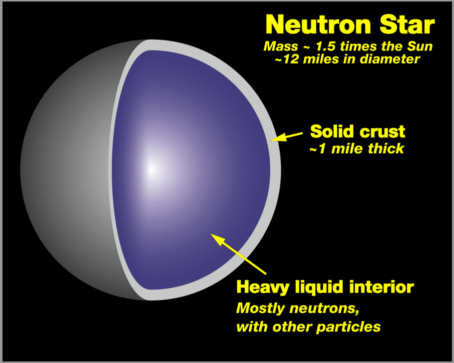
- Decent first approximation for



^{208}Pb, ~ 10 fm, $\sim 10^{-25}$ kg



neutron star, ~ 10 km, $\sim M_{\text{solar}}$

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- Can be used to constrain or eliminate some of the 300+ nuclear energy density functionals
- pedagogically, e.g.

$$E(N,Z) = a_V A - a_S A^{2/3} - a_C \frac{Z(Z-1)}{A^{1/3}} - a_I \frac{(N-Z)^2}{A}$$

can constrain a_V, a_I.

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  - Describe neutron stars and neutron-rich nuclei
  - Extend to symmetric nuclear matter

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- In particular, would like to determine the quasiparticle spectrum of neutron matter.

Outline

What's a quasiparticle

Basic ideas of Fermi Liquid Theory

- Landau assumed a one-to-one correspondence between single particle states of free Fermi gas (FFG) and elementary excitations (quasiparticles) of interacting system:

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$$\delta E = E - E_0 = \sum_p \frac{p^2}{2m} \delta n_p$$

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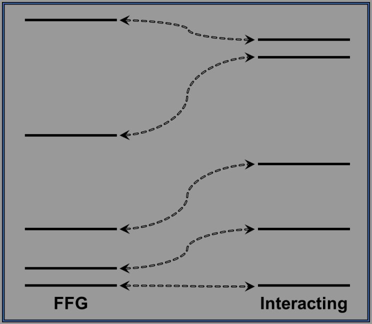

- FFG:

$$\delta E = E - E_0 = \sum_p \frac{p^2}{2m} \delta n_p$$

- Interacting system:

$$\delta E \approx \sum_p \varepsilon_p \, \delta n_p$$

quasiparticle energy

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$$\varepsilon_p \ = E(p, N-1) - \frac{1}{2}\left(E_0(N) + E_0(N-2)\right).$$

and fit parameters such that

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- Fit these
  - effective mass
  - self-energy
  - chemical potential
  - pairing gap

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Quantum Chromodynamics

- QCD is *the* theory of nuclear interactions

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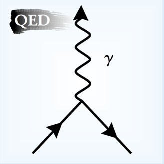

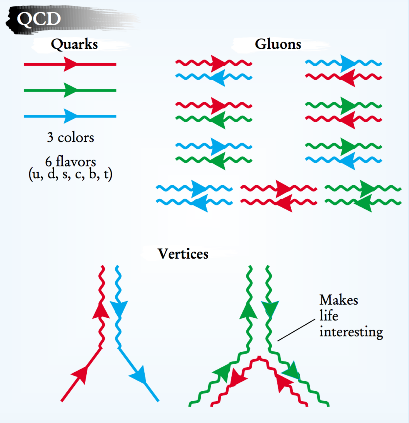

Wilczek, Phys. Today (2000)

Quantum Chromodynamics

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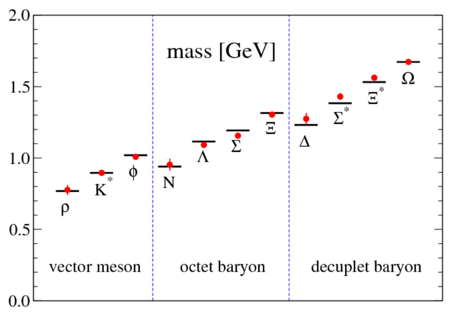

Hayano, Hatsuda, Rev. Mod. Phys. (2010)

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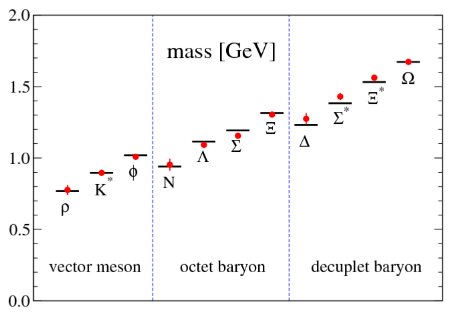

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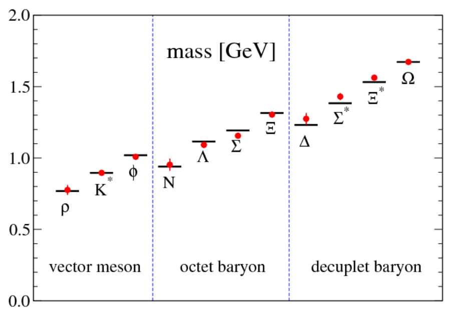

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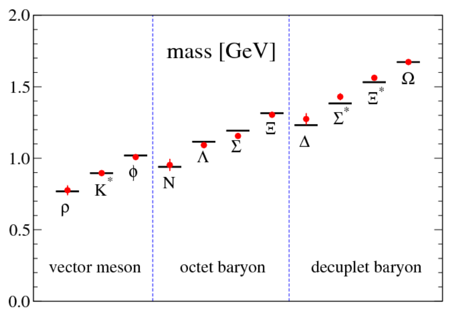

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- Very difficult to calculate things
- Estimates for NNN interaction from LQCD have units of exaflop-years.

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Basic EFT idea:

- pick different degrees of freedom (e.g. quarks $\longrightarrow$ nucleons)
- find two different scales of the problem
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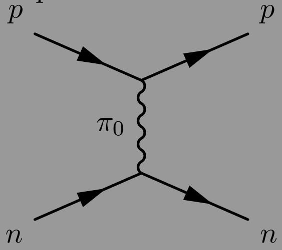

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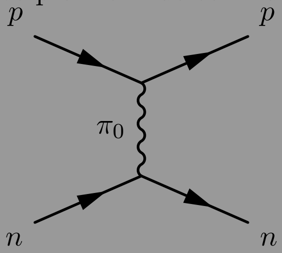

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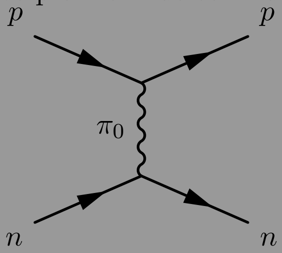

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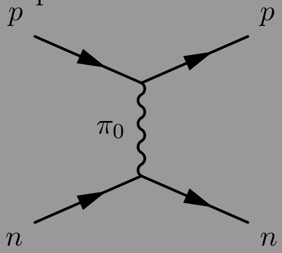

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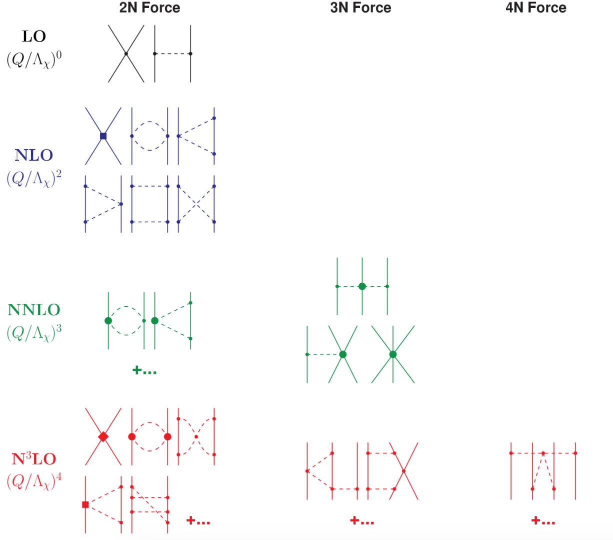
- Expand in powers of $(Q/\Lambda)^\nu$.

Chiral EFT



Machleidt, Entem, Phys. Reports (2011)

Outline

Auxiliary Field Quantum Monte Carlo

- Propagation in imaginary time yields ground state

$$e^{-\tau \widehat{H}} |\psi_T\rangle \xrightarrow{\tau\to\infty} |\psi_0\rangle\,, \qquad \text{assuming } \langle\psi_T|\psi_0\rangle \neq 0.$$

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- In practice we take many small steps (Suzuki-Trotter decomposition):

$$\left|\psi\right\rangle = \prod_{j=1}^{N} e^{\left(-\frac{\Delta\tau\widehat{K}}{2}\right)} e^{\left(-\Delta\tau\widehat{V}\right)} e^{\left(-\frac{\Delta\tau}{2}\widehat{K}\right)}\left|\psi_T\right\rangle + \mathcal{O}\left(\Delta\tau^2\right).$$

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- Use Hubbard Stratonovich Transformation (pedagogical case for operator A):

$$e^{\beta A^2} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{\left(-\sigma^2/2\right)} e^{\left(\sigma\sqrt{2\beta}A\right)} d\sigma$$

Auxiliary field

The Need for MC Integration

Recap:

$$|\psi_0\rangle = \prod_{j=1}^{N} e^{\left(-\frac{\Delta\tau \widehat{K}}{2}\right)} \; e^{\left(-\Delta\tau \widehat{V}\right)} \; e^{\left(-\frac{\Delta\tau}{2}\widehat{K}\right)} |\psi_T\rangle + \mathcal{O}\left(\Delta\tau^2\right).$$

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5x5 possible σ configurations at each site on $N_x N_y N_z N_\tau$ lattice. Massive $25^{N_x N_y N_z N_\tau}$ configurations space.

The Sign Problem

- In QMC, expectation value of some observable A is

$$\langle A \rangle_\sigma = \frac{\int D\sigma A[\sigma] p[\sigma]}{\int D\sigma p[\sigma]},$$

where $A[\sigma] = \langle \psi[\sigma] | A | \psi[\sigma] \rangle$ and $|\psi[\sigma]\rangle = e^{-\mathcal{H}[\sigma]\tau} |\psi_T\rangle$
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- But for fermionic systems, $p[\sigma]$ can be negative in general.
- Importance sampling cannot be used.
- No general solution, NP Hard (Troyer and Wiese, PRL (2005))

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$$\widehat{\mathcal{H}} = \left(\widehat{T} + \widehat{V}_{ev}\right) + \left(\widehat{V}_\chi - \widehat{V}_{ev}\right) = \widehat{\mathcal{H}}_{ev} + \delta\widehat{V}.$$

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  - If $N_\uparrow = N_\downarrow$, $p > 0$

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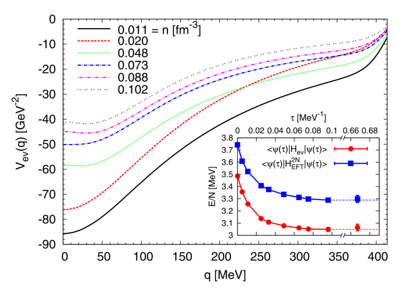

Wlazlowski, et. al. PRL (2014)

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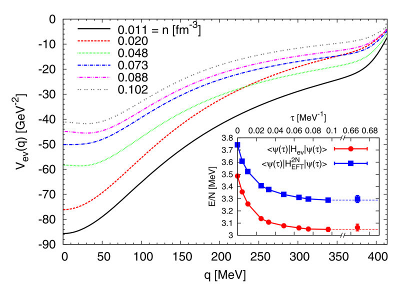

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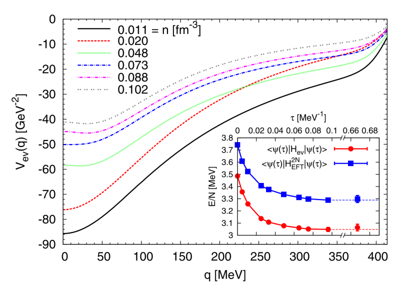

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- This gives us the needed even energies
- What about the odd system?

Re-weighting Methods

Sign problem avoidance strategy #2

Insert 1 in crafty ways to get positive weight factors.

$$
\begin{aligned}
\langle E(N)\rangle &= \frac{\int \mathcal{D}\sigma P_N(\sigma) E(\sigma)}{\int \mathcal{D}\sigma P_N(\sigma)} \\
\langle E(N-1)\rangle &= \frac{\int \mathcal{D}\sigma P_{N-1}(\sigma) E(\sigma)}{\int \mathcal{D}\sigma P_{N-1}}(\sigma) \\
&= \frac{\int \mathcal{D}\sigma P_N(\sigma) \frac{P_{N-1}(\sigma)}{P_N(\sigma)} E(\sigma)}{\int \mathcal{D}\sigma P_N(\sigma)} \frac{\int \mathcal{D}\sigma P_N}{\int \mathcal{D}\sigma P_N \frac{P_{N-1}}{P_N}} \\
&= \left\langle E \frac{P_{N-1}}{P_N} \right\rangle \Big/ \left\langle \frac{P_{N-1}}{P_N} \right\rangle
\end{aligned}
$$

Nakamura, Hatano, and Nishimori J. Phys. Soc. Jpn. (1992)

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- Ratio of expectation values, both with positive weight.

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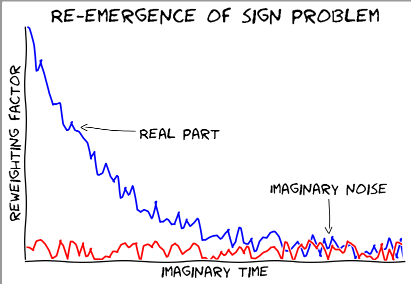
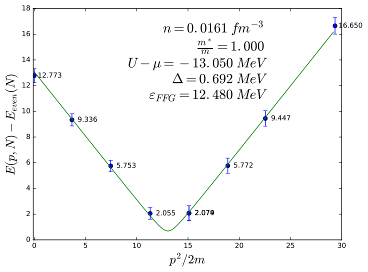


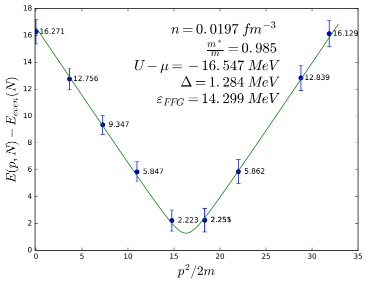
$$\left\langle \frac{P_{N-1}}{P_N} \right\rangle_\sigma \sim \exp\left(-VE\tau\right)$$

- Need a "goldilocks τ": large enough to get ground state, but small enough to delay the sign problem.

Outline

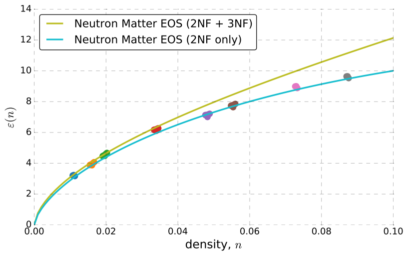
What does the quasiparticle spectrum look like?

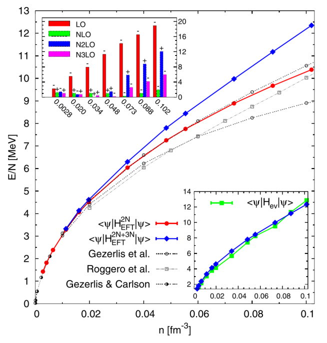




Three body interactions

Large gap due to neglect of three body interactions.

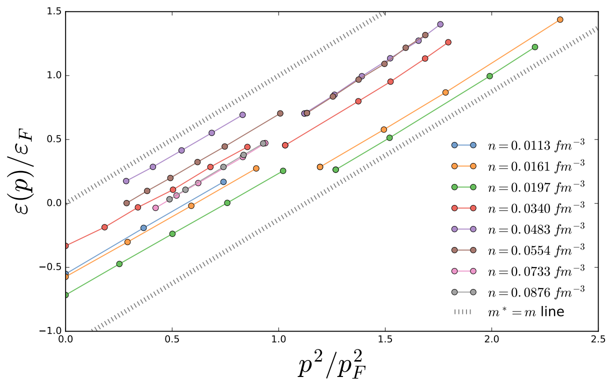




Wlazlowski, et. al. PRL (2014)

What we can say so far

$m^* \approx m_N$ for all simulated densities.



Future work with AFQMC

- Finish this individual study:
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    - Off lattice momenta

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Future work with AFQMC

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  - Three-body interactions
  - Off lattice momenta
- Calculate NM spin susceptibility.
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- Investigate symmetric nuclear matter (i.e. add protons).
- Apply to nuclei, e.g. ^{100}Sn

A CSGF call to arms

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Acknowledgements

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Outline

Appendix A: Pairing Effects in NM

- Why do we average energies for N, $N-2$ in

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Appendix A: Pairing Effects in NM

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- From even-even isobars in nuclei:

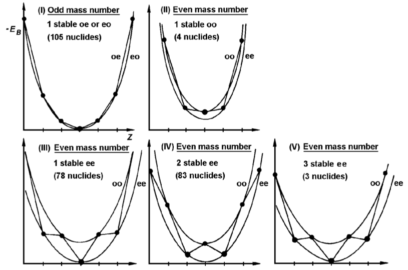

FIG. 3.6. Isobar parabolas for odd mass numbers (I: odd-even or even-odd nuclides) and for even mass numbers (cases II - V). The stable nuclides are indicated by heavier dots.

Choppin, Liljenzin, Rydberg, Radiochemistry and Nuclear Chemistry (2002)

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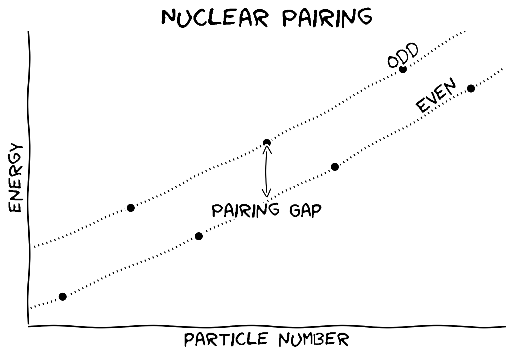
- From even-even isobars in nuclei:
- we expect a gap between even and odd N systems.



Appendix B: Basic Scattering Theory

At large distances assume:

$$\psi \sim e^{ikz} \longrightarrow \psi \sim e^{ikz} + \; f(\theta) \; \frac{e^{ikr}}{r}$$

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For central potential $f(\theta)$ can be expanded as

$$f(\theta) = \frac{1}{2ik} \sum_{\ell} (2\ell + 1) \left(e^{2i\delta_\ell} - 1 \right) P_\ell (\cos\theta)$$

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where δ_ℓ are the phase shifts, and

$$\sigma_{\text{tot}} = \frac{4\pi}{k^2} \sum_{\ell} (2\ell + 1) \sin^2 \delta_\ell(k)$$

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In the low momentum limit

$$k \cot \delta(k) \approx -\frac{1}{a} + \frac{1}{2}\, r_e\, k^2 + \dots$$

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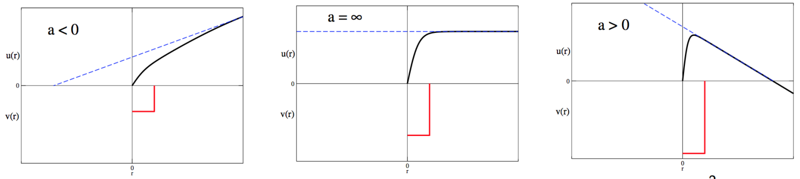
e.g. Attractive square well potential



No bound states | Bound state with E_b=0 | $E_b \sim \frac{\hbar^2}{2m\, a^2}$

Gandolfi, NNPSS (2016)

Appendix C: Low densities

Similar to cold atoms

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- Bertsch proposed model of low density neutron matter with zero-range interaction tuned to infinite scattering length (unitary limit).

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  - Random selection by Monte Carlo methods

$$E_N = (b-a)\langle f \rangle = \frac{(b-a)}{N} \sum_{i=1}^{N} f(x_i) + \mathcal{O}\left(1/\sqrt{N}\right).$$

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where $w(x)$ approximates $f(x)$.

$$E = \int_a^b g(x)p(x)\,dx \approx \frac{1}{N}\sum_{i=1}^{N} g(x_i),$$

where $g(x) = f(x)/p(x)$.

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- Break transition probability into *selection* and *acceptance* probabilities

$$P(\mu \to \nu) = g(\mu \to \nu) A(\mu \to \nu).$$

- Create algorithm which generates random states by $g(\mu \to \nu)$, accept those transitions with $A(\mu \to \nu)$.

Appendix E: More on χEFT

- Use power counting to determine which diagrams to include

$$\nu = -2 + 2A - 2C + 2L + \sum_i \left(d_i + \frac{n_i}{2} - 2 \right)$$

where

- A – nucleons involved in interaction,
- C – separately connected pieces,
- L – pion loops,
- d_i – derivatives or mass insertions, m_π,
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- Adding a nucleon increments ν, so we expect $V_2 \gg V_3 \gg V_4 \gg \ldots$

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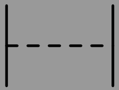

$$A = 2, C = 1, L = 0, d_i = 1, n_i = 2$$
$$\implies \nu = 0 \text{ (LO)}, (Q/\Lambda)^0 .$$

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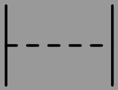

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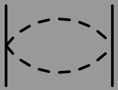

$$A = 2, C = 1, L = 1, d_i = 1, n_i = 2$$
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Appendix F: More on the quasiparticle interaction

Adding/removing only one quasiparticle, we have

$$\delta E = \sum_{p\sigma} \varepsilon_{p\sigma} \delta n_{p\sigma} \qquad \Longrightarrow \qquad \varepsilon_{p\sigma} = \frac{\delta E}{\delta n_{p\sigma}}.$$

For multiple particles

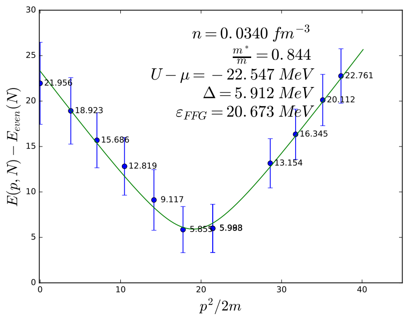
$$\delta E = \sum_{p\sigma} \varepsilon^0_{p\sigma} \delta n_{p\sigma} + \frac{1}{2V} \sum_{p_1\sigma_1 p_2\sigma_2} f_{p_1\sigma_1 p_2\sigma_2} \delta n_{p_1\sigma_1} \delta n_{p_1\sigma_1}$$

$$\varepsilon_{p\sigma} = \varepsilon^0_{p\sigma} + \frac{1}{V} \sum_{p_2\sigma_2} f_{p\sigma p_2\sigma_2} \delta n_{p_2\sigma_2}$$

$$\Longrightarrow f_{p_1\sigma_1 p_2\sigma_2} = V \frac{\delta^2 E}{\delta n_{p_1\sigma_1} \delta n_{p_2\sigma_2}} = V \frac{\delta \varepsilon_{p_1\sigma_1}}{\delta n_{p_2\sigma_2}}$$

Appendix G: Off lattice momenta

Large errors due to difficulty of fitting the minimum of the QPE spectrum.



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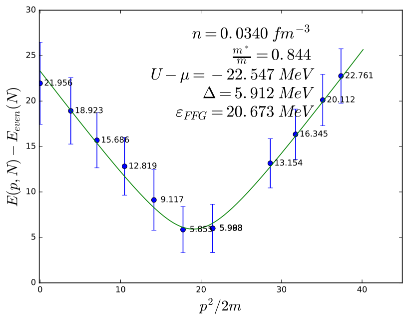

Solution: Add off-lattice momenta

Appendix G: Twisted Boundary Conditions (TBC)

- Instead of using periodic boundary conditions (PBC), where

$$\psi(r_1 + L, r_2, \ldots, r_n) = \psi(r_1, r_2, \ldots, r_N)$$

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- Corresponding momenta

$$p_i = \frac{2\pi n_i}{L} + \frac{\theta}{L}$$

  - On-lattice momenta
  - Shift by arbitrary amount

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- Shifted wavefunctions can be written

$$\psi(x) = \varphi(x)e^{i\frac{\theta}{L}x}, \text{ where } \varphi(x) = \varphi(x+L)$$

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$$i\hbar\partial_t\psi_j = h\psi_j \quad \implies \quad i\hbar\partial_t\varphi_j = \frac{\varphi(p_j+\theta/L)^2}{2m}\varphi + v\varphi_j$$

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- Can keep our existing computational framework
- Time evolve with adjusted kinetic energy operator
- Compute observables with extra phase factor $e^{i\theta/L}$