

Similarity Renormalization Group (SRG)

The essential idea of the SRG is to perform a unitary transformation on our Hamiltonian (and all other operators) to produce an equivalent Hamiltonian which is easier to use in a many-body calculation.

For example, a common application is to use the SRG to "soften" an interaction so that it converges more rapidly as the basis size is increased.

In the next notes, we'll also see that the in-medium formulation of the SRG can be used to directly solve the many-body problem.

Background: The Renormalization Group

As an introduction to the concept of the renormalization group, consider the following simple example from classical electrodynamics.

A point particle with mass m and charge q is at rest

$$\bullet m, q$$

What is the energy of the system? Well, we know the rest mass contributes an energy $U_m = mc^2$. But there is also energy stored in the electric field:

$$U_{\text{EM}} = \frac{\epsilon_0}{2} \int d^3r |\vec{E}(r)|^2$$

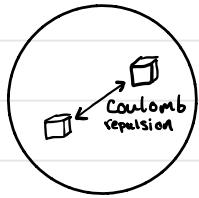
$$= \frac{\epsilon_0}{2} \int_0^\infty 4\pi r^2 dr \left| \frac{q}{4\pi\epsilon_0 r^2} \right|^2$$

$$= \frac{q^2}{8\pi\epsilon_0} \int_0^\infty \frac{1}{r^2} dr = \infty.$$

The energy stored in the field of a point charge is infinite! This is a clear indication that a literal point charge is nonsense. This issue has caused much consternation historically, and basically the same issue shows up in quantum field theory, to the great uneasiness of many physicists.

However, the resolution is actually fairly straightforward: a literal point charge — that is, one with no spatial extent whatsoever all the way down to the tiniest scales imaginable — is indeed nonsense. In order for the theory to make sense (even without quantum effects), the distribution must have some finite extent.

But now we run into another snag: Earnshaw's theorem tells us there can be no stable purely electrostatic configuration. Any two little pieces of charge will repel one another and the whole thing flies apart.



For a stable, finite distribution, there must be some additional physics beyond electrostatics gluing things together. In the case of a proton, this additional physics is the strong force. But in any case there needs to be something holding things together. So to calculate the total energy we add up the mass, electrostatic, and mystery-physics contributions:

$$U = mc^2 + \frac{\epsilon_0}{2} \int d^3r |\vec{E}(r)|^2 + \int d^3r U_m(r)$$

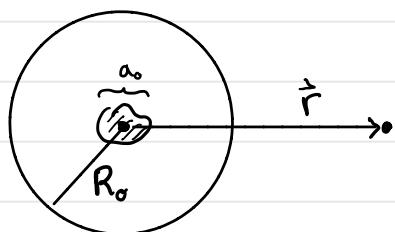
↓
 energy density
 of mystery theory

We still have some problems. First, we need to know the exact charge distribution of our "point charge" to arbitrary precision, with arbitrary spatial resolution. Slight variations at very short distances will have enormous impact on the total energy. Second, we need to know how to calculate the energy content of our mystery theory. In the case of a proton, this is a very painful calculation. In the case of an electron, we have no idea what the theory should even be.

So are we doomed? Not necessarily. Imagine we don't know the mystery theory, and we don't know the charge distribution, but we do know that the distribution is smaller than some characteristic length scale a_0 . Let us also assume that the mystery physics is of sufficiently short range that it is negligible at a distance $r \gtrsim a_0$.

Now, let's draw some imaginary shell of radius $R_0 > a_0$ and split the expression for the energy into two pieces, one for $r \leq R_0$ and one for $r \geq R_0$:

$$U = mc^2 + \frac{e}{2} \int_0^{R_0} dr \left| \vec{E}(r) \right|^2 + \int_0^{R_0} dr U_i(r) + \frac{e}{2} \int_{R_0}^{\infty} dr \left| \vec{E}(r) \right|^2 + \int_{R_0}^{\infty} dr U_i(r)$$



We have assumed that $U_2(\vec{r}) = 0$ for $r \geq R_0$, so we can drop that term. Also, note that the electrostatic integral from R to ∞ is finite:

$$U = mc^2 + \int_0^{R_0} dr \left[\frac{\epsilon_0}{2} |\vec{E}(r)|^2 + U_2(r) \right] + \frac{q^2}{8\pi\epsilon_0 R_0}$$

We still don't know how to handle the integral from 0 to R_0 . However, we do know that it must be some finite number. Furthermore, its only effect will be to produce a constant energy at the location of the particle. This is totally indistinguishable from a mass term, so long as we stay farther away than R_0 .

So we lump that into a renormalized or "physical" mass

$$M_p c^2 = mc^2 + \delta mc^2, \quad \delta mc^2 \equiv \int_0^{R_0} dr \left[\frac{\epsilon_0}{2} |\vec{E}(r)|^2 + U_2(r) \right]$$

"physical"
or
"renormalized"
mass "bare"
mass

$$U = M_p c^2 + \frac{q^2}{8\pi\epsilon_0 R_0}$$

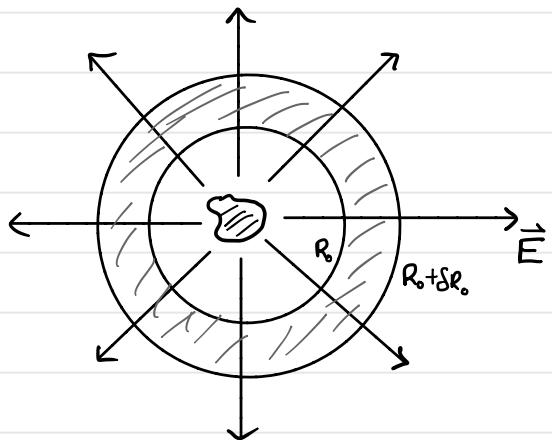
The parameter R_0 , which we used to cut off our integral, is arbitrary — physical predictions should not depend on it. Specifically, the energy should not depend on R_0 :

$$\frac{dU}{dR_0} = \frac{d}{dR_0}(M_p c^2) + \frac{d}{dR_0}\left(\frac{q^2}{8\pi\epsilon_0 R_0}\right) = 0$$

$$\Rightarrow \frac{d}{dR_0}(M_p c^2) = \frac{q^2}{8\pi\epsilon_0 R_0^2}.$$

\leftarrow (Renormalization group equation for $m(R_0)$)

The mass parameter of our theory depends on the cutoff R_0 , but the total energy does not.



If we fix our theory at some R_0 , then $m(R_0)$ is related to the mass we would have found at $R_0 + \delta R_0$ by

$$m(R_0 + \delta R_0) c^2 = m(R_0) c^2 + \int_{R_0}^{R_0 + \delta R_0} d^3 r \frac{e_0}{2} |\vec{E}|^2$$

That is, the mass increases by an amount equal to the electrostatic energy stored between the two shells.

The differential equation dictating how the mass changes with our cutoff R_0 is called a "renormalization group flow equation".

Incidentally, the mass in this problem is an example of what are called "counter terms", absorbing physics beyond the cutoff.

As we vary R_0 , the total energy U is unchanged. However, the relative contributions of mass and electrostatic energy do change. These quantities are called "scale-dependent" and clearly should not be observable individually.

This example outlines the basic philosophy of the renormalization group; applications are typically more complicated, and the integrals are more difficult. We also have not yet touched on the great power of renormalization group ideas to solve difficult problems.

Low-momentum NN potentials: V_{lowk}

As an example of RG concepts applied to nuclear physics, we briefly touch upon the V_{lowk} approach before moving on to the similarity renormalization group.

Consider the scattering of two particles with incoming relative momentum k , interacting by a potential V . The Hamiltonian is $H = T + V$.

If we denote plane wave states $|\phi_k\rangle$ and interacting states $|\gamma_k\rangle$, then the Lippmann-Schwinger equation is

$$|\gamma_k\rangle = |\phi_k\rangle + G_E V |\gamma_k\rangle.$$

Here G_E is the Green's function, or propagator. The form of G_E depends on the boundary conditions we choose, typically incoming/outgoing waves or standing waves.

It turns out to be handy to define the T -matrix

$$\langle \phi_k | \pi | \phi_k \rangle \equiv \langle \phi_k | V | \gamma_k \rangle$$

which obeys its own Lippmann-Schwinger equation,

$$\pi_E = V + G_E V \pi_E.$$

This may be expressed in a partial wave basis as

$$\langle k' | T_E | k \rangle = \langle k' | V | k \rangle + \frac{2}{\pi} P \int_0^\infty dp p^2 \frac{\langle k' | V | p \rangle \langle p | T_E | k \rangle}{E - p^2}$$

Here I use the notation $\langle k' | V | k \rangle = \langle \phi_{k'} | V | \phi_k \rangle$ and I use scattering units $\hbar = c = m = 1$. This means the kinetic energy of $|\phi_k\rangle$ is just k^2 . I also have selected the principal value form of the propagator G_E , which corresponds to standing wave boundary conditions. Note that the integral runs to $p = \infty$.

Realistically, no nuclear potential is valid up to $p = \infty$, so the integral should have some upper limit, which we denote Λ .

$$\langle k | T_{k^2} | k \rangle = \langle k' | V(\Lambda) | k \rangle + \frac{2}{\pi} P \int_0^\Lambda dp p^2 \frac{\langle k' | V | p \rangle \langle p | T_{k^2} | k \rangle}{k^2 - p^2}$$

Our goal is now to change the cutoff Λ while leaving the T-matrix unchanged:

$$\frac{d}{d\Lambda} \langle k' | T_{k^2} | k \rangle = 0$$

Physically, the scattering amplitude is proportional to the T matrix

$$f_E(k' \leftarrow k) = -4\pi\mu \langle k' | T_E | k \rangle$$

so leaving the T-matrix unchanged means that scattering observables, like cross sections, are unchanged. Note that due to energy & momentum conservation, only "on-shell" matrix elements with $k'^2 = k^2$ are observable. Preserving the "half on-shell" terms is an extra requirement.

This "extra" requirement ensures that the low-momentum components of the wave function are unchanged. It also leads to a non-Hermitian potential (though it's typically almost Hermitian).

Taking the derivative of both sides of the equation for T_ϵ , after some manipulation one obtains

$$\frac{d}{ds} \langle k' | V | k \rangle = \frac{2}{\pi} \frac{\langle k' | V | s \rangle \langle s | T_\epsilon | k \rangle}{1 - k^2/\Lambda^2} . \quad (V_{\text{low } k} \text{ flow eq.})$$

This is a renormalization group flow equation for the potential $V(k', k)$. Beginning with some microscopic potential like AV18, CD-Bonn, a chiral potential, etc. which reproduces NN scattering data, we can solve the flow equation to integrate out high-momentum modes while preserving the reproduction of data.

[Note that, technically, the set of transformations that lead to potentials at different scales do not form a group in the mathematical sense because they are not invertible. That is, various high-momentum interactions will collapse to the same low-momentum interaction. We don't have enough information to reconstruct the original interaction from the evolved one, because we threw it out.

On the other hand, Similarity Renormalization Group transformations, which we'll get to shortly, are invertible and so do form a group.]

Why is this useful?

So we've seen that we can eliminate high-momentum modes from our theory without changing observables. But what is the point of doing this?

In short, eliminating modes allows us to work in a smaller model space, which makes calculations feasible.

As a concrete example, consider our calculation of infinite nuclear matter. We of course cannot put literally infinite matter on a computer. In practise we put a finite number of particles in a finite box and truncate the number of momentum modes to, e.g. $n_x^2 + n_y^2 + n_z^2 \leq N_{\max}$. For a fixed particle number A and box size L , we should increase the artificial cutoff N_{\max} until convergence; that is, until further increasing N_{\max} no longer appreciably changes our result.

The size of the single particle basis grows asymptotically as $N_{\max}^{3/2}$, and many-body calculations quickly become expensive - for example, FCI grows factorially with the number of states.

If we are interested in low-energy properties, the value of N_{\max} needed for convergence depends on how strongly the interaction couples low and high momenta. Reducing the strength of the high-low coupling improves the rate of convergence. We'll return to this shortly.

Similarity Renormalization Group (SRG)

Another strategy to suppress high-momentum degrees of freedom is to perform a unitary transformation of the Hamiltonian:

$$\tilde{H} = U H U^\dagger, \quad U^\dagger U = U U^\dagger = \mathbb{1}.$$

Since the transformation is unitary, observables will be unchanged by construction. However, we don't know how to construct U right away. The approach we will take is to parameterize the transformation using a continuous flow parameter s . We label the initial Hamiltonian with $s=0$, so that $U(s=0) = \mathbb{1}$ and

$$H(s) = U(s) H(0) U^\dagger(s).$$

Next, we differentiate with respect to s

$$\begin{aligned} \frac{dH(s)}{ds} &= \frac{dU(s)}{ds} H(0) U^\dagger(s) + U(s) H(0) \frac{dU^\dagger(s)}{ds} \\ &= \frac{dU(s)}{ds} U^\dagger(s) U(s) H(0) U(s) + U(s) H(0) U^\dagger(s) U(s) \frac{dU^\dagger(s)}{ds} \end{aligned}$$

We can make some progress by taking a different derivative

$$\frac{d}{ds}(U(s)U^\dagger(s)) = \frac{dU(s)}{ds}U^\dagger(s) + U(s)\frac{dU^\dagger(s)}{ds} = \frac{d}{ds}(\mathbb{1}) = 0$$

$$\frac{dU(s)}{ds}U^\dagger(s) = -U(s)\frac{dU^\dagger(s)}{ds} = -\left(\frac{dU(s)}{ds}U^\dagger(s)\right)^+$$

We then define: $\eta(s) \equiv \frac{dU(s)}{ds}U^\dagger(s) = -\eta^\dagger(s)$

The anti-hermitian operator $\eta(s)$ is called the generator of the unitary transformation. In terms of $\eta(s)$, our differential equation (or flow equation) is

$$\frac{dH(s)}{ds} = \eta(s) H(s) + H(s) \eta^+(s)$$

$$= \eta(s) H(s) - H(s) \eta(s)$$

$$\boxed{\frac{dH(s)}{ds} = [\eta(s), H(s)]}.$$

(SRG flow equation)

The trick is now to choose a form of the generator η which drives $H(s)$ to a desirable form. As we discussed with V_{bulk} , high momentum modes cause a headache for our many-body methods. We can't eliminate those modes — that would break unitarity. But we can try to decouple high and low momenta.

A choice that does a reasonable job of suppressing coupling to high-momentum modes is the "canonical" generator

$$\eta(s) = [T, H(s)]. \quad (T = \text{kinetic energy})$$

If we define the kinetic energy to be unchanged by the transformation: $H(s) = T + V(s)$, then

$$\frac{dH(s)}{ds} = \frac{dV(s)}{ds} = [[T, V(s)], T + V(s)]$$

$$= TVT + TVV - VTT - VTV - TT V - VT V + TVT + VNT$$

$$= TV^2 + V^2 T - 2VTV - (VT^2 + T^2 V - 2TVT)$$

Writing things explicitly in a plane wave basis, we find

$$\frac{d}{ds} \langle k' | V | k \rangle = \int_0^\infty d^3q (k'^2 + k^2 - 2q^2) \langle k' | V | q \rangle \langle q | V | k \rangle - (k^2 - k'^2)^2 \langle k' | V | k \rangle$$

To understand what this will do, let's assume the first term is small and we can neglect it. Then

$$\frac{d}{ds} \langle k' | V | k \rangle \approx - (k^2 - k'^2)^2 \langle k' | V | k \rangle$$

which we can immediately integrate to obtain

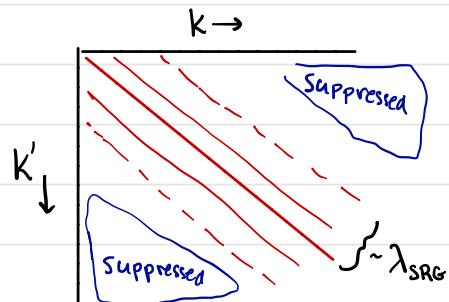
$$\langle k' | V(s) | k \rangle = \langle k' | V(0) | k \rangle e^{-(k'^2 - k^2)s}.$$

We find that off-diagonal matrix elements ($k \neq k'$) are suppressed exponentially, with a strength depending on the difference in the incoming and outgoing momenta. Diagonal matrix elements are unchanged.

We can also observe that we are essentially applying a regulator which suppresses couplings with a momentum difference characterized by the SRG scale

$$\lambda_{\text{SRG}} = s^{-1/4}.$$

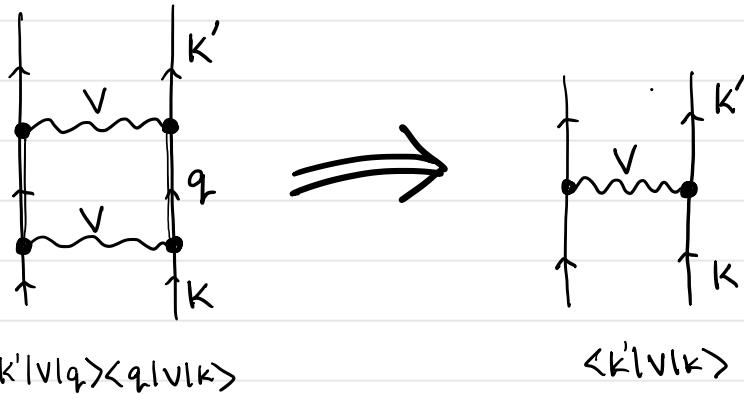
If we view $\langle k' | V | k \rangle$ as a matrix, we are driving V towards a band diagonal form, with a width about the diagonal characterized by λ_{SRG} .



Of course, we can't just ignore the first term in the flow equation. It has to be there to maintain unitarity by absorbing the high momentum physics into a change in the low-momentum parameters. If $k' \approx k$, we ignore the second term and we have

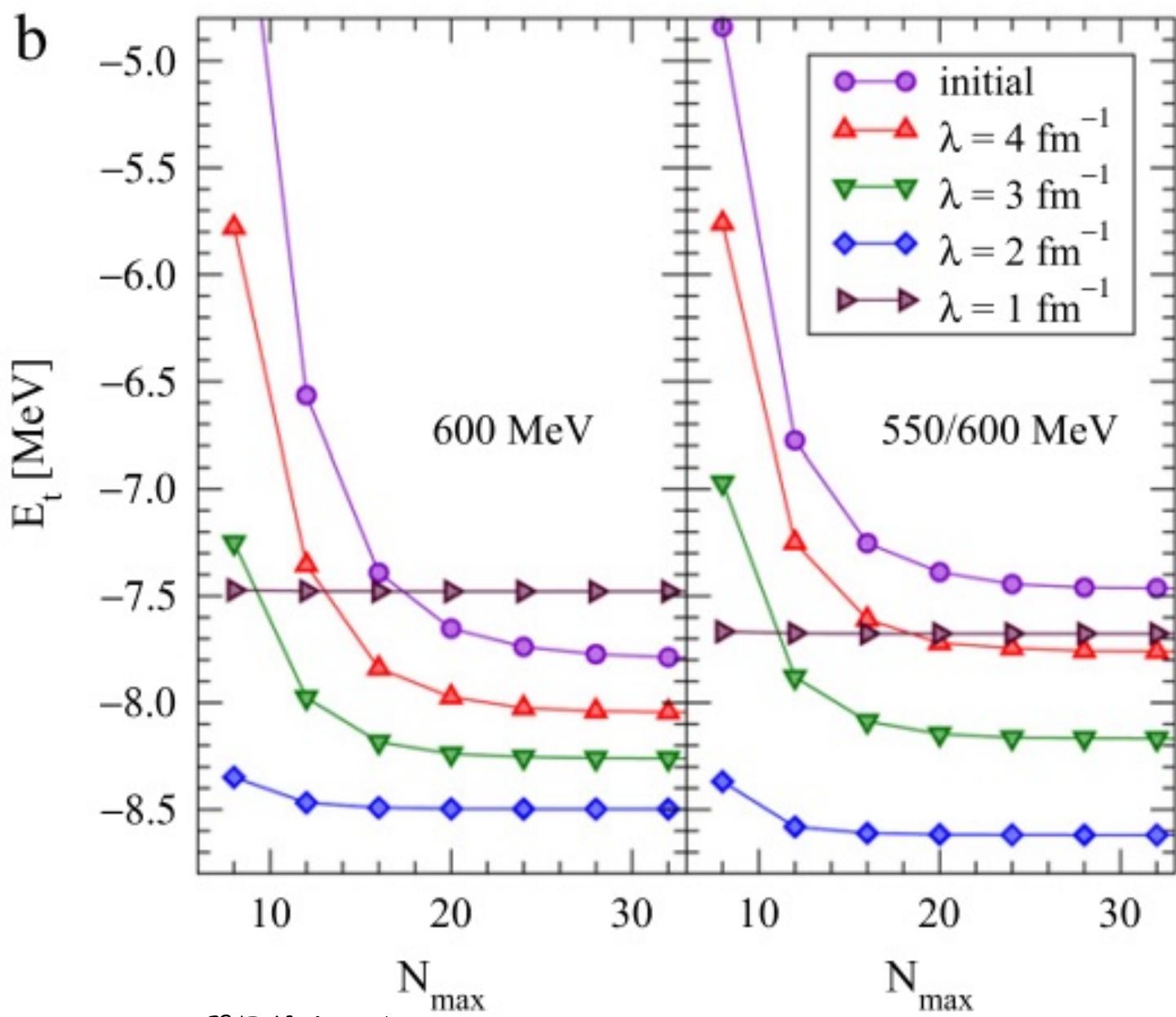
$$\frac{d}{ds} \langle k' | V | k \rangle \approx \int_0^\infty dq (k'^2 + k^2 - 2q^2) \langle k' | V | q \rangle \langle q | V | k \rangle$$

Inside the integral, values of $q \sim k \sim k'$ won't do much because $k'^2 + k^2 - 2q^2 \approx 0$. The change in the potential is dominated by contributions from high momenta $q \gg k$. Schematically, we can think of this in terms of diagrams



As we eliminate low-to-high momentum coupling, a process that would have involved two scatterings with a high momentum intermediate state, is described in the new theory by a single scattering with a renormalized potential.

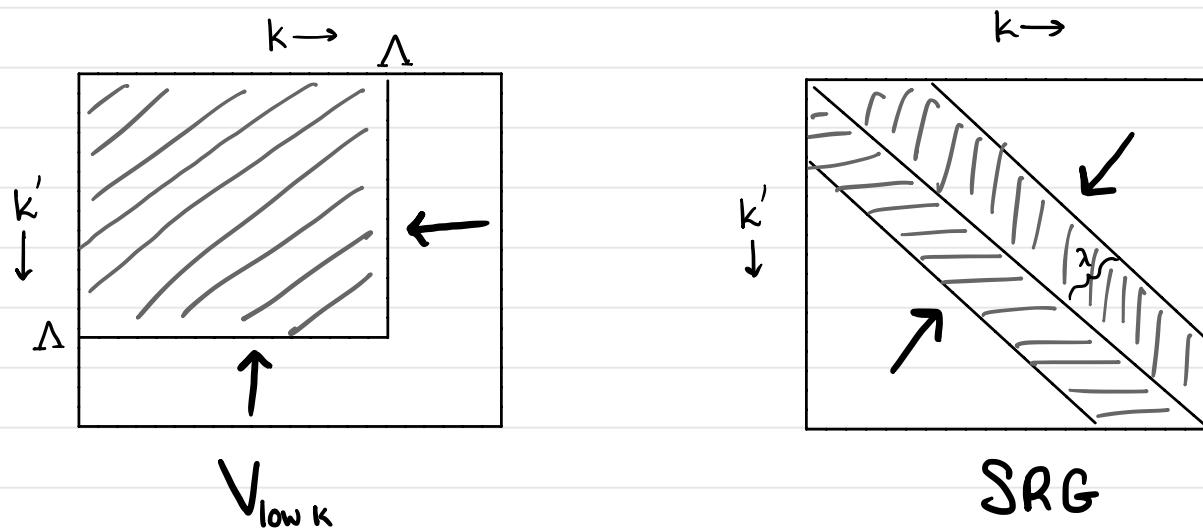
The SRG in this case is performing the same function as $V_{\text{low}k}$, although there are some differences.



From Bognet et. al PPNP 65, 94 (2010)

The first major difference is that $V_{\text{low } k}$ eliminates high momentum modes from the theory, while the SRG suppresses coupling between high and low momenta. The SRG leaves the coupling between high momentum modes largely intact.

Schematically,



Note that the band-diagonal structure of the SRG flow is a consequence of the choice $\eta = [T, H]$, since the kinetic energy is diagonal in k . We could make a different choice and obtain different behavior. For example, $\eta = [P_x H P_x + Q_x H Q_x, H]$, with the projectors

$$P_\Lambda \equiv \int d^3k |k\rangle \langle k|, \quad Q_\Lambda \equiv \int_0^\infty d^3k |k\rangle \langle k| \quad \text{will generate } V_{\text{low } k} \text{-type flow.}$$

Another difference is one of convenience. $V_{\text{low } k}$ requires the solution of the Lippman-Schwinger equation at each step in the flow. SRG requires the evaluation of commutators, which can be cast as a matrix-matrix multiplication — something computers are very good at.

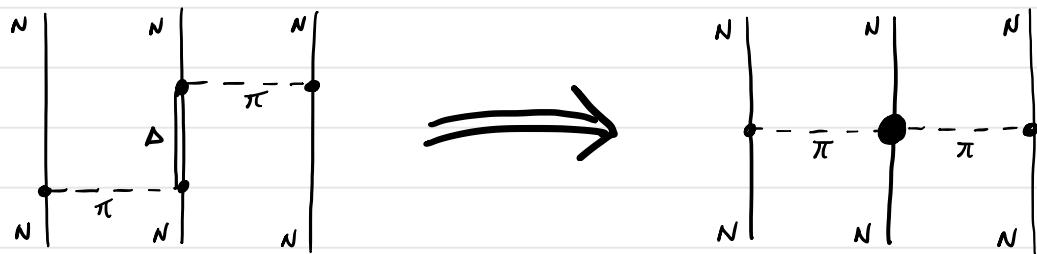
The third difference is in the handling of many-body forces. We can see immediately that they will arise in either formalism by considering the following diagrams



A process in which two low momentum particles P_1 & P_2 scatter into a state with one low momentum P_1' and one high momentum $q \gg P_1, P_2$ will be eliminated by the RG flow (SRG or $V_{\text{low } k}$ decimation) $\frac{1}{2}(q - P_1') > 1$. However, before the elimination, the presence of a third low momentum particle P_3 could allow the high momentum q particle to scatter back down to low momenta P_2', P_3' .

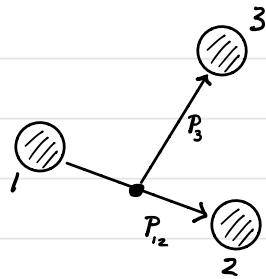
In order to keep the physics unchanged, we need a counter term, which in this case is an irreducible 3-body term in the Hamiltonian. Practically speaking, 3-body terms are more painful to deal with - equations are more complicated, with more integrals/summations, and storage requirements increase rapidly. We might therefore consider the generation of 3-body terms an unacceptable (but inevitable) consequence of eliminating undesired modes. However, in nuclear physics we need to deal with 3N forces anyway, so this actually doesn't impose much of an additional burden.

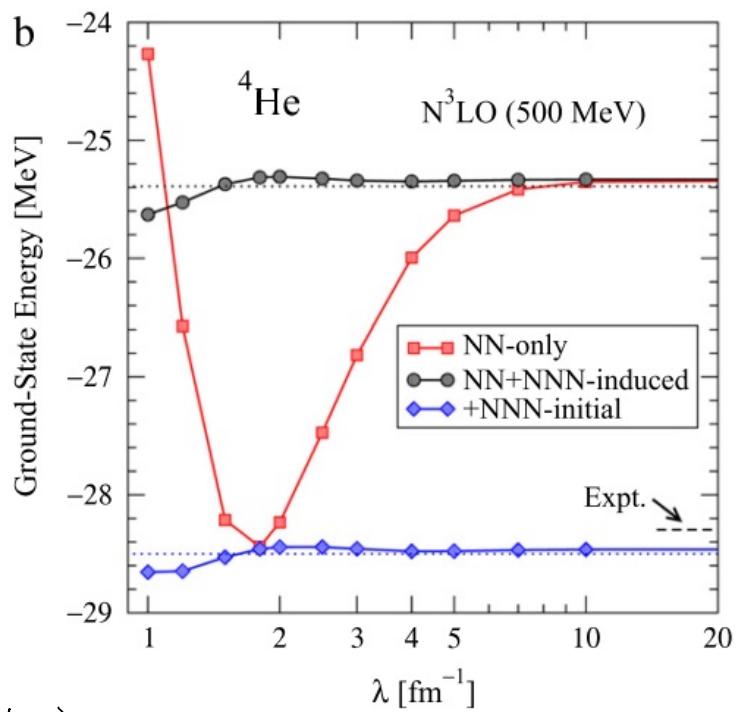
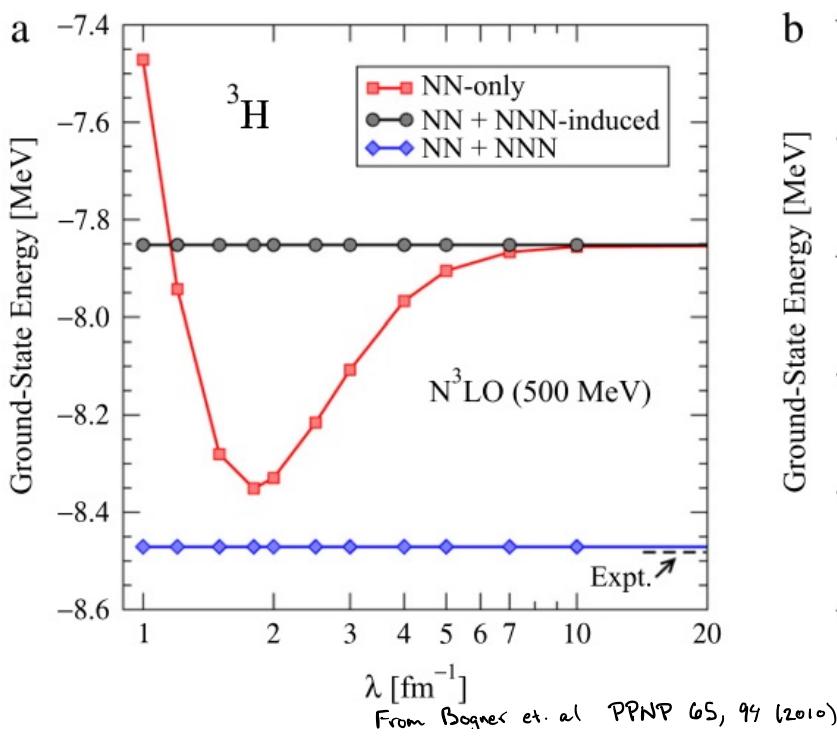
Incidentally, these original 3N forces can be understood in the context of renormalization as having arisen due to "integrating out" other degrees of freedom - not just high momenta this time, but different particles such as the $\Delta(1232)$ excitation of the nucleon, or heavy mesons, e.g.



Both the V_{low_k} and SRG formulations can in principle accommodate 3-body forces. However, especially if we work in momentum space, the V_{low_k} formulation is more awkward. It requires a generalization of the T matrix to 3-body scattering and then requires the solution of the Lippmann-Schwinger equation for all bound and scattering states - including nucleon-deuteron scattering - at every integration step. To my knowledge, this has not been implemented. Further, we now have two Jacobi momenta, and it's not immediately obvious how to consistently regulate them.

One can work in a discrete basis,
eg. harmonic oscillator, but then
this requires us to impose some
artificial trap.





On the other hand, the SRG is formulated as a unitary transformation

$$H(s) = U(s) H(0) U^\dagger(s)$$

and so we may apply exactly the same transformation to the 3N sector unambiguously. There is, of course, no getting around the increase in required storage. But this is manageable.

Example: SRG diagonalization of a 2×2 matrix

Consider a Hamiltonian acting on a 2-state Hilbert space. This can be represented by a Hermitian 2×2 matrix:

$$H(s=0) = \begin{pmatrix} \epsilon_1 & V^* \\ V & \epsilon_2 \end{pmatrix}$$

We wish to drive this matrix towards the diagonal. We could define $H^a \equiv \begin{pmatrix} \epsilon_1 & 0 \\ 0 & \epsilon_2 \end{pmatrix}$ and choose a canonical generator $\eta^{\text{can}} = [H^a, H]$. This will work; however for this case another choice is nicer for an analytic solution:

$$\eta = \frac{V}{\Delta} - \text{h.c.} \quad \text{with} \quad \Delta \equiv \epsilon_2 - \epsilon_1,$$

$$\text{so} \quad \eta = \frac{1}{\epsilon_2 - \epsilon_1} \begin{pmatrix} 0 & -V^* \\ V & 0 \end{pmatrix}.$$

Note that with this choice η is dimensionless. Our flow equation is then

$$\begin{aligned} \frac{d}{ds} H &= [\eta, H] = \frac{1}{\epsilon_2 - \epsilon_1} \left(\begin{pmatrix} 0 & -V^* \\ V & 0 \end{pmatrix} \begin{pmatrix} \epsilon_1 & V^* \\ V & \epsilon_2 \end{pmatrix} - \begin{pmatrix} \epsilon_1 & V^* \\ V & \epsilon_2 \end{pmatrix} \begin{pmatrix} 0 & -V^* \\ V & 0 \end{pmatrix} \right) \\ &= \frac{1}{\epsilon_2 - \epsilon_1} \begin{pmatrix} -2|V|^2 & -(\epsilon_2 - \epsilon_1)V^* \\ -(\epsilon_2 - \epsilon_1)V & +2|V|^2 \end{pmatrix}. \end{aligned}$$

So we have four differential equations

$$\frac{d}{ds} E_1(s) = -2 \frac{|V|^2}{\epsilon_2 - \epsilon_1}, \quad \frac{d}{ds} V^*(s) = -V^*(s)$$

$$\frac{d}{ds} V(s) = -V(s), \quad \frac{d}{ds} E_2(s) = +2 \frac{|V|^2}{\epsilon_2 - \epsilon_1}$$

The solutions for V and V^* are easy

$$V(s) = V(0) e^{-s}.$$

We see that the off-diagonal piece is suppressed exponentially as we flow in s . The equations for E_1 and E_2 can be solved by changing variables

$$\bar{E}(s) = \frac{E_1(s) + E_2(s)}{2}, \quad \Delta(s) = E_2(s) - E_1(s)$$

then $\frac{d}{ds} \bar{E}(s) = \frac{1}{2} \left(\frac{d}{ds} E_1 + \frac{d}{ds} E_2 \right) = 0$,
and

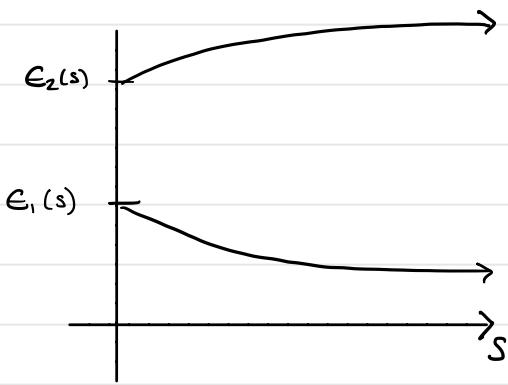
$$\frac{d}{ds} \Delta(s) = \frac{4|V(s)|^2}{\Delta(s)} \Rightarrow \Delta(s) \frac{d}{ds} \Delta(s) = 4|V(0)|^2 e^{-2s}$$

$$\frac{d}{ds} \Delta^2(s) = 8|V(0)|^2 e^{-2s}$$

$$\Delta^2(s) = \Delta^2(0) + 4|V(0)|^2 (1 - e^{-2s})$$

So the gap grows with increasing s , asymptoting to the correct answer

$$\Delta(\infty) = \sqrt{\Delta^2(0) + 4|V(0)|^2}.$$



Fock space formulation

In the 2×2 system we just looked at, as well as the pairing model problem we have considered, it is possible to write the Hamiltonian as a matrix in a Hilbert space. In such a case, the SRG amounts to a method for diagonalizing a matrix, though not a particularly efficient one - it is essentially a generalization of the Jacobi iterative method.

If we do not integrate all the way to the fixed point (where $\frac{d}{dt}H=0$), then we have "pre-diagonalized" the matrix - that is, we have transformed it to a more diagonal form.

Quite often in many-body systems, we deal with systems for which the dimension of the full Hilbert space is so large that it is impractical or impossible to form the relevant matrix and diagonalize it. In such cases, we rely on the few-body character of the Hamiltonian - essentially making a cluster expansion - and express the Hamiltonian and other operators in terms of creation/annihilation operators acting on a Fock space. The Hamiltonian is then

$$H = \sum_{pq} H_{pq} a_p^\dagger a_q + \frac{1}{4} \sum_{pqrs} H_{pqrs} a_p^\dagger a_q^\dagger a_s a_r + \dots$$

where the ... represents (irreducible) 3, 4, 5 etc. body operators, and p, q, r, s run over some discrete single-particle basis.

The SRG generator η can likewise be expressed as a Fock space (or second-quantized) operator

$$\eta = \sum_{pq} \eta_{pq}^{[1]} a_p^+ a_q + \frac{1}{4} \sum_{pqrs} \eta_{pqrs}^{[2]} a_p^+ a_q^+ a_s a_r + \dots$$

The anti-hermiticity of η is encoded by the requirement $\eta_{pq} = -\eta_{qp}$, $\eta_{pqrs} = -\eta_{rspq}$ etc.

Our flow equation,

$$\frac{d}{ds} H = [\eta, H]$$

can be expressed in terms of the coefficients of the creation/annihilation operators by collecting together terms with a given number of creation/annihilation operators. For concreteness, let's assume H and η are initially 2-body operators. Then

$$\begin{aligned} [\eta, H] &= \sum_{\substack{pq \\ rs}} \eta_{pq} H_{rs} [a_p^+ a_q, a_r^+ a_s] \\ &\quad + \frac{1}{4} \sum_{\substack{pqrs \\ tu}} (\eta_{pqrs} H_{tu} - \eta_{tu} H_{pqrs}) [a_p^+ a_q^+ a_s a_r, a_t^+ a_u] \\ &\quad + \frac{1}{16} \sum_{\substack{pqrs \\ tuvw}} \eta_{pqrs} H_{tuvw} [a_p^+ a_q^+ a_s a_r, a_t^+ a_u^+ a_w a_v]. \end{aligned}$$

Beginning with the fundamental anticommutation relations

$$[a_p^+, a_q^+]_+ = [a_p, a_q]_+ = 0, \quad [a_p^+, a_q]_+ = [a_p, a_q^+]_+ = \delta_{pq}$$

we can work out the above commutators.

Relevant commutators:

$$[a_p^+ a_q, a_r^+ a_s] = a_p^+ a_s \delta_{qr} - a_r^+ a_q \delta_{sp}$$

$$[a_p^+ a_q^+ a_s a_r, a_t^+ a_u] = a_p^+ a_q^+ a_s a_u \delta_{rt} + a_p^+ a_q^+ a_u a_r \delta_{st} - a_t^+ a_q^+ a_s a_r \delta_{pu} - a_p^+ a_t^+ a_s a_r \delta_{qu}$$

$$[a_p^+ a_q^+ a_s a_r, a_t^+ a_u^+ a_w a_v] = a_p^+ a_q^+ a_w a_v (\delta_{rt} \delta_{su} - \delta_{ru} \delta_{st}) - a_t^+ a_u^+ a_s a_r (\delta_{pv} \delta_{qw} - \delta_{pw} \delta_{qv})$$

$$\left. \begin{aligned}
& + a_p^+ a_q^+ a_u^+ a_w a_v a_r \delta_{st} + a_t^+ a_p^+ a_q^+ a_s a_w a_v \delta_{ur} \\
& + a_p^+ a_q^+ a_u^+ a_w a_s a_v \delta_{rt} + a_p^+ a_t^+ a_q^+ a_w a_v a_r \delta_{su} \\
& - a_t^+ a_u^+ a_q^+ a_s a_r a_v \delta_{pw} - a_p^+ a_t^+ a_u^+ a_w a_s a_r \delta_{qv} \\
& - a_t^+ a_u^+ a_q^+ a_s a_w a_r \delta_{pv} - a_t^+ a_p^+ a_u^+ a_s a_r a_v \delta_{qw}.
\end{aligned} \right\} \text{induced 3-body terms}$$

We can collect like terms to find

$$\frac{d}{ds} H_{pq} = \sum_a \eta_{pa} H_{aq} - H_{ap} \eta_{qa}$$

$$\begin{aligned}
\frac{d}{ds} H_{pqrs} = & \sum_a \eta_{pqas} H_{ar} + \eta_{pqra} H_{as} - \eta_{qrs} H_{pa} - \eta_{pars} H_{qa} \\
& - H_{pqas} \eta_{ar} - H_{pqra} \eta_{as} + H_{qrs} \eta_{pa} + H_{pars} \eta_{qa} \\
& + \frac{1}{4} \sum_{ab} \eta_{pqab} H_{bars} - \eta_{pqab} H_{bars} - H_{pqab} \eta_{bars} + H_{pqab} \eta_{bars}.
\end{aligned}$$

These expressions can be simplified assuming we work with antisymmetrized matrix elements ($H_{pqrs} = -H_{pqsr}$).

Introducing the index exchange operator P_{ij}

$$P_{ij} H_{p...i...j...} = H_{p...j...i...}$$

We have

$$\frac{d}{ds} H_{pq} = \sum_a \eta_{pa} H_{aq} - H_{ap} \eta_{qa}$$

$$\begin{aligned} \frac{d}{ds} H_{pqrs} = & \sum_a (1 - P_{rs}) (\eta_{pqas} H_{ar} - H_{pqas} \eta_{ar}) - (1 - P_{pq}) (\eta_{pars} H_{qa} - H_{pars} \eta_{qa}) \\ & + \frac{1}{2} \sum_{ab} (\eta_{pqab} H_{abrs} - H_{pqab} \eta_{abrs}). \end{aligned}$$

As we can see from our commutator expressions, we also induce a 3-body piece $H_{pqrsstu}$

$$\frac{d}{ds} H_{pqrsstu} = \sum_a (1 - P_{st} - P_{su}) (\eta_{pqsa} H_{artu} - H_{pqsa} \eta_{artu}).$$

This is a more precise statement of our earlier observation that removing modes (or coupling to modes) will lead to 3-body forces. As soon as H has a 3-body component, then there is a new term in the flow equation

$$\frac{dH}{ds} = \dots + \frac{1}{(2!)^2} \frac{1}{(3!)^2} \sum_{\substack{\text{pqrs} \\ \text{tuvwxy}}} \eta_{pqrs} H_{tuvwxy} [\{a_p^+ a_q^+ a_s a_r\}, \{a_t^+ a_u^+ a_v^+ a_y a_x a_w\}]$$

This commutator will lead to 4-body forces and so on. Keeping track of all these terms is completely infeasible for systems of interest in nuclear physics so

we must make some approximation. A useful choice is to neglect all operators above a given particle rank, e.g. 2-body.

Is this justified? If we start at $s=0$ with the 4-body force equal to zero, at least early in the flow it should stay small. So long as the 4-body term is small, the induced 5-body term must be small, and so on. So it is reasonable that this is a good expansion. Of course, later in the flow the 4-body part could grow larger and spoil everything.

In principle, one should keep enough terms to be sure that higher terms are small. In practice, this is not always feasible and we are left hoping.

We do have at least one diagnostic: if the approximation is a good one, then our computed observables should be independent of the flow parameter s . Any flow parameter dependence is an indication of physics being lost in the truncation.

Note: In practice the SRG is performed not with a Fock space formulation, but in a relative coordinate or Jacobi basis, either using plane waves or an oscillator basis. This is because the Fock space formulation includes the irrelevant center-of-mass motion and so is less efficient.