NN operator conventions

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Abstract

Notes on calculating NN operators in momentum-space documenting our convention in detail.

I. WAVE FUNCTIONS AND POTENTIALS

We implement our calculations in two-particle partial-wave momentum-space with basis states $|klm\rangle$ where k is the magnitude of the relative momentum of the nucleons, l is the orbital momentum associated with the relative motion, and m is the projection of the orbital momentum onto the z-axis in units where $\hbar = 1$. According to Dirac QM2 conventions, the completeness relation is given by

$$\mathbb{1} = \frac{2}{\pi} \sum_{l,m} \int_0^\infty dk k^2 \left|klm\right\rangle \left\langle klm\right| . \tag{1}$$

Projecting onto a partial-wave channel and suppressing the indices reduces this relation to

$$\mathbb{1} = \frac{2}{\pi} \int_0^\infty dk k^2 \left|k\right\rangle \left\langle k\right| . \tag{2}$$

In our situation, we diagonalize a Hamiltonian H for eigenenergies E_α (both of which are in units MeV) and eigenfunctions $|\psi_\alpha\rangle$, that is,

$$H \left|\psi_\alpha\right\rangle = E_\alpha \left|\psi_\alpha\right\rangle . \tag{3}$$

We write Eq. (3) in momentum-space using the completeness relation Eq. (2)

$$\frac{2}{\pi} \int_0^\infty dk' k'^2 \left\langle k|H|k'\right\rangle \left\langle k'|\psi_\alpha\right\rangle = E_\alpha \left\langle k|\psi_\alpha\right\rangle . \tag{4}$$

Numerically, the problem is discrete. We construct an array of momentum values k_i with weights w_i using Gaussian quadrature where $i = 1 \cdots N$. Then Eq. (4) takes the following form,

$$\frac{2}{\pi} \sum_{j=1}^N w_j k_j^2 \left\langle k_i|H|k_j\right\rangle \left\langle k_j|\psi_\alpha\right\rangle = E_\alpha \left\langle k_i|\psi_\alpha\right\rangle . \tag{5}$$

Let's rewrite Eq. (5) such that the momenta and weights are absorbed into the Hamiltonian and wave functions so we can connect to numerically diagonalizing a matrix as is done in practice. Start by multiplying by a factor of $\sqrt{\frac{2w_i}{\pi}} k_i$ on both sides of Eq. (5):

$$\frac{2}{\pi} \sum_{j=1}^N \sqrt{\frac{2w_i}{\pi}} k_i w_j k_j^2 \left\langle k_i|H|k_j\right\rangle \left\langle k_j|\psi_\alpha\right\rangle = E_\alpha \sqrt{\frac{2w_i}{\pi}} k_i \left\langle k_i|\psi_\alpha\right\rangle . \tag{6}$$

Rearranging the momenta and weights, we have

$$\sum_{j=1}^N \left(\frac{2}{\pi} k_i k_j \sqrt{w_i w_j} \left\langle k_i|H|k_j\right\rangle\right) \left(\sqrt{\frac{2w_j}{\pi}} k_j \left\langle k_j|\psi_\alpha\right\rangle\right) = E_\alpha \left(\sqrt{\frac{2w_i}{\pi}} k_i \left\langle k_i|\psi_\alpha\right\rangle\right), \tag{7}$$

$$\sum_{j=1}^{N} \tilde{H}_{ij}(\tilde{\psi_\alpha})_j = E_\alpha(\tilde{\psi_\alpha})_i, \tag{8}$$

where

$$\tilde{H}_{ij} \equiv \frac{2}{\pi} k_i k_j \sqrt{w_i w_j} \left\langle k_i | H | k_j \right\rangle, \tag{9}$$

$$(\tilde{\psi_\alpha})_i \equiv \sqrt{\frac{2w_i}{\pi}} k_i \left\langle k_i | \psi_\alpha \right\rangle. \tag{10}$$

If one does not include the factor of $\sqrt{\frac{2}{\pi}}$ in Eq. (10), then $\langle \psi_\alpha | \psi_\alpha \rangle = \frac{2}{\pi}$ given our completeness relation Eq. (2).

In practice, we diagonalize the Hamiltonian $\tilde{H}$ for normalized eigenvectors which are the wave functions $\tilde{\psi_\alpha}$. Note, both $\tilde{H}$ and $\tilde{\psi_\alpha}$ include the momentum/weight factors. Therefore, in presenting potentials and wave functions that are independent of the momentum-mesh, we must plot quantities with the factors of momenta and weights divided out, $\tilde{V}_{ij} \times \frac{\pi}{2k_i k_j \sqrt{w_i w_j}}$ and $\tilde{\psi}_i \times \frac{\sqrt{\pi}}{k_i \sqrt{2w_i}}$. In Fig. 1 we show deuteron momentum distributions using $\langle k_i | \psi_d \rangle$ for two different momentum meshes.

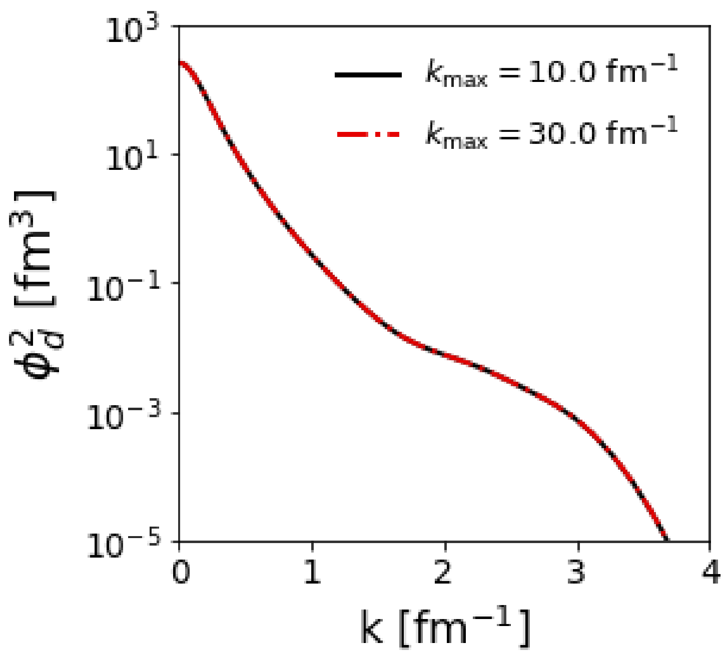

FIG. 1. Deuteron momentum distributions from the EM N^{3}LO 500 MeV potential with two different momentum meshes: $k_{\max} = 10$ and 30 fm^{-1}.

II. MOMENTUM PROJECTION OPERATOR

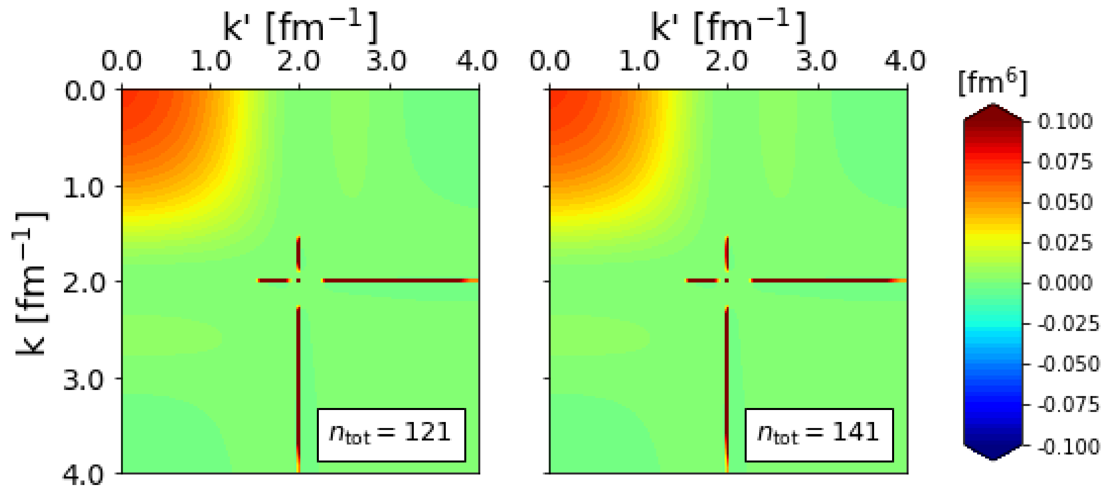

FIG. 2. Momentum projection operators with $q = 2$ fm^{-1} under SRG transformations from EM N^{3}LO 500 MeV potential with two different momentum meshes: $N = 121$ and 141 where $k_{\rm max} = 6$ and $k_{\rm mid} = 2$ fm^{-1}. (This allows for the same value of $q = 1.999$ fm^{-1} in each mesh, so the initial operator is identical.) Here, we use the Wegner generator and set $\lambda = 1.5$ fm^{-1}.

We can connect the momentum projection operator to the normalization of the wave functions $|\psi_\alpha\rangle$. We suppress the state index α in the following,

$$\begin{aligned}
1 &= \langle\psi|\psi\rangle \\
&= \frac{2}{\pi}\int_0^\infty dq q^2 \langle\psi|q\rangle \langle q|\psi\rangle \\
&= (\frac{2}{\pi})^3 \int_0^\infty dq q^2 \int_0^\infty dk k^2 \int_0^\infty dk' k'^2 \langle\psi|k\rangle \; \langle k|a_q^\dagger a_q|k'\rangle \langle k'|\psi\rangle \\
&\approx (\frac{2}{\pi})^3 \sum_{n=1}^N w_n q_n^2 \sum_{i=1}^N w_i k_i^2 \sum_{j=1}^N w_j k_j^2 \langle\psi|k_i\rangle \; \langle k_i|a_{q_n}^\dagger a_{q_n}|k_j\rangle \langle k_j|\psi\rangle \\
&= \sum_{n=1}^N \sum_{i=1}^N \sum_{j=1}^N (\sqrt{\frac{2w_i}{\pi}} k_i \langle\psi|k_i\rangle)(\frac{2}{\pi} w_n q_n^2 \frac{2}{\pi} k_i k_j \sqrt{w_i w_j} \langle k_i|a_{q_n}^\dagger a_{q_n}|k_j\rangle)(\sqrt{\frac{2w_j}{\pi}} k_j \langle k_j|\psi\rangle) \\
&= \sum_{n=1}^N \sum_{i=1}^N \sum_{j=1}^N (\tilde{\psi_\alpha^*})_i \frac{2}{\pi} w_n q_n^2 (\tilde{a}_{q_n}^\dagger \tilde{a}_{q_n})_{ij} (\tilde{\psi_\alpha})_j.
\end{aligned} \tag{11}$$

From this, we identify

$$(\tilde{a}_{q_n}^\dagger \tilde{a}_{q_n})_{ij} = \frac{\pi \delta_{ni}\delta_{nj}}{2 w_n q_n^2}, \tag{12}$$

$$\langle k_i | a^\dagger_{q_n} a_{q_n} | k_j \rangle = \frac{\pi (\tilde{a}^\dagger_{q_n} \tilde{a}_{q_n})_{ij}}{2 k_i k_j \sqrt{w_i w_j}}. \tag{13}$$

For the purposes of presentation, we want to plot mesh-independent results analogous to plotting mesh-independent potentials. This concept should be generalized to *any* operator. Thus, we plot Eq. 13 to visualize the momentum projection operator. In applying SRG transformations to this operator, use Eq. (12), because the transformations are typically constructed out of the normalized eigenvectors of the initial and evolved Hamiltonians meaning the transformation matrix already includes the momenta and weights for "integrating" over dk and dk'. Figure 2 shows SRG-evolved momentum projection operators $\langle k_i | a^\dagger_{q_n} a_{q_n} | k_j \rangle_\lambda$ at $q = 2$ fm^{-1} and $\lambda = 1.5$ fm^{-1} for two different momentum meshes.

Let's do a sanity check by evaluating $\langle \psi | a^\dagger_q a_q | \psi \rangle = |\psi(q)|^2$. Note, this is the squared value of the wave function ψ with momenta and weights divided out, evaluated at some momentum value q where the units are fm^3. In the following check, let q also denote the index of the momentum value q within the momentum array.

$$\begin{aligned}
\langle \psi | a^\dagger_q a_q | \psi \rangle &= (\frac{2}{\pi})^2 \int_0^\infty dk k^2 \int_0^\infty dk' k'^2 \langle \psi | k \rangle \, \langle k | a^\dagger_q a_q | k' \rangle \, \langle k' | \psi \rangle \\
&\approx (\frac{2}{\pi})^2 \sum_{i=1}^N w_i k_i^2 \sum_{j=1}^N w_j k_j^2 \langle \psi | k_i \rangle \, \langle k_i | a^\dagger_q a_q | k_j \rangle \, \langle k_j | \psi \rangle \\
&= (\frac{2}{\pi})^2 \sum_{i=1}^N w_i k_i^2 \sum_{j=1}^N w_j k_j^2 \langle \psi | k_i \rangle \, \frac{\pi^2 \delta_{ni} \delta_{nj}}{4 q_n^2 w_n k_i k_j \sqrt{w_i w_j}} \, \langle k_j | \psi \rangle \\
&= \langle \psi | q \rangle \, \langle q | \psi \rangle \\
&= |\psi(q)|^2.
\end{aligned} \tag{14}$$

Alternative derivation of the momentum projection operator

Let's start by defining the projection operator in Dirac notation for discrete states α. The states are orthogonal and satisfy the completeness relation

$$\langle \alpha | \beta \rangle = \delta_{\alpha\beta}, \tag{15}$$

$$\mathbb{1} = \sum_\alpha |\alpha\rangle \langle \alpha| \equiv \sum_\alpha P_\alpha, \tag{16}$$

where $P_\alpha \equiv |\alpha\rangle \langle \alpha|$ is the projection operator for the state α. We can expand any state $|\psi\rangle$ in terms of the states $|\alpha\rangle$,

$$|\psi\rangle = \sum_\alpha \langle \alpha | \psi \rangle \, |\alpha\rangle = \sum_\alpha P_\alpha \, |\psi\rangle \, . \tag{17}$$

Matrix elements of the projection operator are given by

$$\langle\beta|P_\alpha|\gamma\rangle = \langle\beta|\alpha\rangle\,\langle\alpha|\gamma\rangle = \delta_{\beta\alpha}\delta_{\alpha\gamma}, \tag{18}$$

where we used the orthogonality relation Eq. (15) in the last step. We can make a consistency check with the projection operator P_α by using it to evaluate the normalization of the wave function,

$$\begin{aligned}\sum_\alpha \langle\psi|P_\alpha|\psi\rangle &= \sum_\alpha\sum_\beta\sum_\gamma \langle\psi|\beta\rangle\,\langle\beta|P_\alpha|\gamma\rangle\,\langle\gamma|\psi\rangle \\ &= \sum_\alpha\sum_\beta\sum_\gamma \langle\psi|\beta\rangle\,\langle\beta|\alpha\rangle\,\langle\alpha|\gamma\rangle\,\langle\gamma|\psi\rangle \\ &= \sum_\alpha\sum_\beta\sum_\gamma \langle\psi|\beta\rangle\,\delta_{\beta\alpha}\delta_{\alpha\gamma}\,\langle\gamma|\psi\rangle \\ &= \sum_\alpha \langle\psi|\alpha\rangle\,\langle\alpha|\psi\rangle \\ &= \langle\psi|\psi\rangle\,. \end{aligned} \tag{19}$$

Now, let's do the same derivation but for two-particle partial-wave momentum-space with basis states $|klm\rangle$. In this basis, the orthogonality condition is given by

$$\langle klm|k'l'm'\rangle = \frac{\pi}{2kk'}\delta(k-k')\delta_{ll'}\delta_{mm'}. \tag{20}$$

(This can be verified by taking $|k'l'm'\rangle$ to both sides of Eq. (1).) Likewise we can expand any state $|\psi\rangle$ using the completeness relation Eq. (1),

$$|\psi\rangle = \frac{2}{\pi}\sum_{l,m}\int_0^\infty dkk^2\,\langle klm|\psi\rangle\,|klm\rangle = \frac{2}{\pi}\sum_{l,m}\int_0^\infty dkk^2 P_{klm}\,|\psi\rangle\,, \tag{21}$$

where $P_{klm} \equiv |klm\rangle\,\langle klm|$. Matrix elements of the projection operator are then

$$\begin{aligned}\langle klm|P_{ql''m''}|k'l'm'\rangle &= \langle klm|ql''m''\rangle\,\langle ql''m''|k'l'm'\rangle \\ &= \frac{\pi}{2kq}\delta(k-q)\delta_{ll''}\delta_{mm''}\frac{\pi}{2qk'}\delta(q-k')\delta_{l''l'}\delta_{m''m'}. \end{aligned} \tag{22}$$

If we fix the relative orbital angular momentum and projection to l and m, respectively, we obtain

$$\langle k|P_q|k'\rangle = \frac{\pi^2}{4q^2kk'}\delta(k-q)\delta(q-k'), \tag{23}$$

in agreement with Eqs. (12) and (13). (Note, this has not accounted for the "discrete" numerical problem. Going one step further would introduce sums and weights instead of the integral over dk.) The normalization check is very straight forward and proceeds in the same manner as Eq. (11).

III. RADIUS-SQUARED OPERATOR

In order to plot the r^2 operator in partial-wave momentum-space, we must change the operator from coordinate-space to partial-wave momentum-space. Technically, we could make calculations with the r^2 operator fully in momentum-space where the operator involves derivatives $\frac{d}{dk}$ acting on a wave function. However, we avoid this as the derivatives make it impossible to see the operator directly. In coordinate-space, the operator is given by

$$\langle \mathbf{r}|r^2|\mathbf{r}'\rangle = r^2\delta(\mathbf{r}-\mathbf{r}'). \tag{24}$$

We can transform the operator to partial-wave momentum-space using

$$\langle \mathbf{r}|klm\rangle \equiv i^l j_l(kr)Y_{lm}(\Omega_r), \tag{25}$$

and the completeness relation in coordinate-space,

$$\mathbb{1} = \int d\mathbf{r}\,|\mathbf{r}\rangle\,\langle\mathbf{r}|\,, \tag{26}$$

(see Dirac QM2 for further details.)

Now we can isolate the radius-squared operator in momentum-space,

$$\begin{aligned}
\langle klm|r^2|k'l'm'\rangle &= \int d\mathbf{r}\int d\mathbf{r}'\,\langle klm|\mathbf{r}\rangle\;\langle\mathbf{r}|r^2|\mathbf{r}'\rangle\,\langle\mathbf{r}'|k'l'm'\rangle \\
&= \int d\mathbf{r}\int d\mathbf{r}'[i^l j_l(kr)Y_{lm}(\Omega_r)]^* r^2\delta(\mathbf{r}-\mathbf{r}')[i^{l'} j_{l'}(k'r')Y_{l'm'}(\Omega_{r'})] \\
&= \int_0^\infty dr r^2\int d\Omega_r (i^l)^* j_l(kr)Y^*_{lm}(\Omega_r)r^2 i^{l'} j_{l'}(k'r)Y_{l'm'}(\Omega_r) \\
&= \delta_{ll'}\delta_{mm'}(i^l)^* i^{l'}\int_0^\infty dr r^4 j_l(kr)j_{l'}(k'r),
\end{aligned} \tag{27}$$

where we have used the normalization of the spherical harmonic functions in the last step. Rewriting Eq. (27) for the case $l=l'$ and $m=m'$ gives

$$\langle k|r^2|k'\rangle_{lm} = \int_0^\infty dr r^4 j_l(kr)j_l(k'r). \tag{28}$$

Then switching from a continuous to a discrete basis gives

$$\langle k_i|r^2|k_j\rangle_{lm} = \sum_{m=1}^{M}\Delta r r_m^4 j_l(k_i r_m)j_l(k_j r_m), \tag{29}$$

where we have a linearly spaced array of r values where $dr \to \Delta r$ and M is the number of values in the array. Following the general convention from before, we define the operator with momenta and weights factored in,

$$(\tilde{r}^2_{lm})_{ij} \equiv \frac{2}{\pi} k_i k_j \sqrt{w_i w_j} \, \langle k_i | r^2 | k_j \rangle_{lm} \, . \tag{30}$$

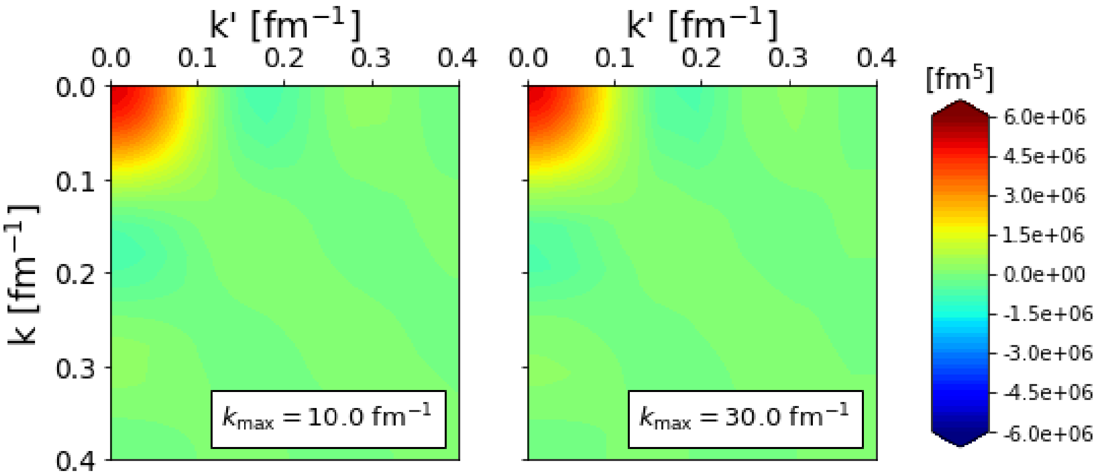

FIG. 3. r^2 operators under SRG transformations from EM N^{3}LO 500 MeV potential with two different momentum meshes: $k_{\max} = 10$ and 30 fm^{-1}. Here, we use the Wegner generator and set $\lambda = 1.5$ fm^{-1}.

This is what is currently in the code in terms of calculating the RMS radius of deuteron. The code reproduces the RKE N^4*LO deuteron radius to high accuracy where we take* $r_{max} =$ 30 *fm (anything less than about* 25 *fm starts to affect the result!) After having written this out, I realized I was applying the SRG transformation matrices (which have momenta and weights factored in) to the wrong form of the* r^2 *operator. I've been applying* $\tilde{U}$ *to Eq.* (29) *whereas it should be applied to Eq.* (30)*! This explains my confusion in looking at the far off-diagonal slices of the operator comparing different transformations. This is now corrected and updated in the paper.*