Infinite Matter Calculations

Coupled Cluster Doubles

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Free-Particle Hamiltonian,

$$\frac{-\hbar^2}{2m}\nabla^2\,\phi(\vec{x}) = \epsilon\,\phi(\vec{x})\,.$$

Periodic Boundary Conditions in L-Box

$$\phi(x,y,z) = \phi(x+L,y,z)$$
$$\phi(x,y,z) = \phi(x,y+L,z)$$
$$\phi(x,y,z) = \phi(x,y,z+L)$$

Single-Particle States

$$\phi_{\vec{k}}(\vec{x}) = \frac{1}{\sqrt{L^3}}e^{i\vec{k}\cdot\vec{x}}, \qquad \vec{k} = \frac{2\pi\vec{n}}{L}, \qquad n_i \in \mathbb{I}$$

Energy Truncation: $n_x^2 + n_x^2 + n_x^2 \leq N_{\mathsf{max}}$

```
n = 0
for shell ∈ {0, ..., N_max} do
    for √N_max ≤ n_x ≤ √N_max do
        for √N_max ≤ n_y ≤ √N_max do
            for √N_max ≤ n_z ≤ √N_max do
                for s_z ∈ {−1/2, 1/2} do
                    if n_x^2 + n_y^2 + n_z^2 = shell then
                        Energy = (4π^2 ħ^2 / 2m) × shell
                        if n < N then
                            type = "hole"
                        else
                            type = "particle"
                        end if
                        STATES ← (n, n_x, n_y, n_z, s_z, Energy, type)
                        n ← n + 1
                    end if
                end for
            end for
        end for
    end for
end for
```

Two-Body Channels

$$\langle pq||rs\rangle \Rightarrow \langle T(pq)\,||\,T(rs)\rangle$$
$$\langle pq||rs\rangle = \langle ps^{-1}||rq^{-1}\rangle \Rightarrow \langle X(ps)\,||\,X(rq)\rangle$$

for sp1 $\in STATES$ **do**
  for sp2 $\in STATES$ **do**
    if $sp1 \neq sp2$ **then**
      $N_i \leftarrow n_{i,1} + n_{i,2}$
      $S_z \leftarrow s_{z,1} + s_{z,2}$
      $T_z \leftarrow t_{z,1} + t_{z,2}$
      i_dir $\leftarrow$ Ind $\left(N_x, N_y, N_z, S_z, T_z\right)$
      $T \leftarrow$ (sp1, sp2, i_dir)
      $N_i' \leftarrow n_{i,1} - n_{i,2}$
      $S_z' \leftarrow s_{z,1} - s_{z,2}$
      $T_z' \leftarrow t_{z,1} - t_{z,2}$
      i_cross $\leftarrow$ Ind $\left(N_x', N_y', N_z', S_z', T_z'\right)$
      $X \leftarrow$ (sp1, sp2, i_cross)
    end if
  end for
end for

One,Three-Body Channels

$$\langle pq||rs\rangle = \langle p||q^{-1}rs\rangle \Rightarrow \langle K(p)\,||\,K_p(qrs)\rangle$$

for Chan $\in T$ **do**
  for tb1 $\in$ Chan **do**
    for tb2 $\in$ Chan **do**
      $K \leftarrow \mathsf{tb1}_1$
      $K_{\mathsf{tb1}_1} \leftarrow \mathsf{tb1}_2, \mathsf{tb2}_1, \mathsf{tb2}_2$
    end for
  end for
end for

$$
\begin{aligned}
t_{ij}^{ab}\epsilon_{ij}^{ab} = \langle ab|\hat{v}|ij\rangle + \frac{1}{2}\sum_{cd}\langle ab|\hat{v}|cd\rangle\, t_{ij}^{cd} + \frac{1}{2}\sum_{kl}\langle kl|\hat{v}|ij\rangle\, t_{kl}^{ab} \\
+ \hat{P}(ij|ab)\sum_{kc}\langle kb|\hat{v}|cj\rangle\, t_{ik}^{ac} + \frac{1}{4}\sum_{klcd}\langle kl|\hat{v}|cd\rangle\, t_{ij}^{cd}t_{kl}^{ab} \\
+ \hat{P}(ij)\sum_{klcd}\langle kl|\hat{v}|cd\rangle\, t_{ik}^{ac}t_{jl}^{bd} - \frac{1}{2}\hat{P}(ij)\sum_{klcd}\langle kl|\hat{v}|cd\rangle\, t_{ik}^{dc}t_{lj}^{ab} \\
-\frac{1}{2}\hat{P}(ab)\sum_{klcd}\langle kl|\hat{v}|cd\rangle\, t_{lk}^{ac}t_{ij}^{db}
\end{aligned}
$$

CCD Intermediates

$$\langle b|\chi|c\rangle = \langle b|f|c\rangle - \frac{1}{2}\sum_{kld} \langle bd|t|kl\rangle \langle kl|v|cd\rangle$$

$$\langle k|\chi|j\rangle = \langle k|f|j\rangle + \frac{1}{2}\sum_{cdl} \langle kl|v|cd\rangle \langle cd|t|jl\rangle$$

$$\langle kl|\chi|ij\rangle = \langle kl|v|ij\rangle + \frac{1}{2}\sum_{cd} \langle kl|v|cd\rangle \langle cd|t|ij\rangle$$

$$\langle kb|\chi|cj\rangle = \langle kb|v|cj\rangle + \frac{1}{2}\sum_{dl} \langle kl|v|cd\rangle \langle db|t|lj\rangle$$

$$\langle ab|\chi|cd\rangle = \langle ab|v|cd\rangle$$

CCD Equations with Intermediates

$$
\begin{aligned}
t_{ij}^{ab}\epsilon_{ij}^{ab} = \langle ab|\hat{v}|ij\rangle + \hat{P}(ab)\sum_{c}\langle b|\chi|c\rangle\, t_{ij}^{ac} - \hat{P}(ij)\sum_{k}\langle k|\chi|j\rangle\, t_{ik}^{ab} \\
+\frac{1}{2}\sum_{cd}\langle ab|\chi|cd\rangle\, t_{ij}^{cd} + \frac{1}{2}\sum_{kl}\langle kl|\chi|ij\rangle\, t_{kl}^{ab} \\
+ \hat{P}(ij|ab)\sum_{kc}\langle kb|\chi|cj\rangle\, t_{ik}^{ac}
\end{aligned}
$$

Intermediates as Matrix-Matrix Multiplications

$$\langle b|\chi|c\rangle \Rightarrow f^{b}_{c}\left(K(b),K(c)\right) - \frac{1}{2} t^{bd}_{kl}\left(K(b),K_b(kld)\right) \cdot v^{kl}_{cd}\left(K_c(kld),K(c)\right)$$

$$\langle k|\chi|j\rangle \Rightarrow f^{k}_{j}\left(K(k),K(j)\right) + \frac{1}{2} v^{kl}_{cd}\left(K(k),K_k(cdl)\right) \cdot t^{cd}_{jl}\left(K_j(cdl),K(j)\right)$$

$$\langle kl|\chi|ij\rangle \Rightarrow v^{kl}_{ij}\left(T(kl),T(ij)\right) + \frac{1}{2} v^{kl}_{cd}\left(T(kl),T(cd)\right) \cdot t^{cd}_{ij}\left(T(cd),T(ij)\right)$$

$$\langle kb|\chi|cj\rangle \Rightarrow v^{kb}_{cj}\left(X(kc),X(jb)\right) + \frac{1}{2} v^{kl}_{cd}\left(X(kc),X(dl)\right) \cdot t^{db}_{lj}\left(X(dl),X(jb)\right)$$

$$\langle ab|\chi|cd\rangle \Rightarrow v^{ab}_{cd}\left(T(ab),T(cd)\right)$$

CCD Equations as Matrix-Matrix Multiplications

$$\sum_{c} \langle b|\chi|c\rangle \langle ac|t|ij\rangle \Rightarrow \chi^{b}_{c}\left(K(b), K(c)\right) \cdot t^{ac}_{ij}\left(K(c), K_c(ija)\right)$$

$$\sum_{k} \langle k|\chi|j\rangle \langle ab|t|ik\rangle \Rightarrow \chi^{k}_{j}\left(K(j), K(k)\right) \cdot t^{ab}_{ik}\left(K(c), K_c(ija)\right)$$

$$\sum_{cd} \langle ab|\chi|cd\rangle \langle cd|t|ij\rangle \Rightarrow \chi^{ab}_{cd}\left(T(ab), T(cd)\right) \cdot t^{cd}_{ij}\left(T(cd), T(ij)\right)$$

$$\sum_{kl} \langle ab|t|kl\rangle \langle kl|\chi|ij\rangle \Rightarrow t^{ab}_{kl}\left(T(ab), T(kl)\right) \cdot \chi^{kl}_{ij}\left(T(kl), T(ij)\right)$$

$$\sum_{kc} \langle ac|t|ik\rangle \langle kb|\chi|cj\rangle \Rightarrow t^{ac}_{ik}\left(X(ia), X(kc)\right) \cdot \chi^{kb}_{cj}\left(X(kc), X(jb)\right)$$

$$V(r) = \frac{1}{2}\left(V_R + \frac{1}{2}\left(1 + P_{12}^{\sigma}\right)V_T + \frac{1}{2}\left(1 - P_{12}^{\sigma}\right)V_S\right)\left(1 - P_{12}^{\sigma}P_{12}^{\tau}\right),$$

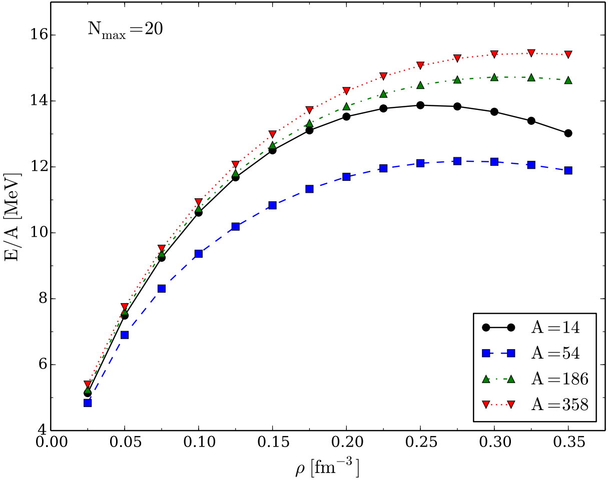
$$V_\alpha\left(r\right) = V_\alpha e^{-\kappa_\alpha r^2},\ P_{12}^{\sigma} = \frac{1}{2}\left(1 + \sigma_1 \cdot \sigma_2\right),\ P_{12}^{\tau} = \frac{1}{2}\left(1 + \tau_1 \cdot \tau_2\right)$$

α	V_α	κ_α
R	200 MeV	1.487 fm^{-2}
T	178 MeV	0.639 fm^{-2}
S	91.85 MeV	0.465 fm^{-2}

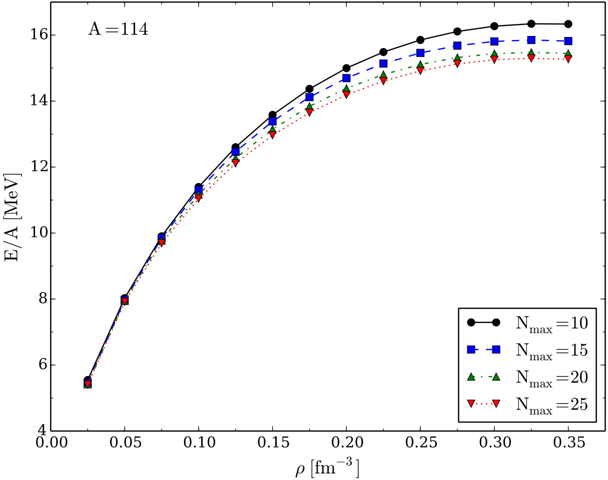
$$\langle pq|V_\alpha|rs\rangle = \frac{V_\alpha}{L^3}\left(\frac{\pi}{\alpha}\right)^{3/2} e^{\frac{-q^2}{4\alpha}} \delta_{\vec{k}_p+\vec{k}_q,\vec{k}_r+\vec{k}_s}$$

$$\vec{q} = \frac{1}{2}\left(\vec{k}_p - \vec{k}_q - \vec{k}_r + \vec{k}_s\right)$$

Pure Neutron Matter



Pure Neutron Matter



$$\phi_{\vec{k}}(\vec{x}+\vec{L}) \rightarrow e^{i\vec{\theta}}\phi_{\vec{k}}(\vec{x})$$

$\theta_i = 0$ for PBC and $\theta_i = \pi$ for APBC

$$\vec{k} \rightarrow \vec{k} + \frac{\vec{\theta}}{L}$$

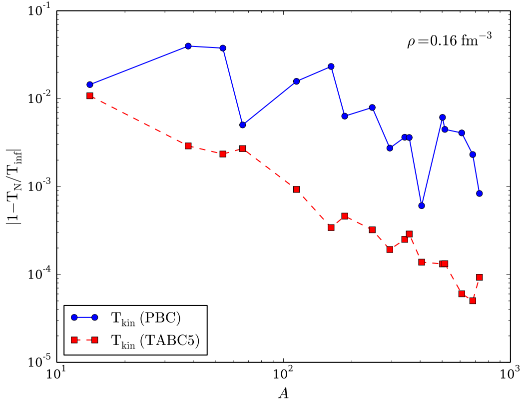
$$\epsilon_{\vec{k}} \rightarrow \epsilon_{\vec{k}} + \frac{\pi}{L}\vec{k}\cdot\vec{\theta} + \frac{\pi^2}{L^2}$$

Build Gauss-Legendre Mesh for Each Direction, $\{\theta_i, w_i\}$

$E_{\text{twist}} = 0$
for $(\theta_x, w_x) \in \{\theta_x, w_x\}$ **do**
    for $(\theta_y, w_y) \in \{\theta_y, w_y\}$ **do**
        for $(\theta_z, w_z) \in \{\theta_z, w_z\}$ **do**
            Build Basis States with $k_i \to k_i + \frac{\theta_i}{L}$
            Order States by Energy and Fill Holes
            Get Result E (T,HF,CCD)
            $E_{\text{twist}} = E_{\text{twist}} + \frac{1}{\pi^3} w_x w_y w_z E$
        end for
    end for
end for

Pure Neutron Matter - Twist Averaging

$$\mathsf{T}_{\mathsf{inf}} = \frac{3\hbar^2 k_f^2}{10m}$$



$$\mathrm{HF_{inf}} = \frac{1}{(2\pi)^6}\frac{L^3}{2\rho}\int_0^{k_f} d\vec{k}_1 \int_0^{k_f} d\vec{k}_2 \, \langle \vec{k}_1\vec{k}_2|\hat{v}|\vec{k}_1\vec{k}_2\rangle$$