Nearly-isentropic Energy Conversion with Quantum Excitation Transfer

Sponsors
Draper Laboratory

Project Staff
M. J. Wu, P. L. Hagelstein, K. P. Sinha, A. Meulenberg, R. S. Dimatteo, C. G. Fonstad

Introduction

We have previously proposed a new device concept in addressing the problem of thermal to electric energy conversion. The device consists of a hot-side emitter, a cold-side converter, and a vacuum gap in between. See Figure 1 for the scheme. The hot-side is at a higher temperature, and it has a two-level quantum well to which the electron is provided from an electron reservoir. The cold-side has one two-level quantum well which is at close proximity to the hot-side well such that electrons in these two wells couple through Coulombic force. The cold-side has a second one-level quantum well which is separated from the first well by a potential barrier. Each well on the cold-side also communicates with a reservoir, which is connected through a load. The high temperature on the hot-side provides an excited electron in the well. Energy transfer occurs through the Coulombic coupling which results in a ground-state electron on the hot-side and an excited electron on the cold-side. This excited electron in turn tunnels through the barrier to the other quantum well before relaxing into the reservoir to provide electrical work.

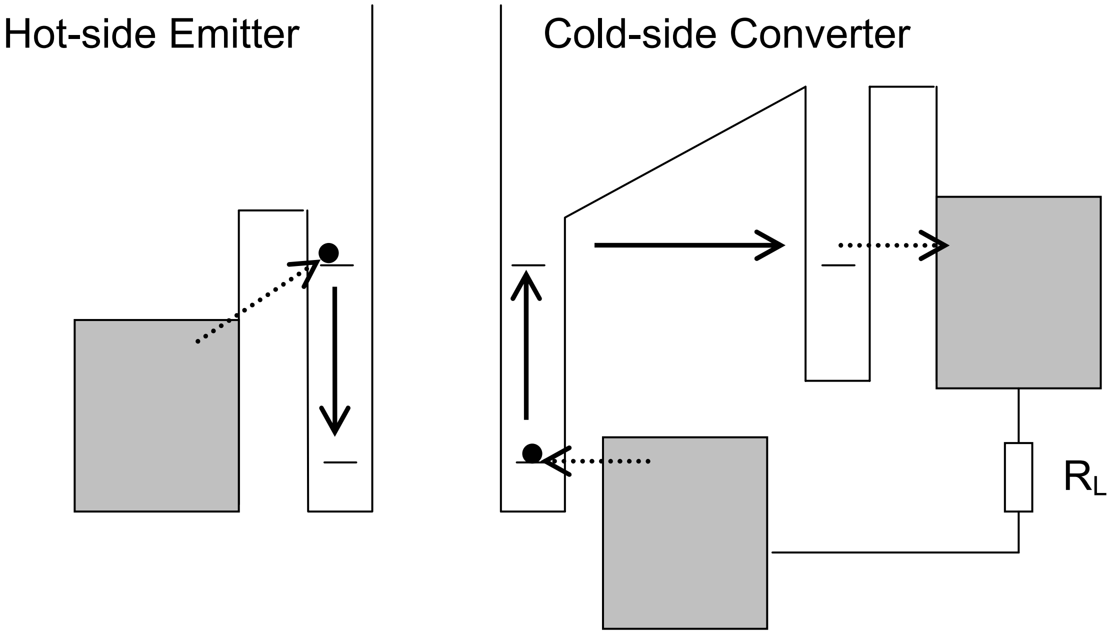


Fig. 1: Schematic of an idealized device structure

Modeling

The scheme under discussion here is interesting theoretically because it has both quantum mechanical components (two-level systems, tunneling and a Coulombic coupling effect) and statistical mechanics components (relaxation to and from the reservoirs). To model this device, we start with Ehrenfest's Theorem for the Coulombic coupling and the tunneling. Then we combine it with classical rate equations for the analysis of relaxations to and from reservoirs. The full set of equations is fairly complex, but the essential features can be captured in the following example. Suppose we have a two-level system with two states, state 1 and state 2, with energy E_1 and E_2, respectively. A coupling between the two states occurs and is termed V. We denote N_1 and N_2 as the occupation probabilities of the two states, and P, Q as the polarization terms caused by coupling V. Both states communicate with a reservoir which gives each state an associated equilibrium occupation value N_1^0 and N_2^0, and an associated relaxation time τ_1 and τ_2. The polarization terms have an associated coherence time τ. The Bloch equations for this simple example would be:

$$\frac{d}{dt}N_1 + \frac{N_1 - N_1^0}{\tau_1} = \frac{V}{\hbar}P$$

$$\frac{d}{dt}N_2 + \frac{N_2 - N_2^0}{\tau_2} = -\frac{V}{\hbar}P$$

$$\frac{d}{dt}P + \frac{P}{\tau} = -\left(\frac{E_2 - E_1}{\hbar}\right) Q + \frac{2\,V}{\hbar}\left[N_2 - N_1\right]$$

$$\frac{d}{dt}Q + \frac{Q}{\tau} = \frac{E_2 - E_1}{\hbar}P$$

To obtain the full model for the device, we extend the above model to account for all the couplings and relaxations that occur between quantum states and reservoirs.

Current

If we denote the energy difference between the two levels in a quantum well as ΔE, the voltage drop between the two cold-side reservoirs as ΔV, the temperature of the hot-side as T_h, the temperature of the cold-side as T_c, and the Boltzmann's constant as k, the current in the cold-side turns out to be proportional to the following expression:

$$current = forward\,current - reverse\,current \sim e^{-\frac{\Delta E}{k\ T_h}} - e^{-\frac{\Delta E}{k\ T_c}} e^{\frac{q \cdot \Delta V}{k\ T_c}} \quad (1)$$

Energy transfer across the vacuum gap can go both ways. When the excitation is transferred from the hot-side to the cold-side, forward current occurs. When energy transfers in the opposite direction, reverse current occurs. The net current is hence the difference between the forward and the reverse currents. The forward current basically depends on the amount of excited electrons in the well, and it has a Boltzmann dependence on the temperature. The reverse current is also dependent on the temperature, but the voltage across the load contributes to the reverse current as well. The higher the voltage drop, the more reverse current is driven by the load.

Efficiency

For each excitation transfer, ΔE amount of energy is lost on the hot-side and ΔE is gained on the cold-side. However, only $q\Delta V$ amount of energy is done on the load, where q is the electron charge. Hence, the efficiency of the device is the ratio of the two quantities:

$$efficiency = \frac{q \cdot \Delta V}{\Delta E} \quad (2)$$

The excitation transfer process is isentropic, and electron tunneling (in the absence of scattering) is also isentropic. However, entropy is introduced when an electron thermalizes into the reservoir. Therefore, the device is nearly-isentropic and becomes isentropic in the limit that no electron thermalizes into the reservoir, that is, no current flows. Figure 2 shows a current vs voltage plot of the device. We can see that the working region of the device (when positive power is providing to the load) is when voltage resides in the following range:

$$0 \le \Delta V \le \frac{\Delta E \cdot Carnot\ limit}{q} = \frac{\Delta E}{q}\left(\frac{T_h - T_c}{T_h}\right)$$

Our previous argument indicates that current goes to zero when the efficiency is at the isentropic limit – the Carnot limit. Indeed this is the case. From Figure 2 we see that current vanishes at voltage

$$\Delta V = \frac{\Delta E}{q}\left(\frac{T_h - T_c}{T_h}\right)$$

and the efficiency at this voltage is the Carnot limit.

$$efficiency = \frac{q \cdot \Delta V}{\Delta E} = \frac{T_h - T_c}{T_h}$$

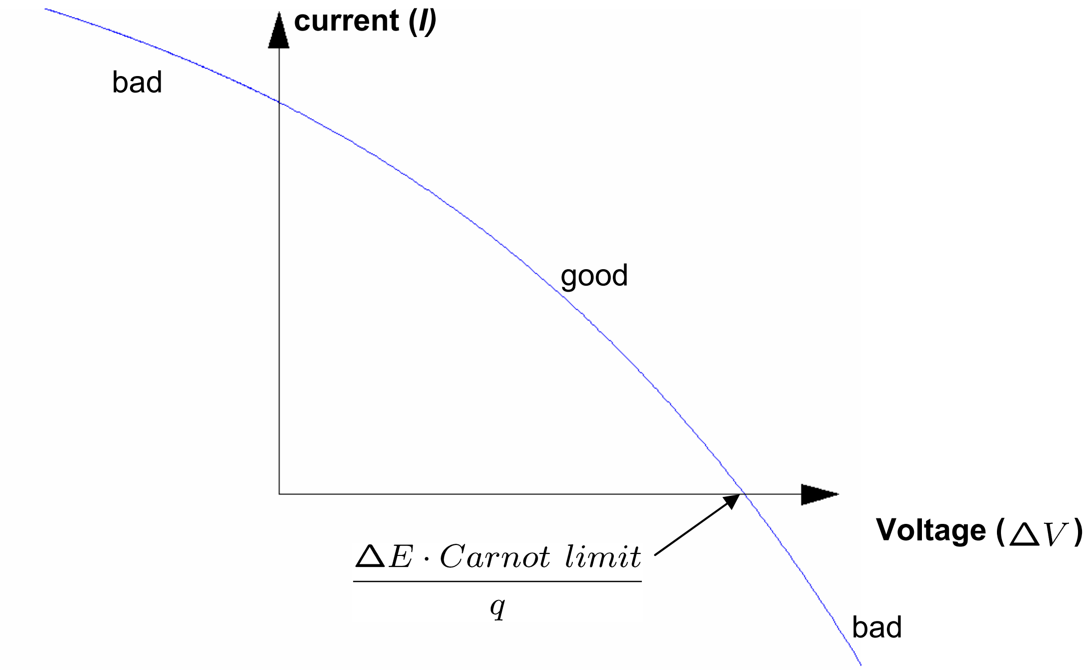


Fig. 2: Three regions of operation

Carnot Limit

The efficiency of any heat engine is constrained by the Carnot limit. A general heat engine consists of a hot heat-reservoir at temperature T_h, a cold heat-reservoir at temperature T_c, and a converter that converts heat to work. The hot heat-reservoir provides the converter with heat q_h; the converter performs work w and rejects heat q_c into the cold heat-reservoir. Energy conservation requires

$$q_h = w + q_c \tag{3}$$

The second law of thermodynamics requires that the total entropy change of the two reservoirs to be non-decreasing

$$\Delta S = \frac{-q_h}{T_h} + \frac{q_c}{T_c} \geq 0 \tag{4}$$

Substituting equations (3) and (4) give s a limit on the efficiency

$$efficiency = \frac{w}{q_h} \leq \frac{T_h - T_c}{T_h}$$

Carnot limit is achieved when the entropy change is zero. Therefore, Carnot limit is the efficiency under isentropic condition.

Throughput Power

The simulation of the model shows that decent power can be provided by the device. Plotted in Figure 3 is the throughput power versus load voltage for three cases of coupling strength. In this calculation, the temperature on the hot-side is assumed to be 600K and the temperature on the cold-side is 300K. The energy difference between the two levels in a quantum well, ΔE, is 0.1eV. Relaxation times are assumed to be one pico-second. The three coupling strengths used are 0.0021, 0.0042, and 0.0084eV, which are so chosen to give Rabi frequency on the order of pico-seconds.

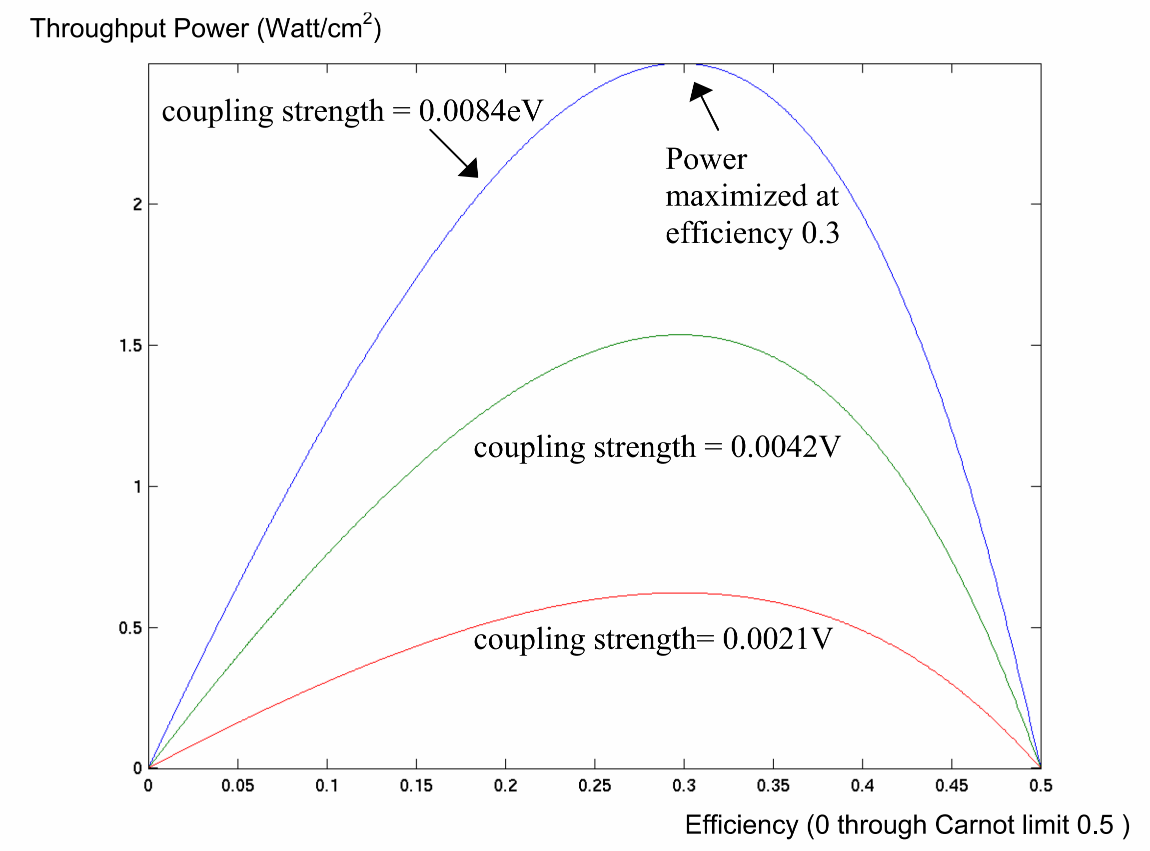
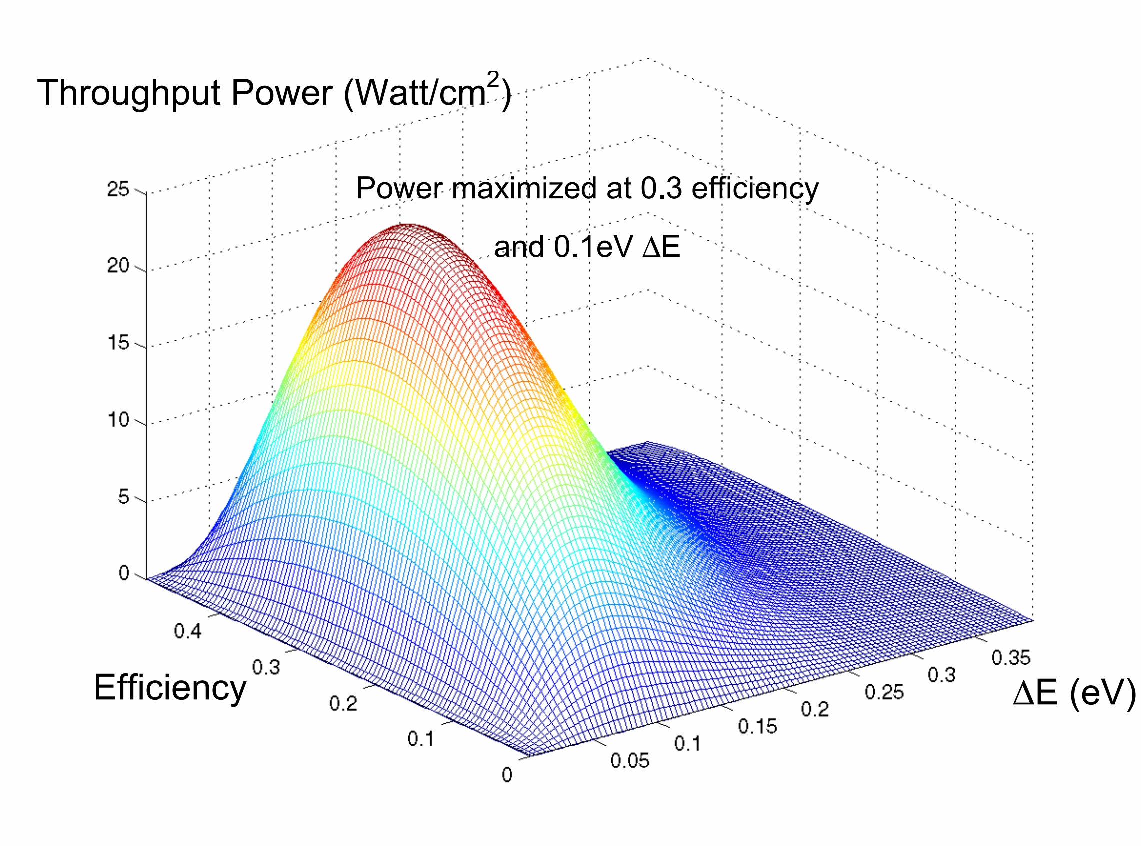


Fig. 3: Power versus efficiency

Design Issue

The device parameters that give optimal throughput power depend on the temperatures. As apparent from equation (1), the current has exponential dependence on the parameters and hence it is critical to optimize device parameters for the temperatures chosen. Figure 4 shows that the throughput power is maximized at ΔE=0.1eV and 0.3 efficiency for the temperature pair (600K, 300K). The coupling strength is assumed to be 0.0084eV in the calculation.



Discussion

This device looks promising because the simulations show that it gives a decent power at fairly high efficiencies. The next step would be to verify the device parameters experimentally and move towards a physical realization of the device.

Few-Body Nuclear Wavefunctions

Sponsors
Bose Foundation

Project Staff
I. Chaudhary and P. L. Hagelstein

Introduction

We have been interested in the problem of the coupling of vibrational degrees of freedom with nuclear degrees of freedom in the case of interacting nuclei embedded in a lattice. For nuclear problems without such coupling, there exist standard methods based on Racah algebra for evaluating interaction matrix elements that result from an analysis of the associated scattering problem. These methods take advantage of conservation of spin, isospin, and angular momentum based on fixed single particle orbitals. For the new problems that we are considering where the nuclear interactions occur with phonon exchange, the interaction of the lattice comes into the problem in a way perhaps better treated with approximate many-particle Gaussian wavefunctions, and a description based on single particle orbitals is inconvenient. For these problems, we are developing a new formulation in which the spin and isospin algebra is treated much as in the case of Racah algebra, but the spatial part of the wavefunction is left unspecified, other than the underlying symmetry properties under particle exchange.

In this work we generalize the standard method of building two-particle atomic wave functions to multi-particle nuclear systems. The most widely used method for building many-body nuclear wave functions is based on *Racah Algebra*. We propose a method based on *Clebsch-Gordan coefficients* (CG coefficients) of the *symmetric group*. Broadly speaking all we are doing is to write out

$$\psi = \sum_{j} C_j [R]_j \, [S]_j \, [T]_j$$

where $[R]$, $[S]$ and $[T]$ are respectively the spatial, spin and isospin parts of the nuclear wave functions and C_j are some coefficients which can be calculated by using Clebsch-Gordan techniques. To understand this calculation we need to understand the representation theory of

$$S(n) = \{\text{Group of permutations of } n \text{ objects}\}$$
$$SU(m) = \{\text{Group of } m\times m \text{ unitary matrices of determinant } 1\}$$

$S(n)$ is called the symmetric group and $SU(m)$ the special unitary group. Before we begin a discussion of the Clebsch-Gordan method, we note the salient features of the Racah Algebra.

Racah Algebra

It was developed in a series of important papers by Racah in the 1940s and 1950s [1-4]. It was later on extended to nuclear problems by Jahn and others [5,6]. A typical example of a nuclear wave function constructed using Racah's method would be

$$\psi(j^n,\alpha,I,J) \;=\; \sum_{\alpha_1,I_1,J_1} [j^{n-1}(\alpha_1,I_1,J_1), j, I, J]\} j^n,\alpha,T,J]\,\psi[j^{n-1}(\alpha_1,T_1,J_1), j^n, T, J] \qquad (1)$$

where $[j^{n-1}(\alpha_1, I_1, J_1), j, I, J]\} j^n, \alpha, T, J]$ are the coefficients of fractional parentage (CFP), and where $\psi[j^{n-1}(\alpha_1, T_1, J_1), j^n, T, J]$ is the result of coupling a completely antisymmetric $n-1$ particle wavefunction to the n^{th} particle. The main advantages of Racah algebra are that it is easy to use, since known standard formulas exist. Also it can be used to construct wave functions for arbitrarily large N. However the main drawback of Racah's method is that it assumes particles in angular momentum eigenstates. This is a serious difficulty in theories which include phonon exchange with nuclear degrees of freedom. An aesthetic objection for nuclear wave functions in LST coupling is that we are forced to do L-(ST) coupling (i.e. one has to consider S-T super-multiplets) and cannot treat all degrees of freedom on the same footing. In order to overcome these difficulties, we propose using the Clebsch-Gordan methods.

Clebsch-Gordan approach

The Clebsch-Gordan approach is the obvious generalization of the naive way of constructing two-particle atomic wave functions. It overcomes the main drawback of Racah Algebra (as applied to systems in which angular momentum is not conserved) in that it does not assume anything about particles being in angular momentum eigenstates. It also cleanly separates space, spin and isospin portions of the nuclear wave functions, and treats them on par with each other. The main disadvantage is that as of now, no standard formulas exist for wave functions or for matrix elements. However, using Wigner-Eckart type theorems, the matrix element calculations should simplify somewhat. To warm up, we start with the well known two-electron system.

Two-Electron System

This is the simplest example in which we see the Clebsch-Gordan coefficients work. The coefficients are 1, so the calculation is trivial. However, please note that we are talking about the CG coefficients of the *S(2)* and not *SU(2)*. Normally physicists encounter the CG-coefficients of *SU(2)* when learning about angular momentum addition. The construction of product wave functions for two-electron systems is a standard topic in quantum mechanics textbooks. It is based on the *Pauli exclusion principle*. The results are the usual

Spin	→	*Space*
Symmetric		antisymmetric
Antisymmetric		symmetric

If we denote $m_S = 1/2$ by α, $m_S = -1/2$ by β then the actual wavefunctions are

$$Spin\ Symmetric = \begin{cases} \alpha(1)\alpha(2) \\ 1/\sqrt{2}\{\alpha(1)\beta(2) + \beta(1)\alpha(2)\} \\ \beta(1)\beta(2) \end{cases}$$

$$Spin\ Antisymmetric = 1/\sqrt{2}\{\alpha(1)\beta(2) - \beta(1)\alpha(2)\}$$

$$Space\ Symmetric = f(r_1, r_2) + f(r_2, r_1)$$

$$Space\ Antisymmetric = f(r_1, r_2) - f(r_2, r_1)$$

The complete wave function is constructed by taking appropriate products e.g.

$$\alpha(1)\alpha(2)\{f(r_1,r_2)-f(r_2,r_1)\}$$

Please note that this is not normalized since $f(r_1,r_2)+f(r_2,r_1)$ cannot be normalized until we know the form of the f. This inability to normalize will be a constant feature of this construction. However, this is not a serious draw back, since given any spatial wavefunction, it can be normalized. The next simple system we consider is the two-nucleon system.

Two-Nucleon System

The construction of the two-particle nuclear wave functions takes places in a completely similar manner to the two-electron case except that we include isospin. It is based on the *Generalized Pauli Exclusion Principle* which states that the total wave function (including isospin) has to be antisymmetric under the exchange of any two particles. Hence the results are

Spin	*Isospin*	→	*Space*
Symmetric	symmetric		antisymmetric
Symmetric	antisymmetric		symmetric
Antisymmetric	symmetric		symmetric
Antisymmetric	antisymmetric		antisymmetric

If we denote $m_S = 1/2$ by α, $m_S = -1/2$ by β, $m_I = 1/2$ by μ, $m_I = -1/2$ by ν, then the explicit wave functions are

$$Spin\ Symmetric = \begin{cases} \alpha(1)\alpha(2) \\ 1/\sqrt{2}\{\alpha(1)\beta(2)+\beta(1)\alpha(2)\} \\ \beta(1)\beta(2) \end{cases}$$

$$Spin\ Antisymmetric = 1/\sqrt{2}\{\alpha(1)\beta(2)-\beta(1)\alpha(2)\}$$

$$Isospin\ Symmetric = \begin{cases} \mu(1)\mu(2) \\ 1/\sqrt{2}\{\mu(1)\nu(2)+\mu(2)\nu(1)\} \\ \nu(1)\nu(2) \end{cases}$$

$$Isospin\ Antisymmetric = 1/\sqrt{2}\{\mu(1)\nu(2)-\mu(2)\nu(1)\}$$

$$Space\ Symmetric = f(r_1,r_2)+f(r_2,r_1)$$

$$Space\ Antisymmetric = f(r_1,r_2)-f(r_2,r_1)$$

The complete (unnormalized) wave function is constructed by taking appropriate products e.g.

$$\alpha(1)\alpha(2)\frac{1}{\sqrt{2}}\{\mu(1)\nu(2)-\nu(1)\mu(2)\}\{f(r_1,r_2)+f(r_2,r_1)\}$$

Again the wave function cannot be normalized until we know the explicit form of f . These examples seem completely straight forward, and use no knowledge of group theory. However, when we try and generalize to the 3-body problem, we very quickly encounter some serious difficulties. So let us explicitly consider the problem of construction of the Triton wavefunctions [7].

The Triton Wavefunction

We consider ^{3}H as a three-particle system with $M_s = 1/2$ and isospin $I = 1/2$. There are three linearly independent wavefunctions with $M_s = 1/2$. There are three wavefunctions because two correspond to $S = 1/2$ (when we add three $s = 1/2$ particles, we get two total spin $S = 1/2$ states) and one to $S = 3/2$. Similarly there are two isospin wavefunctions corresponding to $M_I = 1/2$ or $M_I = -1/2$. We can use the standard algebra of angular momentum addition to construct these states. While the $S = 3/2$ are completely symmetric, unlike the two particle case, the lower S and I states seem to be neither symmetric nor antisymmetric. We have a total of 6 possible states of products of spin and isospin. While there is no symmetry constraint imposed on these 6 states, the total wavefunctions (including the spatial part) have to be completely antisymmetric. There seems to be no clean separation nor a systematic way for constructing these wavefunctions as we did for the two particle case. Our naive way of constructing product wavefunctions breaks down.

We still want to continue our naive way of constructing wavefunctions. However, as we have seen, the direct approach does not yield the required results. By staring at the wavefunctions of the two-particle case, we see that there seems to be strong connections between the symmetry properties of the spin/isospin wavefunctions and total S/I . This is the connection we will exploit to construct the multi-particle wavefunctions.

Note that the product wavefunctions are rigorously true when spin and isospin are good quantum numbers. In that case we know that eigenfunctions have to be products of spin, isospin and space. Now spin eigenfunctions can be chosen so that they have prescribed symmetry properties. Same can be done for isospin wavefunctions. To make sure that the total wavefunction is anti-symmetric, severe restrictions are then imposed on the spatial part of the wavefunction. This has been carried out for 3-particle and 4-particle nuclei.

Results for the Three-Body Wavefunction

In the results given below q is used for spin, v for isospin and f for the space part of the wave function. The superscripts on the q 's, v 's and f 's represent the particular Young-Yamanouchi basis vector with

[2 1 1] = 1 mixed symmetry
[1 2 1] = 2 mixed symmetry
[1 1 1] = 3 symmetric
[3 2 1] = 4 antisymmetric

The results are:

S=3/2 I=3/2 $\psi = f^4 q^3 v^3$
S=3/2 I=1/2 $\psi = \frac{1}{\sqrt{2}}\{f^1 q^3 v^2 - f^2 q^3 v^1\}$
S=1/2 I=3/2 $\psi = \frac{1}{\sqrt{2}}\{f^1 q^2 v^3 - f^2 q^1 v^3\}$
S=1/2 I=1/2 $\psi = \frac{1}{\sqrt{2}}\{f^1(-\frac{1}{\sqrt{2}})(q^1 v^2 + q^2 v^1) - f^2(\frac{1}{\sqrt{2}})(q^1 v^1 - q^2 v^2)\}$
S=1/2 I=1/2 $\psi = f^4(\frac{1}{\sqrt{2}})(q^1 v^1 + q^2 v^2)$
S=1/2 I=1/2 $\psi = f^3(\frac{1}{\sqrt{2}})(q^1 v^2 - q^2 v^1)$

The details of the various symbols and wavefunctions are given in the following subsections.

1. Spin Wave functions

Let us define spin wave functions corresponding to various m_S values and permutation symmetries. We will denote them by $q^a_{m_S}$, where the subscript refers to the value of m_S and the superscript labels the various Yamanouchi basis vectors.

1. m_S = 3/2

$$[111]_{3/2} = q^3_{3/2} = \alpha(1)\alpha(2)\alpha(3)$$

2. m_S = 1/2

$$[211]_{1/2} = q^1_{1/2} = \frac{1}{\sqrt{6}}\{\beta(1)\alpha(2) + \alpha(1)\beta(2)\}\alpha(3) - \sqrt{\frac{2}{3}}\alpha(1)\alpha(2)\beta(3)$$

$$[121]_{1/2} = q^2_{1/2} = \frac{1}{\sqrt{2}}\{\beta(1)\alpha(2) - \alpha(1)\beta(2)\}\alpha(3)$$

$$[111]_{1/2} = q^3_{1/2} = \frac{1}{\sqrt{3}}\{\alpha(1)\alpha(2)\beta(3) + \alpha(1)\beta(2)\alpha(3) + \beta(1)\alpha(2)\alpha(3)\}$$

3. m_S = -1/2

$$[211]_{-1/2} = q^1_{-1/2} = \frac{1}{\sqrt{6}}\{\beta(1)\alpha(2) + \alpha(1)\beta(2)\}\beta(3) - \sqrt{\frac{2}{3}}\beta(1)\beta(2)\alpha(3)$$

$$[121]_{-1/2} = q^2_{-1/2} = \frac{1}{\sqrt{2}}\{\beta(1)\alpha(2) - \alpha(1)\beta(2)\}\beta(3)$$

$$[111]_{-1/2} = q^3_{1/2} = \frac{1}{\sqrt{3}}\{\alpha(1)\beta(2)\beta(3) + \beta(1)\alpha(2)\beta(3) + \beta(1)\beta(2)\alpha(3)\}$$

4. m_S = -3/2

$$[111]_{-3/2} = q^3_{-3/2} = \beta(1)\beta(2)\beta(3)$$

2. Isospin Wave functions

In a completely analogous way to the spin wave functions, we can define isospin wave functions with the q 's replaced by the v 's.

3. Space Wave functions

$$[111]_R = f^3 = f(123) + f(132) + f(213) + f(321) + f(231) + f(312)$$

$$[211]_R = f_1^1 = f(123) + f(213) - 1/2 f(132) - 1/2 f(321) - 1/2 f(231) - 1/2 f(312)$$

$$[121]_R == f_1^2 = \frac{\sqrt{3}}{2}\{f(132) - f(321) - f(231) + f(312)\}$$

Or we can use the other pair

$$[211]_R = f_2^1 = \frac{\sqrt{3}}{2}\{f(132) - f(321) + f(231) - f(312)\}$$

$$[121]_R = f_2^2 = f(123) - f(213) + 1/2 f(132) + 1/2 f(321) - 1/2 f(231) - 1/2 f(312)$$

and

$$[321]_R = f^4 = f(123) + f(231) + f(312) - f(132) - f(321) - f(213)$$

Please note that these pairs can turn out to be linearly dependent if the functions have certain symmetries. Hence they are not normalized.

Ground State Matrix Elements

However, these wavefunctions are not well-suited for calculating matrix elements. It is better to use wavefunctions that are explicitly symmetric or antisymmetric in the coordinates (spin and isospin only) of the last two particles. This makes evaluation of the matrix elements easy because the nuclear force is explicitly symmetric under the exchange of spin (or isospin) of two particles. This would mean that states with the same permutation symmetry couple to states with the same permutation symmetry. This simplifies matters signifcantly. Please note that these are not new wavefunctions. They are the old ones, except that we choose certain linear combinations to make sure that they are symmetric or antisymmetric in the last two particles.

We have been examining the Hamada-Johnston potential to calculate the matrix elements for the Deuteron, ^{3}He, ^{3}H, and ^{4}He. The Hamada Johnston potential between nucleon 1 and nucleon 2 can be written in the form

$$V = V_C + V_T S_{12} + V_{LS}\vec{L}.\vec{S} + V_{LL}L_{12} \tag{1}$$

where

$$\begin{aligned}
V_C &= \vec{\tau}_1.\vec{\tau}_2 \\
V_T &= \vec{\tau}_1.\vec{\tau}_2 y_T(r_{12}) \\
V_{LS} &= y_{LS}(r_{12}) \\
V_{LL} &= y_{LL}(r_{12}) \\
S_{12} &= 3(\vec{\sigma}_1.\vec{r})(\vec{\sigma}_2.\vec{r}) - \vec{\sigma}_1.\vec{\sigma}_2 \\
L_{12} &= (\vec{\sigma}_1.\vec{\sigma}_2)\vec{L}^2 - \frac{1}{2}\{\vec{\sigma}_1.\vec{L}\vec{\sigma}_2.\vec{L} + \vec{\sigma}_2.\vec{L}\vec{\sigma}_2.\vec{L}\}
\end{aligned}$$

For now we are only considering diagonal matrix elements, from where we expect the maximum contribution. The off-diagonal ones will be considered later on.

Two-Particle Matrix Elements

Before we begin evaluating the matrix elements for the various nuclei, let us calculate the two-body matrix elements for the nuclear force. They will be very useful in calculating the two, three and four-body matrix elements. Since we are, in this chapter, concerned with the ground state, we expect the spatial part of the wavefunction to be completely symmetric (since we are dealing with low-mass nuclei). The wavefunction for the 2-body case then looks like

$$\Psi = \{f(r_1,r_2) + f(r_2,r_1)\}\left\{\begin{matrix} \uparrow\uparrow \\ \frac{1}{\sqrt{2}}(\uparrow\downarrow + \downarrow\uparrow) \\ \downarrow\downarrow \end{matrix}\right\}_S \left\{\begin{matrix} \uparrow\uparrow \\ \frac{1}{\sqrt{2}}(\uparrow\downarrow + \downarrow\uparrow) \\ \downarrow\downarrow \end{matrix}\right\}_T$$

Now let us consider different parts of the nuclear force. We will call $\frac{1}{2}\{\vec{\sigma}_1.\vec{L}\vec{\sigma}_2.\vec{L} + \vec{\sigma}_2.\vec{L}\vec{\sigma}_1.\vec{L}\}$ as $\vec{\sigma}.\vec{L}$. The diagonal matrix elements can be written as

$$\begin{aligned}
\langle \text{triplet}|\vec{\sigma}\cdot\vec{\sigma}|\text{triplet}\rangle &= -1 \\
\langle \text{singlet}|\vec{\sigma}\cdot\vec{\sigma}|\text{singlet}\rangle &= -3
\end{aligned}$$

$$\langle\uparrow\uparrow|(\vec{\sigma}_1\cdot\mathbf{r})(\vec{\sigma}_2\cdot\mathbf{r})|\uparrow\uparrow\rangle = z^2$$

$$\left\langle \frac{\uparrow\downarrow-\downarrow\uparrow}{\sqrt{2}} \right| (\vec{\sigma}_1\cdot\mathbf{r})(\vec{\sigma}_2\cdot\mathbf{r}) \left| \frac{\uparrow\downarrow-\downarrow\uparrow}{\sqrt{2}} \right\rangle = x^2+y^2-z^2$$

$$\left\langle \downarrow\downarrow \right| (\vec{\sigma}_1\cdot\mathbf{r})(\vec{\sigma}_2\cdot\mathbf{r}) \left| \downarrow\downarrow \right\rangle = z^2$$

$$\left\langle \frac{\uparrow\downarrow+\downarrow\uparrow}{\sqrt{2}} \right| (\vec{\sigma}_1\cdot\mathbf{r})(\vec{\sigma}_2\cdot\mathbf{r}) \left| \frac{\uparrow\downarrow+\downarrow\uparrow}{\sqrt{2}} \right\rangle = -x^2-y^2-z^2$$

$$\left\langle \uparrow\uparrow \right| \mathbf{L}\cdot\mathbf{S} \left| \uparrow\uparrow \right\rangle = 2L_z$$

$$\left\langle \frac{\uparrow\downarrow+\uparrow\uparrow}{\sqrt{2}} \right| \mathbf{L}\cdot\mathbf{S} \left| \frac{\uparrow\downarrow+\uparrow\uparrow}{\sqrt{2}} \right\rangle = 0$$

$$\left\langle \downarrow\downarrow \right| \mathbf{L}\cdot\mathbf{S} \left| \downarrow\downarrow \right\rangle = -2L_z$$

$$\left\langle \frac{\uparrow\downarrow-\uparrow\uparrow}{\sqrt{2}} \right| \mathbf{L}\cdot\mathbf{S} \left| \frac{\uparrow\downarrow-\uparrow\uparrow}{\sqrt{2}} \right\rangle = 0$$

$$\left\langle \uparrow\uparrow \right| \vec{\sigma}\cdot\mathbf{L} \left| \uparrow\uparrow \right\rangle = L_z^2$$

$$\left\langle \frac{\uparrow\downarrow+\uparrow\uparrow}{\sqrt{2}} \right| \vec{\sigma}\cdot\mathbf{L} \left| \frac{\uparrow\downarrow+\uparrow\uparrow}{\sqrt{2}} \right\rangle = L_x^2+L_y^2-L_z^2$$

$$\left\langle \downarrow\downarrow \right| \vec{\sigma}\cdot\mathbf{L} \left| \downarrow\downarrow \right\rangle = L_z^2$$

$$\left\langle \frac{\uparrow\downarrow-\uparrow\uparrow}{\sqrt{2}} \right| \vec{\sigma}\cdot\mathbf{L} \left| \frac{\uparrow\downarrow-\uparrow\uparrow}{\sqrt{2}} \right\rangle = -L_x^2-L_y^2-L_z^2$$

Now that we have the two-body matrix elements in this form, we can explicitly write the matrix elements for the deuteron, ^{3}He, ^{3}H, and ^{4}He.

Deuteron Matrix Elements

The deuteron ground state is spatially symmetric, S = 1 and T= 0. We may write

$$\left\langle \Psi \right| V_C \left| \Psi \right\rangle = -3\int \psi^*(\mathbf{r}_1,\mathbf{r}_2) y_C(\mathbf{r}_{12}) \psi(\mathbf{r}_1,\mathbf{r}_2)$$

$$\langle\Psi|V_T|\Psi\rangle \;=\; 3\int\psi^*(\mathbf{r}_1,\mathbf{r}_2)y_T(\mathbf{r}_{12})\psi(\mathbf{r}_1,\mathbf{r}_2)\;-9\int\int\psi^*(\mathbf{r}_1,\mathbf{r}_2)y_T(\mathbf{r}_{12})\begin{bmatrix} z^2 \\ x^2+y^2-z^2 \\ z^2 \end{bmatrix}\psi(\mathbf{r}_1,\mathbf{r}_2)$$

$$\langle\Psi|V_{LS}|\Psi\rangle \;=\; \int\psi^*(\mathbf{r}_1,\mathbf{r}_2)y_{LS}(\mathbf{r}_{12})\begin{bmatrix} 2L_z \\ 0 \\ -2L_z \end{bmatrix}\psi(\mathbf{r}_1,\mathbf{r}_2)$$

$$\langle\Psi|V_{LL}|\Psi\rangle \;=\; \int\psi^*(\mathbf{r}_1,\mathbf{r}_2)y_{LL}(\mathbf{r}_{12})\psi(\mathbf{r}_1,\mathbf{r}_2)\;-\;\int\psi^*(\mathbf{r}_1,\mathbf{r}_2)y_{LL}(\mathbf{r}_{12})\begin{bmatrix} L_z^2 \\ L_x^2+L_y^2-L_z^2 \\ L_z^2 \end{bmatrix}\psi(\mathbf{r}_1,\mathbf{r}_2)$$

where

$$\psi(\mathbf{r}_1,\mathbf{r}_2)=f(\mathbf{r}_1,\mathbf{r}_2)+f(\mathbf{r}_2,\mathbf{r}_1)$$

Triton Matrix Elements

We first need to write down the ^3He wavefunction using two-particle CFPs. We will write out the wavefunctions so that each spin, isospin part is either completely symmetric or completely antisymmetric in the last two particles. This makes calculations of the matrix elements easier. ^3He ground state is again spatially symmetric and has S = 1/2 and T = 1/2.

$$\Psi=\psi_3([111],R)\frac{\phi_3([12]1)\Gamma_3(\{12\}1)+\phi_3(\{12\}1)\Gamma_3([12]1)}{\sqrt{2}}$$

where

$$\phi_3([12]1)=\phi_3(\sigma^1,S''=1/2;\sigma_2=1/2,\sigma_3=1/2,S_2=1;S=1/2,M_S)$$
$$\phi_3(\{12\}1)=\phi_3(\sigma^1,S''=1/2;\sigma_2=1/2,\sigma_3=1/2,S_2=0;S=1/2,M_S)$$

More explicitly, in the $\phi_3([12]1)$ we couple particles 2 and 3 to form S = 1. Then couple particle particle to this S = 1 to get a S = 1/2 state. (Exactly the same holds for Γ.) The convention used is that $\phi_3([12]_1)$ is symmetric and $\phi_3(\{12\}1)$ is antisymmetric in the last two particles. Exactly the same conventions apply to Γ as well.

We obtain for the matrix elements the following results:

$$\frac{1}{3}\langle\Psi|V_C|\Psi\rangle \;=\; -3\int\psi^*(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)y_C(\mathbf{r}_{12})\psi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)$$

$$\frac{1}{3}\langle\Psi|V_T|\Psi\rangle = 3\int\psi^*(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)y_T(\mathbf{r}_{12})\psi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)$$

$$-3\int\int\psi^*(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)y_T(\mathbf{r}_{12})\left(x^2+y^2+z^2\right)\psi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)$$

$$\frac{1}{3}\langle\Psi|V_{LS}|\Psi\rangle = \pm\frac{2}{3}\int\psi^*(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)y_{LS}(\mathbf{r}_{12})L_z\psi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)$$

$$\frac{1}{3}\langle\Psi|V_{LL}|\Psi\rangle = -\frac{2}{3}\int\psi^*(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)y_{LL}(\mathbf{r}_{12})\vec{L}^2\psi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)$$

for $M_S = \pm 1/2$.

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