RESONANT TUNNELING AND RESONANT EXCITATION TRANSFER

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Issues involved in the tunneling of deuterons in metal deuterides are considered in relation to experimental claims of anomalies in metal deuterides. From earlier studies, screening is thought to be similar to the case of molecular D_2. Resonant tunneling has been advocated in the literature as a possible mechanism to achieve tunneling enhancements. We develop a two-level system for a piecewise constant potential model for resonant tunneling that matches the energy levels in the vicinity of a level crossing, arguing that such models are applicable for more general potential models. Resonant tunneling effects and dynamics, including acceleration due to coherence, are accounted for in the model. The model is extended to include relaxation effects, and it is found that one would not expect to find coherent effects associated with tunneling in the case of two deuterons in a metal lattice. We present a simple model for the transfer of excitation from a collection of deuterons to a collection of helium nuclei, a model closely related to resonant tunneling and also to new phonon-coupled SU(N) models under development. The excitation transfer models show coherent enhancements as well as collective effects.

1. Introduction

Perhaps the most fundamental theoretical problem associated with the various experimental claims of anomalies in metal deuterides is how the deuterons manage to come together at a sufficiently high rate to produce observable reaction rates. There was speculation in 1989 that screening effects might be enhanced in metal deuterides, and that this might account for the low-level neutron emission claimed by Jones and colleagues at BYU.[1] Over the years, papers have been published arguing for, and against, enhanced screening effects. Koonin and Nauenberg[2] argued that the screening should be similar to that of molecular D_2. As screening effects are weak in the D_2 molecule, the associated tunneling rate for the ground state is more than 50 orders of magnitude too small to account for the low-level fusion rates claimed in the initial BYU experiments.

The most popular line of argument in favor of enhanced screening effects in 1989 proposed that an increase in the effective electron mass was present in some metal deuterides. An increase in the effective mass reduces the screening length, according to the early proposals, and increases the tunneling rate dramatically. A weakness of the argument is that the effective mass approximation describes electron and hole dynamics over many sites in a periodic lattices, and is not applicable to the screening problem.

There have appeared other discussions of screening between deuterons in metal deuterides, but we will consider such works as largely being out of the scope of this paper. Our position is in general agreement with the arguments of Koonin and Nauenberg, that one would not expect large deviations from the molecular problem. From our perspective, the highest tunneling probabilities are expected when two deuterons occupy a single octahedral site in PdD. Although double site occupancy may have a low associated probability, the tunneling rate is tens of orders of magnitude larger than when deuterons are at different sites. The two-deuteron wavefunction associated with double occupancy is reasonably well approximated by the molecular D_2 wavefunction, and the modifications of the two-deuteron wavefunction by the surrounding lattice is not so great. Hence, we would expect the molecular D_2 problem to be very relevant for developing estimates for tunneling rates for double occupancy, which we expect to dominate the tunneling rate over all other processes under normal conditions.

We note that there has appeared very recently measurements of dd-fusion cross sections at low energy which appear to show significant enhancements[3] (see also [4] Earlier measurements in TiD produced reaction rates similar to that of D_2, while the new measurements show very large enhancements. We await experimental confirmation of the effect. Our position is that if real, this effect is most likely a recoil effect in which fast incident deuterons push deuterons at rest into tightly bound electron orbitals, where very strong screening effects would be expected. If this line of argument is correct, then one would not expect the enhancements to extend to the case of deuterons nearly at rest. The screening implied by these measurements is sufficiently large that the metal deuterides would be highly unstable against dd-fusion if the same screening model applied naively to all deuterons (with thermal energy) in the lattice.

In the absence of screening enhancements and exotic effects that create fast deuterons in the lattice, the only way that a modification of the tunneling rate can come about is if something changes on the nuclear scale. There have appeared proposals for modifications of the tunneling rate due to the presence of nuclear states that are nearly resonant with the molecular state (this idea has been pursued in previous years by X. Z. Li and colleagues at Tsinghua University, and also by Y. E. Kim and colleagues at Purdue). It is a relatively simple calculation to show that in fact a nuclear state with appropriate properties could in fact produce a significant modification in the tunneling problem, and lead to large enhancements in the tunneling rate. In spite of this attractive feature of this kind of model, we note that the four nucleon system has been the focus of many theoretical and experimental studies over many years, and it is known that there are no states present that are sufficiently close in energy and sufficiently long-lived to make any impact on the tunneling rate in the way proposed.

In what follows, we will examine the modification in the tunneling rate due to a resonant nuclear state using the simplest possible relevant model. Based on the discussion above, there might seem to to be little motivation for pursuing such a model, since we already know that there are no relevant four nucleon states to which the model might be applied. However, we find several reasons to pursue this model: (1) It is useful to demonstrate cleanly that there is more to the problem of tunneling between deuterons than simple Golden Rule transition rate physics as is normally assumed; (2) it is possible to develop a two-level approximation for this kind of problem, which allows us to study coherent and incoherent effects on an equal footing; and (3) this kind of model appears to have some relevance to the new phonon-coupled SU(N) models that we have proposed for the anomalies in metal deuterides. The results that we present lead one to conclude that resonant tunneling models for the four nucleon system are not relevant to the problem of anomalies in metal deuterides. However, the notion of tunneling as a coherent process that is part of something larger going on in the lattice is in our view extremely important.

2. Piecewise Constant Potential Model

We have over the years become convinced of the utility of simple models that embody the relevant physical principles as a way of developing understanding and intuition about complex phenomena. Consequently, to study resonant tunneling, we propose the simplest of piecewise constant potentials that has two wells separated by a potential barrier. We adopt the radial ($l = 0$) Hamiltonian

$$\hat{H} \;=\; -\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} \;+\; V(r) \tag{1}$$

where

$$V(r) \;=\; \begin{cases} -V_n & 0 \leq r \leq R_n \\ V_0 & R_n < r < R_a \\ 0 & R_a \leq r \leq R \\ \infty & R < r \end{cases} \tag{2}$$

We see an attractive nuclear potential for relative separation less than a nuclear radius R_n, a zero potential between an atomic radius R_a and an outer radius R, and a barrier of height V_0 that separates the two wells. An advantage of developing a simple model such as this one is that it is relatively easy to solve. We focus first on developing eigenfunctions and eigenvalues of the time-independent Schrödinger equation

$$EP(r) \;=\; -\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}P(r) \;+\; V(r)P(r) \tag{3}$$

Solutions are constructed using

$$P(r) \;=\; \begin{cases} A\sin k_n r & 0 \le r \le R_n \\ Be^{\alpha r} \;+\; Ce^{-\alpha r} & R_n < r < R_a \\ D\sin k_a(r-R) & R_a \le r \le R \\ 0 & R < r \end{cases} \tag{4}$$

2.1. *Limit of Perfect Isolation*

If the wells are isolated from one another, then things simplify further. The energies of each well in isolation can be determined from matching the appropriate point and slope of the assumed solutions at R_n and at R_a. We obtain the constraints

$$\frac{1}{k_n}\;\tan k_n R_n \;=\; -\frac{1}{\alpha} \tag{5}$$

$$\frac{1}{k_a}\;\tan k_a(R_a - R) \;=\; \frac{1}{\alpha} \tag{6}$$

We note that k_n, k_a and α are functions of the energy eigenvalue E that satisfy

$$E \;=\; \frac{\hbar^2 k_n^2}{2\mu} - V_n \qquad\qquad E \;=\; \frac{\hbar^2 k_a^2}{2\mu} \qquad\qquad E \;=\; -\frac{\hbar^2\alpha^2}{2\mu} \;+\; V_0$$

We assume that the energy eigenvalues of the wells in isolation are E_n and E_a.

2.2. *Coupled Wells*

Now we consider what happens when the wells are coupled. The energy eigenvalue in this case satisfies

$$e^{-2\alpha R_n}\,\frac{\dfrac{1}{k_n}\tan k_n R_n + \dfrac{1}{\alpha}}{\dfrac{1}{k_n}\tan k_n R_n - \dfrac{1}{\alpha}} \;=\; e^{-2\alpha R_a}\,\frac{\dfrac{1}{k_a}\tan k_a(R_a - R) + \dfrac{1}{\alpha}}{\dfrac{1}{k_a}\tan k_a(R_a - R) - \dfrac{1}{\alpha}} \tag{7}$$

Although this constraint may appear to be composed of lots of factors that have to be sorted out, upon further inspection, one sees that it has a specific form that will be useful to us. We see terms that correspond to the individual energy eigenvalue equations in isolation that appear on both sides. We can collect these and write

$$\left[\frac{1}{k_n}\tan k_n R_n + \frac{1}{\alpha}\right]\left[\frac{1}{k_a}\tan k_a(R_a - R) - \frac{1}{\alpha}\right]$$
$$= e^{-2\alpha(R_a - R_n)}\left[\frac{1}{k_n}\tan k_n R_n - \frac{1}{\alpha}\right]\left[\frac{1}{k_a}\tan k_a(R_a - R) + \frac{1}{\alpha}\right] \quad (8)$$

If the coupling between the wells is weak (as we assume), then the energies will be close to the unperturbed energies of the wells in isolation. Hence

$$\left[\frac{1}{k_n}\tan k_n R_n + \frac{1}{\alpha}\right] = \frac{d}{dE}\left[\frac{1}{k_n}\tan k_n R_n + \frac{1}{\alpha}\right]_{E_n}(E - E_n) + \cdots \quad (9)$$

$$\left[\frac{1}{k_a}\tan k_a(R_a - R) - \frac{1}{\alpha}\right] = \frac{d}{dE}\left[\frac{1}{k_a}\tan k_a(R_a - R) - \frac{1}{\alpha}\right]_{E_a}(E - E_a) + \cdots \quad (10)$$

We are therefore able to develop a simpler approximate version of the eigenvalue equation which is of the form

$$(E-E_n)(E-E_a) = e^{-2\alpha(R_a-R_n)}$$
$$\times \left[\frac{\frac{1}{k_n}\tan k_n R_n - \frac{1}{\alpha}}{\frac{d}{dE}\left(\frac{1}{k_n}\tan k_n R_n + \frac{1}{\alpha}\right)_{E_n}}\right]\left[\frac{\frac{1}{k_a}\tan k_a(R_a - R) + \frac{1}{\alpha}}{\frac{d}{dE}\left(\frac{1}{k_a}\tan k_a(R_a - R) - \frac{1}{\alpha}\right)_{E_a}}\right] \quad (11)$$

This is interesting because it is of the same form as the eigenvalue equation for a two-level system, as long as the terms on the right hand side are presumed to be energy independent in the vicinity of the resonance. The static two-level system eigenvalue equation can be written in the form

$$\det\begin{vmatrix} E_n - E & Ve^{-G} \\ Ve^{-G} & E_a - E \end{vmatrix} = 0 \quad (12)$$

which is equivalent to

$$(E - E_n)(E - E_a) = V^2\, e^{-2G} \quad (13)$$

We identify the Gamow tunneling factor with the exponential on the RHS of equation (11)

$$e^{-G} = e^{-\alpha(R_a - R_n)}$$

There is nothing particularly special in this regard about the piecewise constant potential that we have selected for this discussion in this regard. Other potentials which might be proposed for this kind of problem, including Coulomb and more realistic nuclear potential models, would produce a qualitatively similar relation for the energy eigenvalue under conditions that both wells in isolation have states that are nearly matched in energy.

3. Equivalent Two-Level System for the Coupled-Well Problem

The analysis of the previous section indicates that we can think of the coupling between nearly degenerate states in a potential well using a two level model.[5] A Hamiltonian appropriate for the associated two-level model is

$$\hat{H}_2 \;=\; |\phi_n\rangle E_n \langle\phi_n| \;+\; |\phi_a\rangle E_a \langle\phi_a| \;+\; Ve^{-G}\Bigg[|\phi_n\rangle\langle\phi_a| \;+\; |\phi_a\rangle\langle\phi_n|\Bigg] \qquad (14)$$

where ϕ_n is a basis state for the well at the nuclear scale, and where ϕ_a is a basis state for the well at the atomic scale.

3.1. *Rabi Oscillations*

The two-level model appears in a wide variety of applications, and its properties are well known. We focus briefly on the dynamical problem

$$i\hbar\frac{\partial}{\partial t}\psi \;=\; \hat{H}_2\psi \qquad (15)$$

To analyze this, one approach is to expand in terms of basis states

$$\psi \;=\; c_n(t)|\phi_n\rangle \;+\; c_a(t)|\phi_a\rangle \qquad (16)$$

This approach leads to the coupled equations

$$\frac{d}{dt}c_n(t) \;=\; E_n c_n(t) \;+\; Ve^{-G}c_a(t) \qquad (17)$$

$$\frac{d}{dt}c_a(t) \;=\; E_a c_a(t) \;+\; Ve^{-G}c_n(t) \qquad (18)$$

These equations are of course well known, and are readily solved. Suppose we assume that the system is initialized at $t = 0$ such that $c_a(0) = 1$ and $c_n(0) = 0$, which corresponds to the two deuterons being initially in a molecular state. Then we may compute the probability that the two deuterons are in the nuclear states at some time later

$$|c_n(t)|^2 \;=\; \frac{4V^2e^{-2G}}{(E_n - E_a)^2 + 4V^2e^{-2G}}\;\sin^2\frac{\Omega t}{2} \qquad (19)$$

where

$$\Omega = \sqrt{\left(\frac{E_n - E_a}{\hbar}\right)^2 + \frac{4V^2 e^{-2G}}{\hbar^2}} \tag{20}$$

3.2. *Resonance*

On resonance ($E_n = E_a$), the probability oscillates between the two states sinusoidally with a frequency

$$\Omega = \frac{2Ve^{-G}}{\hbar} \tag{21}$$

The Rabi oscillation frequency associated with this coherent effect is very fast as compared to the decay rate associated with incoherent transitions

$$\gamma = \frac{2\pi}{\hbar} V^2 e^{-2G} \rho \tag{22}$$

We see that Ω is proportional to e^{-G}, while γ is proportional to e^{-2G}. This is important when each Gamow tunneling factor e^{-G} is on the general order of 10^{-40}.

3.3. *Discussion*

Incoherent dd-fusion from molecular D_2 is governed by Golden Rule decay dynamics, and is very slow because the expression is proportional to e^{-2G}. The Rabi oscillation frequency that would be associated with a resonant nuclear state is much faster since it is linear in the Gamow tunneling factor. This essential difference between coherent and incoherent reaction rates has been noted many times since 1989. Moreover, the low-level neutron emission rate reported by the BYU group in 1989 is roughly consistent with the Rabi oscillation frequency for this problem. Since 1989, the resonant tunneling model has been argued for by many authors as being relevant to metal deuterides, and have proposed that the experimental results support the existence of a resonant nuclear state.

In what follows, we would like to argue that in spite of the nice features of the model, that the naive resonant tunneling model suffers from very severe problems associated with maintaining coherence long enough for a Rabi oscillation to occur.

4. Relaxation Effects

In many areas of applied physics where the two-level model is used, the predictive capabilities of the model are often extended to include relaxation effects in a simple way.[5] As applied to the present discussion, two deuterons in a molecular state may begin tunneling as described by the formulas given above, but this tunneling may be interrupted if the two deuterons separate and hop to other sites. We wish to add such physics to our model, and understand what the resulting predictions of the extended model are.

4.1. *Bloch equations*

To proceed, some authors define real variables from quadratic combinations of the expansion coefficients. We define the Bloch variables

$$Q(t) \;=\; c_n^*(t)c_a(t) \;+\; c_a^*(t)c_n(t) \tag{23}$$

$$P(t) \;=\; \frac{1}{i}\left[c_n^*(t)c_a(t) \;-\; c_a^*(t)c_n(t)\right] \tag{24}$$

$$N(t) \;=\; |c_a(t)|^2 \;-\; |c_n(t)|^2 \tag{25}$$

By taking time derivatives of the Bloch variables, it is straightforward to show that the Bloch equations are obtained

$$\frac{d}{dt}Q(t) \;=\; \omega_0 P(t) \tag{26}$$

$$\frac{d}{dt}P(t) \;=\; -\,\omega_0 Q(t) \;+\; \frac{2Ve^{-G}}{\hbar}N(t) \tag{27}$$

$$\frac{d}{dt}N(t) \;=\; -\,\frac{2Ve^{-G}}{\hbar}P(t) \tag{28}$$

where $\hbar\omega_0 \;=\; E_a - E_n$. These equations are equivalent to the evolution equations for the amplitudes given in equations (17) and (18).

4.2. *Bloch Equations with Relaxation*

Following the literature, we may extend the Bloch equations by adding relaxation terms

$$\frac{d}{dt}Q(t) \;+\; \frac{Q(t)}{T_2} \;=\; \omega_0 P(t) \tag{29}$$

$$\frac{d}{dt}P(t) \;+\; \frac{P(t)}{T_2} \;=\; -\,\omega_0 Q(t) \;+\; \frac{2Ve^{-G}}{\hbar}N(t) \tag{30}$$

$$\frac{d}{dt}N(t) \;+\; \frac{N(t) - N_0}{T_1} \;=\; -\,\frac{2Ve^{-G}}{\hbar}P(t) \tag{31}$$

where T_1 and T_2 are empirical relaxation times associated with populations and with polarizations, respectively.

4.3. *Solution*

The Bloch equations are linear and hence relatively straightforward to solve. The solutions simplify considerably in the case where the relaxation times are equal, so we focus on a model problem in which $T_1 = T_2 = T$. We consider one such solution in the case where the two deuterons are initialized in $|\phi_a\rangle$ so that $N(0) = 1$, with no initial polarization $Q(0) = P(0) = 0$. The solution in this case is

$$Q(t) = \frac{2U\omega_0}{\hbar\Omega^2}[1-\cos(\Omega t)]e^{-t/T} + \frac{N_0}{1+(\Omega T)^2}\frac{2U\omega_0}{\hbar\Omega^2}\left\{(\Omega T)^2[1-e^{-t/T}]-[1-\cos(\Omega T)]e^{-t/T}-\Omega T\sin(\Omega t)\ e^{-t/T}\right\} \quad (32)$$

$$P(t) = \frac{N_0}{1+(\Omega T)^2}\frac{2UT}{\hbar}[1-\cos(\Omega t)\ e^{-t/T}] + \frac{2U}{\hbar\Omega}\left[1-\frac{N_0}{1+(\Omega T)^2}\right]\sin(\Omega t)\ e^{-t/T} \quad (33)$$

$$N(t) = \frac{\omega_0^2+\left[\frac{2U}{\hbar}\right]^2\cos(\Omega t)}{\Omega^2}e^{-t/T} + \frac{N_0}{1+(\Omega T)^2}\left[\frac{2U}{\hbar\Omega}\right]^2\Omega T\ \sin(\Omega T)\ e^{-t/T} + \frac{N_0}{1+(\Omega T)^2}\left\{1+(\omega_0 T)^2-\left[\frac{2U}{\hbar\Omega}\right]^2\cos(\Omega t)\ e^{-t/T}-\left[\frac{\omega_0}{\Omega}\right]^2[1+(\Omega T)^2]\ e^{-t/T}\right\} \quad (34)$$

In writing these equations, we have used

$$U = Ve^{-G} \quad (35)$$

and

$$\Omega = \sqrt{\omega_0^2+\left[\frac{2U}{\hbar}\right]^2} \quad (36)$$

4.4. *Discussion*

One sees in the solution terms that are oscillatory with frequency Ω, and damping terms that decay with the relaxation time T. If we consider the on-resonance case where the energy levels are matched ($\omega_0 = 0$), then Rabi oscillations occur with a frequency $\frac{2U}{\hbar}$ while the damping occurs with a decay rate of $\frac{1}{T}$. The relaxation time T that one would associate with the dissociation of the molecular state in the metal is not so well known, but one would expect times well below a second. The Rabi oscillation frequency that would correspond to the fastest coherent tunneling transition that might be expected is on the order of 10^{25} seconds. Consequently, under these conditions one sees that all of the oscillations are completely damped before they execute even a small fraction of a cycle.

The degree of resonance required for coherent processes to be seen in this model is enormous. One case see this from the appearance of Lorentzian factors in the expression, which could be rewritten as

$$\frac{1}{(E_n - E_a)^2 \; + \; V^2 e^{-2G} \; + \; \dfrac{\hbar^2}{T^2}}$$

If relaxation processes were somehow suppressed, to observe nearly full Rabi oscillations would require

$$E_n - E_a \;\sim\; V e^{-G} \tag{37}$$

which is not practical. In the presence of relaxation processes, we require instead

$$E_n - E_a \;\sim\; \frac{\hbar}{T} \tag{38}$$

to be resonant, which is a big improvement. The effect under these conditions is very much reduced. To obtain a full cycle of oscillation requires that somehow Ve^{-G} is commensurate. This would require a coupling matrix element very much larger than what is plausible.

We conclude from these arguments that the resonant tunneling approach does indeed exhibit an enormous increase in the tunneling rate as a coherent process theoretically, but that the approach suffers from many problems. Among these are the absence of resonant states in the four nucleon system, an extreme sensitivity to any process that causes destruction of the coherence, and very stringent resonance requirements.

5. Excitation Transfer Model

We are presently considering models for anomalies in metal deuterides in which nuclear reactions are assumed to take place exchanging phonons with the lattice. In this case, there is the possibility of second-order (as well as higher order) reactions in which a reaction at one site is coupled with reactions at one (or more) other sites. Progress on these models is discussed elsewhere in this conference proceedings.[6] Here, we are interested in examining one aspect of the models that is relevant to our general discussion of tunneling effects in this paper.

5.1. *Simplified Model*

We consider a simple model in which reactions at different sites are coupled together. We assume in this model that we have N_1 deuteron pairs (with double occupation of a site) which may fuse with phonon exchange to make ^{4}He. The excitation energy from the reactions is used to drive excitations elsewhere within the coherence domain of a highly excited phonon. For simplicity, we will assume that these reactions involve transitions from N_2 different ^{4}He nuclei to compact states.[a]

In the SU(N) models, the coupling between the compact states, helium nuclei and the highly excited phonon mode produce a very large number of states, some of which are resonant with the initial molecular deuterium states. In the simple model under discussion here, we will include only resonant states. Excitation transfer of the general kind under discussion here is present in the phonon-SU(N) models, but the details of the coupling are not quite the same. Nevertheless, the simple model under discussion here has associated dynamics that are similar to what the phonon-SU(N) are presently believed to possess.

We consider then a model in which a population of molecular deuterons at one set of sites react to make helium at those sites, coupled to a set of helium nuclei at other sites which can be excited to make resonant states. Written using a notation similar to that used above, the associated Hamiltonian is

$$\begin{aligned}
\hat{H} \;=\; & \sum_j^{N_1} \Big[|\Phi_j[D_2]\rangle E_{D_2} \langle \Phi_j[D_2]| \;+\; |\Phi_j[{}^4He]\rangle E_{{}^4He} \langle \Phi_j[{}^4He]| \Big] \\
& + \sum_k^{N_2} \Big[|\Phi_k[com]\rangle E_{com} \langle \Phi_k[com]| \;+\; |\Phi_k[{}^4He]\rangle E_{{}^4He} \langle \Phi_k[{}^4He]| \Big] \\
& + V e^{-G} \Bigg[\sum_j^{N_1} \Big[|\Phi_j[{}^4He]\rangle \langle \Phi_j[D_2]| \;+\; |\Phi_j[D_2]\rangle \langle \Phi_j[{}^4He]| \Big] \Bigg] \\
& \times \Bigg[\sum_k^{N_2} \Big[|\Phi_k[{}^4He]\rangle \langle \Phi_k[com]| \;+\; |\Phi_k[com]\rangle \langle \Phi_k[{}^4He]| \Big] \Bigg] \qquad (39)
\end{aligned}$$

In this expression the notation D_2 refers to double site occupation within the metal and "com" refers to two-deuteron compact states that are nearly resonant with the D_2 states.

[a]The notion of a compact state requires some explanation. Our early models for phonon exchange showed clearly that if reactions at two sites involved phonon exchange with a highly excited phonon mode, then the two reactions could be coupled together as a second-order quantum process. Early data for fast alpha emission supported this notion, where the energy of two deuterons fusing to ^{4}He was proposed to be available to ionize an alpha particle out of Pd nuclei. The fastest site-other-site process was predicted to be one in which the energy from two deuterons fusing went into dissociating a ^{4}He nucleus. After analysis of this process, it was noticed that following the dissociation, that two deuterons would have difficulty dissociating, and that they might be observed close together. Experiments by Kasagi provides evidence for such an effect. We term the resulting states "compact states".

5.2. *Pseudostate Operator Formulation*

The model described above can be written more compactly in terms of pseudostate operators

$$\hat{H} \ = \ \frac{\Delta E}{2}\hat{\Sigma}_z^{(1)} \ + \ \frac{\Delta E}{2}\hat{\Sigma}_z^{(2)} \ + \ Ve^{-G}\left[\hat{\Sigma}_+^{(1)}+\hat{\Sigma}_-^{(1)}\right]\left[\hat{\Sigma}_-^{(2)}+\hat{\Sigma}_+^{(2)}\right] \tag{40}$$

This Hamiltonian differs from that of Equation (39) by an constant energy offset, which does not change the dynamics of observable quantities. The $\hat{\Sigma}_z$ pseudostate operators are defined according to

$$\hat{\Sigma}_z^{(1)} \ = \ \sum_j^{N_1} \left[|\Phi_j[D_2]\rangle\langle\Phi_j[D_2]| \ - \ |\Phi_j[^4He]\rangle\langle\Phi_j[^4He]|\right] \tag{41}$$

$$\hat{\Sigma}_z^{(2)} \ = \ \sum_k^{N_2} \left[|\Phi_k[com]\rangle\langle\Phi_k[com]| \ - \ |\Phi_k[^4He]\rangle\langle\Phi_k[^4He]|\right] \tag{42}$$

The $\hat{\Sigma}_\pm$ pseudostate operators are defined according to

$$\hat{\Sigma}_-^{(1)} \ = \ \sum_j^{N_1} |\Phi_j[^4He]\rangle\langle\Phi_j[D_2]| \qquad \hat{\Sigma}_+^{(1)} \ = \ \sum_j^{N_1} |\Phi_j[D_2]\rangle\langle\Phi_j[^4He]|$$

$$\hat{\Sigma}_-^{(2)} \ = \ \sum_k^{N_2} |\Phi_k[^4He]\rangle\langle\Phi_k[com]| \qquad \hat{\Sigma}_+^{(2)} \ = \ \sum_k^{N_2} |\Phi_k[com]\rangle\langle\Phi_k[^4He]|$$

The energy difference ΔE is

$$\Delta E \ = \ E[D_2] \ - \ E[^4He] \tag{43}$$

which is taken to be resonant with $E[com] - E[^4He]$.

5.3. *Solution*

We can develop an approximate solution by forming a superposition of resonant states within the model

$$\Psi \ = \ \sum_n c_n(t) \ |N_1, n\rangle|N_2, N_1 - n\rangle \tag{44}$$

where we used basis states formed of products of Dicke states $|N, n\rangle$. Our notation assumes N nuclei with n in the excited state. These states are consistent with

$$\hat{\Sigma}_z|N, n\rangle \ = \ (2n - N)|N, n\rangle \tag{45}$$