A Theoretical Formulation for Problems in Condensed Matter Nuclear Science

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Abstract

Over the years theorists have adopted a wide variety of approaches to theoretical problems in condensed matter nuclear science. If one starts with a formulation adapted to condensed matter, then the resulting model may be well adapted to describing electrons and phonons, but perhaps less well adapted to describing nuclear states. If one starts with a formulation adapted to nuclear calculations, then the resulting model may be well adapted to structure and reaction calculations, but perhaps less well adapted to phonon or plasmon modes. We discuss here the use of a more general formulation based on nucleons and electrons which can be used for problems in condensed matter physics, nuclear physics, or for problems that involve interactions between nuclear and condensed matter systems.

1. Introduction

Excess heat in the Fleischmann-Pons experiment appears to be the result of a new kind of nuclear process [1]. The experimental arguments supporting this include: (a) the amount of energy measured greatly exceeds that which could be stored conventionally, or which could be of chemical origin; (b) ^{4}He is observed as an ash in amounts commensurate with the energy produced, where the amount of energy observed per ^{4}He is near 24 MeV (which is the mass difference between two deuterons and ^{4}He); and (c) low-level nuclear emissions have been observed in samples at low current density which produce excess heat at high current density. However, the excess heat is produced without commensurate energetic particle production, which is unprecedented. In a conventional exothermic nuclear reaction, the reaction energy is expressed as kinetic energy in the reaction products. In the Fleischmann-Pons experiment the excess heat is thought to be due to an exothermic nuclear process, but experiment shows an absence of corresponding energetic emissions.

If the energy does not appear as kinetic energy, then it must be expressed through other channels, since ultimately it is seen in thermal measurements. The only available non-kinetic channels into which the energy might go are those of the host metal deuterides structure, which are condensed matter modes. From the results of single and dual laser experiments, there is indirect evidence that some of the energy may be going into plasmon or optical phonon modes prior to thermalization. As such, it seems reasonable to consider the theoretical question as to

what kind of coupling occurs between these modes and the local nuclear systems which have been put forth in proposed reaction mechanisms.

More generally, there are by now numerous experiments which show anomalies of one sort or another (beyond excess heat), in which nuclear and condensed matter effects are probably connected. To address such issues, theorists over the years have been using a variety of tools to develop models, and to make predictions. However, if a condensed matter approach is adopted, then there are issues associated with including nuclear effects. If the starting point is some kind of nuclear physics calculation, then there are issues as to how one includes condensed matter effects. Within the literature one finds a variety of approaches which have been employed, so far with no systematic formulation. For each problem and each author, one must often put in effort to understand both the underlying formulation as well as the result.

Because of this, it seems worthwhile to see whether a formulation might be constructed which has a foundation sufficiently general to encompass aspects of condensed matter and nuclear physics on a uniform footing. If so, then we might be able to use it to advantage in modeling problems in areas where both are equally important in accounting for physical effects that are observed. In what follows, we describe one approach to such a formulation. In essence, if we do nothing more than start from a set of fundamental building blocks, such as electrons and nucleons, then the resulting formulation has the potential to speak to problems in the two disciplines on equal footing starting from a common foundation. Armed with such a foundation, we would be able to bring in results from the relevant literature in both disciplines within a unified framework to address problems of interest. Workers with backgrounds in either discipline could then have a common language that could be used to address such problems.

2. Electrons and nucleons

As a foundation, we consider models at the outset composed of a set of electrons and a set of nucleons. Within the isospin formalism, neutrons and protons are considered to be simply nucleons; identical particles differing only by whether they are isospin up (proton) or isospin down (neutron). This is similar to a set of electrons, which are identical particles, and which may have spin up or spin down.

Computations of nuclear structure or dynamics can in many cases be described adequately from such a starting place, and over the years good models have been developed that describe the interaction between nucleons. Restricting ourselves to a description based on nucleons bars us from addressing more sophisticated problems in which quarks become important. However, given the difficulty of working with QCD at present in association with bound state problems, this limitation seems a good trade off against a much improved ability to perform calculations much more easily.

Condensed matter computations in general assume electrons and nuclei, so that breaking down nuclei into their component nucleons greatly increases the complexity of what is already a pretty complicated theoretical problem. If one needs to account for the nuclear structure of every nucleus in a solid at the outset, then one would expect that subsequent calculations will quickly become a mess. Since the expanded formulation includes condensed matter physics as a subset, we are sure that it will be capable of address relevant problems in principle. However,

at some point we will require tools to reduce our description in order to allow us to focus on important parts of a problem. Hence, using a starting point of a set of electrons and nucleons at the outset will have to be viewed as formal for condensed matter calculations, and we will need a way to collect the nucleons back into their constituent nuclei for those that are not directly involved in a reaction under consideration.

Consequently, we require of our formulation a basic definition for the electron-nucleon Hamiltonian, and then we will need a systematic way to reduce problems so that we can focus on those parts which are particularly important for a specific calculation.

2.1. The electronic part

Focusing first on the electronic part, it seems clear that the place to start in general is with QED, which describes electrons and photons (the focus on electrons above is simplistic, since the interaction with electromagnetic fields is ubiquitous in condensed matter systems). In the literature over the years, one can find problems worked in configuration space (relativistic and nonrelativistic), in **k**-space, in second quantization, and using a wide range of approaches. We have no plans here to restrict in any way which part or formulation of QED to be used, and we would consider configuration space models that include only Coulomb interactions to be a good low-end example of a useful subset of QED.

2.2. The nucleon part

One can find much literature on structure and dynamics calculations of nuclei presented in configuration space, with empirical nucleon-nucleon potentials and Coulomb interactions. This would constitute a useful low-end example of the nucleon part of the problem. At the other end of the spectrum, there have been published nucleon-based field theories which are empirical generalizations of QED, including relativistic effects and coupling with the electromagnetic field (see for example [2] which discusses QHD). Such models would equivalently be suitable for the general formulation under discussion in this paper. In order to model beta decay, we assume that such models are augmented as needed with neutrinos and their associated weak interactions.

2.3. A simple example of a configuration space Hamiltonian

As an example of a minimal low-end model, we might adopt a Hamiltonian of the form

$$\hat{H} \;=\; -\sum_i \frac{\hbar^2}{2m}\nabla_i^2 - \sum_\alpha \frac{\hbar^2}{2M}\nabla_\alpha^2 + \sum_{i<j}\frac{e^2}{\left|\mathbf{r}_i-\mathbf{r}_j\right|} + \sum_{\alpha<\beta} V_n\left(\left|\mathbf{r}_\alpha-\mathbf{r}_\beta\right|\right) + \sum_{\substack{i,\alpha \\ protons}}\frac{e^2}{\left|\mathbf{r}_i-\mathbf{r}_\alpha\right|}$$

In this model, the first two terms account for the (nonrelativistic) kinetic energies of the electrons (with mass m) and nucleons (with mass M); the third term describes Coulomb interactions between electrons; the fourth term describes strong force and Coulomb interactions between nucleons; and the final term describes the attractive Coulomb interaction between electrons and protons.

2.3. The nucleon-nucleon interaction

The nucleon-nucleon potential is far more complicated than the simple Coulomb interaction (which could be used as a first approximation for the electron-electron potential). This is because nucleons are composite particles made up of quarks. In the past decades, nuclear physicists have developed empirical nucleon-nucleon potentials that are accurate for "low energy" (below a few hundred MeV) applications by fitting scattering data and bound state energies to appropriate functional forms [3]. One such potential that was proposed early on was the Hamada-Johnston potential [4]. A more modern example is the Argonne potential, which is now widely used [5]. More complicated nonlocal potential models have been developed in recent years [6,7].

2.4 Antisymmetrization

Electrons are identical fermionic particles, so that the overall wavefunction must be antisymmetric under the exchange of any two electrons, which leads to constraints on the spin and spatial pieces. Nucleons in this kind of model are also identical fermionic particles, so that once again the overall wavefunction must be antisymmetric under the exchange of any two nucleons, which in this case leads to constraints on the spin, isospin, and spatial parts of the problem. The extra degree of freedom in the nucleon part of the problem makes the construction of properly antisymmetrized nuclear wavefunctions a more complicated exercise than in the electronic case.

In the case of two electrons, there are two ways to construct an antisymmetric wavefunction:

$$\Psi = \begin{cases} (\text{antisymmetric in spin})(\text{symmetric in space}) \\ (\text{symmetric in spin})(\text{antisymmetric in space}) \end{cases}$$

In the case of two nucleons, there are three ways to construct an antisymmetric wavefunction:

$$\Psi = \begin{cases} (\text{antisymmetric in spin})(\text{symmetric in isospin})(\text{symmetric in space}) \\ (\text{symmetric in spin})(\text{antisymmetric in isospin})(\text{symmetric in space}) \\ (\text{symmetric in spin})(\text{symmetric in isospin})(\text{antisymmetric in space}) \end{cases}$$

For three-nucleon or four-nucleon wavefunctions, there are many more combinations, and one needs to make use of group theory for classification and construction [8]. This issue is much more important for the nucleon part of the problem than for the electron part of the problem, since the Coulomb interaction is scalar, and since an independent particle approximation can provide a useful starting place. The independent particle approximation is a much poorer starting place in the case of few-nucleon problems due to the absence of a fixed attractive core.

3. Matrix element example

The approach under discussion is very powerful, and to illustrate this we consider a formal example in the case of a phonon exchange matrix element. The discussion that follows is a brief summary of one given previously in Ref. [9]. We consider phonon exchange associated with a nuclear transition mediated by the nucleon-nucleon interaction. We assume that the initial and final nucleon states are nearly stationary in the lattice, which means that the associated physical process is not energy conserving, so that the matrix element would describe a piece of a more complicated physical process that does conserve energy.

3.1. Formal initial and final state wavefunctions

We take as a formal starting place initial and final state wavefunctions that are much more general than will be needed, but which are consistent with the formulation under discussion

$$\Psi_i = \Psi_i\left(\{\mathbf{r}_j\},\{\sigma_j\},\{\mathbf{r}_\alpha\},\{\sigma_\alpha\},\{\tau_\alpha\}\right)$$
$$\Psi_f = \Psi_f\left(\{\mathbf{r}_j\},\{\sigma_j\},\{\mathbf{r}_\alpha\},\{\sigma_\alpha\},\{\tau_\alpha\}\right)$$

Where the subscript j is used for electron position and spin variables, and α is used for nucleon position and spin variables. The matrix element under discussion can be written formally as

$$M_{fi} = \left\langle \Psi_f \middle| V_n \middle| \Psi_i \right\rangle$$

where V_n is the nucleon-nucleon interaction. At this point, since the wavefunctions are assumed to be properly antisymmetrized functions of the nucleon spin, isospin, and position variables, the matrix element is expressed appropriately for a calculation of the nucleon-nucleon interaction. Unfortunately, there is no hope of describing phonon exchange or condensed matter effects at this level with such a description. Starting from this formulation as a formal starting place, we need to reduce the problem systematically so that it might be amenable to computation.

3.2. Spectator nuclei

One thing that complicates matters is that most of the nuclei in the lattice do not participate in the reaction of interest, and contribute only through their center of mass coordinates. For example, consider a nuclear rearrangement of a local four nucleon system involving two deuterons; in this case, none of the host metal nuclei participate, and we should not need to carry around a description of the internal structure at the nucleon level. Hence, our first task is to eliminate individual nucleon coordinates of the spectator nuclei, and replacing them by a smaller number of nuclear center of mass coordinates. This can be done rigorously by expressing the parts of the spectator wavefunctions in terms of center of mass coordinates and relative coordinates, and then integrating over relative coordinates. In the end, we can denote this through

$$\Psi_i\left(\{\mathbf{r}_j\},\{\sigma_j\},\{\mathbf{r}_\alpha\},\{\sigma_\alpha\},\{\tau_\alpha\}\right) \rightarrow \Psi_i\left(\{\mathbf{r}_j\},\{\sigma_j\},\{\mathbf{r}_\alpha\},\{\sigma_\alpha\},\{\tau_\alpha\},\{\mathbf{R}_k\}\right)$$

The electron variables remain the same, but now the set of nucleon coordinates under consideration is reduced, and we have explicit center of mass coordinates for the spectator nuclei. In this form, we are now much closer to a problem formulation suitable for the condensed matter part of the problem.

3.3. Born-Oppenheimer approximation

As long as we are interested in processes assumed to be adiabatic relative to electron dynamics, we can make use of a Born-Oppenheimer approximation in order to reduce the problem further. The associated product wavefunction can be written as

$$\Psi_i\left(\{\mathbf{r}_j\},\{\sigma_j\},\{\mathbf{r}_\alpha\},\{\sigma_\alpha\},\{\tau_\alpha\},\{\mathbf{R}_k\}\right) = \Phi_i\left(\{\mathbf{r}_j\},\{\sigma_j\};\{\mathbf{r}_\alpha\},\{\sigma_\alpha\},\{\tau_\alpha\},\{\mathbf{R}_k\}\right)\Psi_i\left(\{\mathbf{r}_\alpha\},\{\sigma_\alpha\},\{\tau_\alpha\},\{\mathbf{R}_k\}\right)$$

Where the first term is the electronic wavefunction given fixed nucleon and nuclei positions, and the second is the adiabatic nucleon and nuclei wavefunctions. If our focus is on phonon exchange, then we are interested in the second term, and it may be possible to integrate out the electronic part of the problem if we have some reason to believe that the electronic wavefunctions in the initial and final states are sufficiently alike. If not, then the overlap integral coupling to the relevant electronic states in the final state will have to be estimated. For simplicity, we will assume in the matrix element under consideration that there are no important electronic or plasmon excitations. This approximation has the effect of reducing the wavefunction according to

$$\Psi_i\left(\{\mathbf{r}_j\},\{\sigma_j\},\{\mathbf{r}_\alpha\},\{\sigma_\alpha\},\{\tau_\alpha\},\{\mathbf{R}_k\}\right) \rightarrow \Psi_i\left(\{\mathbf{r}_\alpha\},\{\sigma_\alpha\},\{\tau_\alpha\},\{\mathbf{R}_k\}\right)$$

3.4. Phonons

Our goal was to develop a description for phonon exchange, and we require yet one more modification of the problem in order to bring phonons into our description. One way to do this is to recast the local nucleon problem in terms of relevant center of mass and relative coordinates. For example, if there are two deuterons present, then two different center of mass coordinates would be appropriate. If a helium nucleus is present, then only a single center of mass coordinate would be appropriate. We can denote this through

$$\{\mathbf{r}_\alpha\} \rightarrow \{\mathbf{R}\},\{\boldsymbol{\xi}_i\}$$

This change in coordinates then leads to wavefunctions that we may denote through

$$\Psi_i\left(\{\mathbf{r}_\alpha\},\{\sigma_\alpha\},\{\tau_\alpha\},\{\mathbf{R}_k\}\right) \rightarrow \Psi_i\left(\{\boldsymbol{\xi}_i\},\{\sigma_\alpha\},\{\tau_\alpha\},\{\mathbf{R}_k\}\right)$$

Now the wavefunction on the RHS has a full set of center of mass coordinates, and from the Born-Oppenheimer approximation (or from experiment) we can in principle develop equilibrium positions and force constants, so that we can recast the center of mass position operators in terms of phonon mode amplitudes. This we can denote according to

$$\Psi_i\left(\{\boldsymbol{\xi}_i\},\{\sigma_\alpha\},\{\tau_\alpha\},\{\mathbf{R}_k\}\right) \rightarrow \Psi_i\left(\{\boldsymbol{\xi}_i\},\{\sigma_\alpha\},\{\tau_\alpha\},\mathbf{q}_i\right)$$

where $\mathbf{q}_i$ is a vector that contains all of the initial state phonon mode amplitudes. The nucleon center of mass coordinates in this case can be expressed as phonon operators.

3.5. Matrix element integrations

We now have wavefunctions in a form suitable for describing phonon exchange matrix elements, at least formally. The matrix element can be written as [9]

$$M_{fi} = \iint\!\!\iint \Psi_f^*\left(\{\boldsymbol{\xi}_f\},\{\sigma_\beta\},\{\tau_\beta\},\mathbf{q}_f\right) V_n \Psi_i\left(\{\boldsymbol{\xi}_i\},\{\sigma_\alpha\},\{\tau_\alpha\},\mathbf{q}_i\right) \times \Delta\left(\mathbf{q}_i,\mathbf{q}_f\right)\Delta\left(\boldsymbol{\xi}_i,\boldsymbol{\xi}_f\right) d\mathbf{q}_i d\mathbf{q}_f d\boldsymbol{\xi}_i d\boldsymbol{\xi}_f$$

where the center of mass coordinates of the initial state lattice must agree with the center of mass coordinates in the final state lattice

$$\Delta\left(\mathbf{q}_i,\mathbf{q}_f\right) = \delta\left(\mathbf{q}_i - \mathbf{A}\cdot\mathbf{q}_f - \mathbf{b}\right)$$

This is consistent with the linear relation between vibrational coordinates that is sometimes used in the case of Franck-Condon factors in polyatomic molecules [10,11]

$$\mathbf{q}_f = \mathbf{A}\cdot\mathbf{q}_i + \mathbf{b}$$

In addition, the individual nucleon coordinates in the initial state must agree with those for the same nucleons in the final state, which is imposed through

$$\Delta\left(\boldsymbol{\xi}_i,\boldsymbol{\xi}_f\right) = \prod_\alpha \delta\left(\mathbf{r}_\alpha^f - \mathbf{r}_\alpha^i\right)$$

3.6. Coupling between phonons and internal nuclear coordinates

In the expression for the matrix element M_{fi} above, the initial state and final state wavefunctions are expressed in terms of phonon coordinates and internal relative nuclear coordinates. To within an excellent approximation, these two degrees of freedom are independent, so that we could reasonably use product wavefunctions for both. If so, then the issue of the origin of coupling between them becomes of interest. The coupling between these degrees of freedom comes about implicitly in this formulation through the nucleon-nucleon interaction, which depends on the relative position of two nucleons. The nucleon coordinates themselves depend on the local nuclear center of mass coordinate (which itself is a function of the phonon mode coordinates), and the relative coordinates. As a result, under certain

conditions (for example, if the intial state contains two deuterons, and the final state contains a ^{4}He nucleus), V_n can cause a mixing between the phonons and internal relative coordinates.

4. Discussion

We can use this approach to address problems systematically in condensed matter nuclear science which involve both nuclear and condensed matter pieces. In order to handle nuclear models, we begin with a description at the outset in terms of nucleons and electrons. This allows us to specify the problem in a way that is consistent with the requirements for the nuclear part of the calculation. However, the wavefunctions and matrix elements that result initially are far too complicated to work with for the condensed matter part of the problem. The idea is to subsequently reduce the problem into a form suitable for condensed matter calculations by using successive transformations.

We illustrated this in a formal example involving a phonon exchange matrix element. From this example, we see that the nucleon-electron starting place does indeed provide for a suitable starting point for a nuclear calculation. If the strong force is involved, then we need fully antisymmetric nucleon wavefunctions expressed in terms of nucleon variables, and the formalism outlined here provides for this. The utility of the approach for the condensed matter part of the problem is that it allows for a well-defined foundation that can be used as a starting point for approximations and transformations commonly used in condensed matter calculations. In the end, the formalism allows us to see explicitly how mixing between phonon modes and internal nuclear coordinates come about.

Limitations imposed on the conference proceedings restrict us from any detailed consideration of other problems, but it should be clear that we can apply the method generally to problems that have arisen within the field. Should we wish to describe condensed matter screening effects in the same computation with deuteron-deuteron fusion reactions, the formulation outlined here can handle the problem systematically. If we are interested in coupling nuclear reactions with plasmon mode excitation, then we can start from the same place, but make different approximations and transformations to obtain a formula for a matrix element in a form suitable for computation.

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