RESEARCH REVIEW JOURNALS
Volume-03
Issue-03
March-2018
ISSN: 2455-3085 (Online)
RESEARCH REVIEW International Journal of Multidisciplinary
www.rrjournals.com [UGC Listed Journal]

The Study of Quantum Mechanics and Statistical Mechanics of A Linear Chain in the Solid State Physics

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ARTICLE DETAILS

Article History

Published Online: 30 March 2018

Keywords

quantum mechanics, linear, chain, nonlinear, solid state, physics, etc.

ABSTRACT

The establishments of Statistical Mechanics and Thermodynamics structure a hidden microscopic theory, specifically Quantum Mechanics. The methodology is genuine quantum as in statistical conduct is an outcome of target quantum uncertainties because of entrapment and uncertainty relations. Quantum Mechanics professes to be a basic theory. A huge writing on these nonlinear excitations, called solitons in integrable frameworks and lone excitations in non-integrable models in the event that they have certain soundness in regular Statistical Mechanics probabilities, assumption esteems, differences and higher snapshots of observables are figured through ensemble averages. by removing a ^{12}C atom, replacing it by a ^{13}C atom in the tetrahedral configuration of the diamond, and doing this cycle periodically a linear way, one could get a linear chain of nuclear spins one half which can function as a quantum computer.

1. INTRODUCTION

The methodology is genuine quantum as in statistical conduct is an outcome of target quantum uncertainties because of entrapment and uncertainty relations. No extra randomness is added by hand and no presumptions about from the earlier probabilities are made, instead measure focus results are utilized to legitimize the techniques for Statistical Physics. Quantum Mechanics professes to be a basic theory. As such it ought to be equipped for providing us with a microscopic clarification for all wonders we see in plainly visible frameworks, including irreversible cycles like thermalization. Yet, its unitary time advancement is by all accounts incompatible with irreversibility leading to an obvious logical inconsistency between Quantum Mechanics and Thermodynamics. This obvious logical inconsistency is essential for the long standing issue of the development of traditionally from Quantum Mechanics. To defeat this issue numerous creators have proposed modifying Quantum Theory, either by adding nonlinear terms to the von Neumann equation or by postulating a periodical unconstrained breakdown of the wave work. Others have thought about compelling, Markovian, time advancements for open Quantum frameworks and it has been demonstrated that framework shower models that develop under an extraordinary type of Hamiltonian will in general advance into states that are traditional super positions of supposed pointer states a wonder called earth induced super determination, a term because of Zurek. Depending on the creator subsets of these methodologies are subsumed under the term decoherence theory. In face of the tremendous accomplishment of standard Quantum Mechanics in explaining microscopic wonders and the extra troubles that emerge when the von Neumann equation is changed and the presence of plainly visible quantum frameworks from one viewpoint, and the expansive relevance of Statistical Mechanics and Thermodynamics on the other, we feel that neither an adjustment of Quantum Theory, nor contemplations limited to uncommon circumstances can give an agreeable clarification of the statistical and thermodynamic conduct of our perceptible world.

2. NONLINEAR STRUCTURES IN SOLID STATE PHYSICS

Nonlinear excitations as naturally visible wonders have been known for quite a while, since the early revelation of Russell and the surmised treatment of the Navier Stokes equation by Korteweg and de Vries. In the microscopic solid state theory the primary endeavors with a nonlinear model were done regarding the portrayal of disengagements in the supposed Prandtl-Dehlinger-Frenkel-Kont0rova model using the Sine-Gordon equation (named contrastingly later). An interesting survey with recorded notes was given by Seeger. Today there exists a huge writing on these nonlinear excitations, called solitons in integrable frameworks and lone excitations in non-integrable models in the event that they have certain soundness. In this survey it is difficult to cover all the various parts of nonlinear structures and elements. We won't examine the different perspectives and utilizations of the Sine-Gordon equation; this was magnificently assessed by Bak. He additionally gives an excellent diagram of record results for magnetic frameworks. We likewise don't focus on the different parts of nonlinear excitations in conducting polymers. Two late surveys cover these interesting zones totally. We focus here on those structures where a polarizable particle offers ascend to nearby nonlinearities. As in the frameworks referenced over, these harmonicities lead to singular excitations and, much more interestingly, to different grid structures whose presence and strength relies upon the accessibility of competing interactions with different neighbors. It ought to be noticed that the aftereffects of our study can be found in relationship to other nonlinear frameworks, since there is a wide comparability between the different nonlinearities.

3. QUANTUM STATISTICAL MECHANICS

Another interpretation of the establishments of Statistical Mechanics following Seth Lloyd we called this methodology pure state quantum Statistical Mechanics. In what follows we give a compact and independent audit of the consequences of these and other related works in a bound together and reliable documentation.

3.1 Ensemble averages and pure state quantum Statistical Mechanics

In regular Statistical Mechanics probabilities, assumption esteems, differences and higher snapshots of observables are figured through ensemble averages. Depending on the circumstance viable one should utilize the microcanonical, sanctioned or the proper grand standard ensemble. The legitimacy of this methodology is past all uncertainty and the outcomes obtained using it has been affirmed by innumerous trials. Then again, the part of likelihood in Physics, the issue of ergodicity and particularly the microscopic defense of the Second Law of Thermodynamic are inconspicuous issues and numerous major inquiries concerning them are as yet open notwithstanding numerous times of exploration. The starting point of our conversation will be to show how the materialness of ensemble averages can be legitimized using Quantum Mechanics and measure fixation methods with no additional suppositions.

- **Microcanonical ensemble:**

The microcanonical ensemble is in some sense the most central ensemble. In old style Statistical Physics it is applied to shut frameworks in harmony. Different ensembles, accepted and grand sanctioned can be gotten from it. In the quantum setting the microcanonical ensemble is utilized in circumstances where each of the one thinks about a shut actual framework is that the estimation of some recognizable A, which relates to a rationed amount, i.e (, A) = 0, lies in some interval I[3]. Let |ai be the eigenvectors of An and $_R$ the confined subspace spread over by those eigenvectors that have eigenvalues in the interval. The microcanonical assumption estimation of any noticeable B as for $_R$ is then defined to be

$$\langle B\rangle_{\mathrm{mc}} = \frac{1}{d_R}\sum_{|a\rangle\in\mathcal{H}_R}\langle a|B|a\rangle = \mathrm{Tr}[\frac{\Pi_R}{d_R}B] \quad (1)$$

Where

$$\Pi_R = \sum_{|a\rangle\in\mathcal{H}_R}|a\rangle\langle a|$$

Is the projector onto the subspace $_R$ of Eigen states of A with Eigen esteems in I. Knowing just that measuring A would give an incentive in I we attribute to the framework the blended state?

$$\rho_{\mathrm{mc}} = \frac{\Pi_R}{d_R} = \frac{1}{d_R}\sum_{|a\rangle\in\mathcal{H}_R}|a\rangle\langle a|. \quad (2)$$

Equation (1) and (2) are the quantum adaptation of the equal a cloister probability postulate, which is the fundamental postulate of convectional Statistical Mechanics. All compatible states are assigned the same a monastery probability. It is past all uncertainty that this approach to calculate expectation values has demonstrated to be incredibly helpful and yields brings about great agreement with tests. Anyway it remains puzzling why dynamically evolving and intrinsically quantum mechanical frameworks may be portrayed by the static, exceptionally blended state (2).

4. QUANTUM MECHANICS OF A LINEAR CHAIN

As a toy model of a solid, let us think about a linear chain of masses m associated by springs with spring constant B. Assume that the balance spacing between the masses is a. The balance positions define a 1D lattice. The lattice 'vectors', j, are defined by:

j = ja (3)

They interface the origin to all points of the lattice. On the off chance that and 0 are lattice vectors, at that point + are also lattice vectors. A bunch of basis vectors is a minimal arrangement of vectors which generate the full arrangement of lattice vectors by taking linear combinations of the basis vectors. In our 1D lattice, is the basis vector? Let ui be the displacement of the ith mass from its harmony position and let pi be the corresponding momentum. Allow us to assume that there are N masses, and we should force an occasional boundary condition, $u_i = u_{i+N}$. The Hamiltonian for such a framework is:

$$H = \frac{1}{2m}\sum_i p_i^2 + \frac{1}{2}B\sum_i (u_i - u_{i+1})^2 \quad (4)$$

Allow us to utilize the Fourier transform representation:

$$u_j = \frac{1}{\sqrt{N}}\sum_k u_k\, e^{ikja}$$
$$p_j = \frac{1}{\sqrt{N}}\sum_k p_k\, e^{ikja} \quad (5)$$

Because of the intermittent boundary condition, the allowed k's are:

$$k = \frac{2\pi n}{Na} \quad (6)$$

We can invert (5):

$$\frac{1}{\sqrt{N}}\sum_j u_j e^{ik'ja} = \frac{1}{N}\sum_k\sum_j u_k\, e^{i(k-k')ja}$$
$$\frac{1}{\sqrt{N}}\sum_j u_j e^{ik'ja} = u_{k'} \qquad (7)$$

Note that $u^\dagger_k$ = u_k, $p^\dagger_k$ = p_k since $u^\dagger_j = u_j$, $p^\dagger_j = p_j$. They satisfy the commutation relations:

$$\begin{aligned}[p_k, u_{k'}] &= \frac{1}{N}\sum_{j,j'} e^{ikja}e^{ik'j'a}\,[p_j, u_{j'}] \\ &= \frac{1}{N}\sum_{j,j'} e^{ikja}e^{ik'j'a} - i\hbar\delta_{jj'} \\ &= -i\hbar\frac{1}{N}\sum_j e^{i(k-k')ja} \\ &= -i\hbar\delta_{kk'} \end{aligned} \qquad (8)$$

Thus, p_k and $u_{k'}$ drive except if k = k'.

4.1 Statistical Mechnics of a Linear Chain

The case of a linear chain of masses m separated by springs of power constant B, at balance distance a. The excitations of this framework are phonons which can have momenta k ∈ [−π/a, π/a] (since k ≡ k + 2πm/a), corresponding to energies

$$\hbar\omega_k = 2\left(\frac{B}{m}\right)^{\frac{1}{2}}\left|\sin\frac{ka}{2}\right| \qquad (9)$$

Phonons are bosons whose number isn't monitored, so they comply with the Planck appropriation. Subsequently, the energy of a linear chain at finite temperature is given by

$$\begin{aligned} E &= \sum_k \frac{\hbar\omega_k}{e^{\beta\hbar\omega_k}-1} \\ &= L\int_{\frac{-\pi}{a}}^{\frac{\pi}{a}} \frac{dk}{(2\pi)}\,\frac{\hbar\omega_k}{e^{\beta\hbar\omega_k}-1} \end{aligned} \qquad (10)$$

Changing variables from k to ω,

$$\begin{aligned} E &= 2\cdot\frac{L}{2\pi}\int_0^{\sqrt{4B/m}}\frac{2}{a}\,\frac{d\omega}{\sqrt{\frac{4B}{m}-\omega^2}}\,\frac{\hbar\omega}{e^{\beta\hbar\omega}-1} \\ &= \frac{2N}{\pi}\int_0^{\sqrt{4B/m}}\frac{d\omega}{\sqrt{\frac{4B}{m}-\omega^2}}\,\frac{\hbar\omega}{e^{\beta\hbar\omega}-1} \\ &= \frac{2N}{\pi}\frac{(k_BT)^2}{\hbar}\int_0^{\beta\hbar\sqrt{4B/m}}\frac{1}{\sqrt{\frac{4B}{m}-\left(\frac{x}{\beta\hbar}\right)^2}}\,\frac{x\,dx}{e^x-1} \end{aligned} \qquad (12)$$

On the off chance that we had alternating masses on springs, at that point the articulation for the energy would have two integrals, one over the acoustic modes and one over the optical modes.

5. DIAMOND AS A SOLID STATE QUANTUM COMPUTER BY LINEAR CHAIN OF NUCLEAR SPINS SYSTEM

Up until this point, the idea of having a working quantum computer with enough number of qubits (at least 1000) has faced two main issues: the decoherence due the interaction of the climate with the quantum system, and technological limitations (get signal from NMR quantum computer, laser control capability in particle trap quantum computer, physical development for more than two qubits like in photons cavities, atoms traps, Josephson's joint particles, Aronov-Bhom gadgets, diamond NV gadget, or high field and high field gradients in linear chain of paramagnetic atoms with spin one half). In particular, the linear chain of paramagnetic atoms of spin one half became a decent mathematical model to make investigations of quantum gates, quantum algorithms, and decoherence which could be applied to other quantum computers. One set up the ideas of using the diamond stable structure and the linear chain of spin one half nucleuses. To do this, on the tetrahedral ^{12}C (with nuclear spin zero) configuration of the diamond main structure, one eliminates a ^{12}C component of this configuration and replace it by a ^{13}C (with nuclear spin one half) atom, and one repeats this replacement along a linear course of the crystal. By doing this replacement, one obtains a linear chain of atoms of nuclear spin one half which is shielded from the climate by the crystal structure and the electrons cloud. Hence, one could have a quantum computer profoundly tolerant to climate interaction and maybe not all that hard to construct it, from the technological point of view.

5.1 $^{12}C^{13}C$ Diamond and spin-spin interaction

The above idea is spoken to in Figure 1, where the ^{13}C atoms are place on the situation of some ^{12}C atoms. This replacement should be possible using the same methods used to build the diamond NV structure, or using particle implantation methods and neutralization of ^{13}C in the diamond. It is assumed in this paper that this configuration can be constructed by one way or another. Presently, as one can see, the important interaction on this configuration is the spin-spin interaction between the nucleuses of the ^{13}C atoms. This interaction is notable and is given by

$$U = \frac{\mu_o}{4\pi}\frac{(\boldsymbol{m}_1\cdot\boldsymbol{x})(\boldsymbol{m}_2\cdot\boldsymbol{x}) - \boldsymbol{m}_1\cdot\boldsymbol{m}_2}{|\boldsymbol{x}|^3}, \qquad (13)$$

Where the magnetic moment, m_i, i =1, 2 of ^{13}C's is related with the nuclear spin as

m_i= S_i (14)

Being γ the proton gyromagnetic ratio γ ≈2.675×10^8 rad T.s). Without losing the main idea, it will be assumed here that ^{13}C magnetic second is because of proton. The variable x indicates the separation vector between two ^{13}C nucleus, which has magnitude a = |x| 10^{-10}. Aligning the chain of ^{13}C nucleus along the x-axis of the reference system and assuming

Ising interaction between ^{13}C nucleuses, this energy can be composed as

$$U = \frac{J}{\hbar} S_1^z S_2^z, \quad (15)$$

Where the coupling constant J has been defined as

$$J = \frac{\mu_o \gamma^2 \hbar}{4\pi a^3} \quad (16)$$

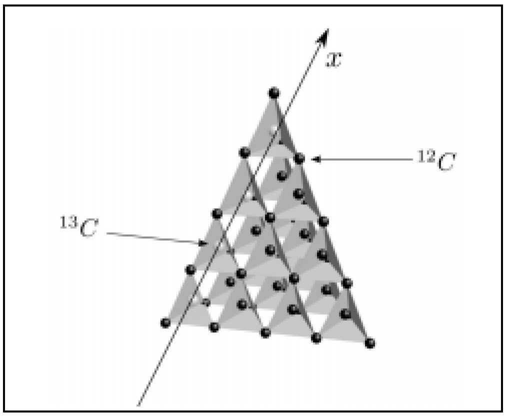

Figure 1: Diamond ^{12}C-^{13}C

By removing a ^{12}C atom from the tetrahedral configuration of the diamond, replacing it by a ^{13}C atom, and repeating this linear way, it is conceivable to have a linear chain of nuclear spins one half and to construct a solid state quantum computer.

6. CONCLUSION

We can conclude that that various structural properties of insulating systems have their origin in the nonlinear local electron-particle interaction. It was demonstrated that by removing a ^{12}C atom, replacing it by a ^{13}C atom in the tetrahedral configuration of the diamond, and doing this cycle periodically a linear way, one could get a linear chain of nuclear spins one half which can function as a quantum computer. In particular, the linear chain of paramagnetic atoms of spin one half became a decent mathematical model to make investigations of quantum gates, quantum algorithms, and decoherence which could be applied to other quantum computers. The foundations of Statistical Mechanics and Thermodynamics structure an underlying microscopic theory, namely Quantum Mechanics. In regular Statistical Mechanics probabilities, assumption esteems, differences and higher snapshots of observables are figured through ensemble averages.

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