# Special Topic Paper

Scientist: Hans Bethe

# Paper: On the Theory of Metals

**I. Eigenvalues and Eigenfunctions of a Linear Chain of Atoms**

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# Introduction

Hans Bethe was a German-American physicist who made seminal contributions to nuclear physics, astrophysics and solid-state physics and won the Nobel Prize in physics for his work on the theory of stellar nucleosynthesis.

His other works include Bethe formula which involves treatment of collision problems using a Fourier transform. His biggest contribution to solid-state physics is Bethe Ansatz, a method for finding the exact solutions for the eigenvalues for the eigenvalues and eigenvectors of certain one-dimensional quantum many-body models. This is the celebrated paper titled “On the Theory of Metals” on which I am writing my special topic paper. This paper, although mathematically very rigorous, gives us a clear idea about incorporating many body physics into solid-state physics and subsequently extracts all the exact solutions for a system of linear atomic chains. This marked an amazing development in understanding the metals in the sense that in previous model, the calculations were mainly single conduction, while electron-electron interactions were hardly taken into account. But Bethe resolved all these issues in this paper. I will mainly give a brief discussion some of the mathematical formulations and their results in this paper. Next, I will talk some of the developments in this field and report some of the future directions as well.

# Theory of Metals: Other Theories and Issues

Metals have been always at the center of interest of physicists because of the wide use in many aspects of condensed matter physics. The theory of metal is by far, one of the most intriguing topics. In the previous theories given by Sommerfeld or Bloch, only the movement of single conduction has been taken into account while electron-electron interaction has been ignored. In other words, it has not been treated as a many-body physics problem. Although, the single conduction treatment has been effective in describing various phenomena in metals, yet it cannot completely describe ferromagnetism and superconductivity [1]. In addition, the calculation of cohesion forces has been impossible in this scheme. This is why, a new theory was needed to resolve all these theoretical obstacles and give us a clear view about the physics of metals.

As we know that the exchange forces between electrons are relevant for the size of the first of the first-order terms in the perturbation series for the energy. And order of magnitudes of these forces are same as the zero-point energy of the electron gas. This phenomenon is anomalous in the sense that here the movement of individual electrons is considered to be more important than the interaction energy. As a solution, Slater and Bloch considered the interaction as perturbation, same as London-Heitler approximation for molecules [2][3]. But the difference is that while Slater calculated for non-ferromagnetic materials, where interaction term $J < 0$ (antiferromagnetic) in London-Heitler method [4]. Slater's technique gives us an effective insight about calculation of the ground states of such metals. On the contrary, Bloch took $J > 0$ (ferromagnetic). The problem with this method was that he found too many eigenvalues. That is where Bethe's calculation comes handy to find all the eigenstates and eigenvalues correctly.

# Bethe's Method to Find Eigenstates of Metals

Basically, Bethe's method is an upgrade of Bloch's calculations. His aim was to demonstrate a method for the calculation for all the eigenvalues of the metals with arbitrary precision in a linear chain of atoms. In this method, he obtained solutions of a different type in a way that total number of eigenvalues is the exactly correct one.

Let us consider a linear chain of N identical atoms. Each atom has, apart from closed shells, one conduction electron in s-orbit. Also, we disregard the interaction between them for the simplicity of the problem. We consider the spins to be either pointing to right or left directions. As by simple math, we that

if we have N identical atoms with spins either in right or left directions, then the degeneracy of the system is $2^N$. To describe the problem, we describe the state of the atom by indicating for which atoms, the spin points to the right. We assume that atoms with numbers $m_1, m_2, \dots, m_r$ are pointing to the right. Let the corresponding eigenfunction is $\psi(m_1, \dots, m_r)$. The correct eigenfunction is

$$\Psi = \sum_{m_1,\dots,m_r} a(m_1, \dots, m_r)\, \psi(m_1, \dots, m_r)$$

Here, $1 \leq m_1, m_2, \dots, m_r \leq N$ and $m_1 < m_2 < \cdots < m_r$

Calculating the matrix elements of the interaction energy with respect to the states defined by $m_1, m_2, \dots, m_r$ we find the diagonal elements and off-diagonal elements. If the spin distribution $m_1, m_2, \dots, m_r$ has $N'$ neighboring pairs of parallel spins, then

$$W_{m_1,m_2,\dots,m_r} = E_0 - N'J$$

Here, $E_0$ = interaction due to the charged clouds of atoms. $J$ is the London-Heitler exchange integral between neighboring atoms which is ignored for non-neighboring atoms.

Also, the off-diagonal elements occur between two states which can be obtained from one-another by exchanging two nearest-neighbor spins with opposite spins. All these integrals give $-J$.

We acquire the following equations in this mechanism,

$$2\epsilon a(m_1, \dots, m_r) + \sum_{m_1',\dots,m_r'} [a(m_1', \dots, m_r') - a(m_1, \dots, m_r)] = 0 \qquad (1)$$

Where

$$2\epsilon J = e - E_0 + NJ \qquad (2)$$

e is the total perturbed energy to first approximation and $m_1', \dots, m_r'$ is the new distribution after exchanging neighboring spins. This must satisfy the periodic boundary condition

$$a(m_1, \dots, m_i, \dots, m_r) = a(m_1, \dots, m_i + N, \dots, m_r)$$

We can verify this for the case where r = 1 in the following paragraph,

Consider the N atom atomic chain where only the m-th atom spin is oriented to the right. As it must satisfy the periodic boundary condition mentioned above. Then we have from (1)

$$2\epsilon a(m) + a(m-1) + a(m+1) - 2a(m) = 0$$

If,

$$a(m) = e^{ikm}$$

Then we obtain,

$$2\epsilon + e^{ik} + e^{-ik} - 2 = 0$$

$$\epsilon = 1 - \cos k$$

From periodicity, we have

$k = \frac{2\pi}{N}\lambda$ , where $\lambda$ is an integer

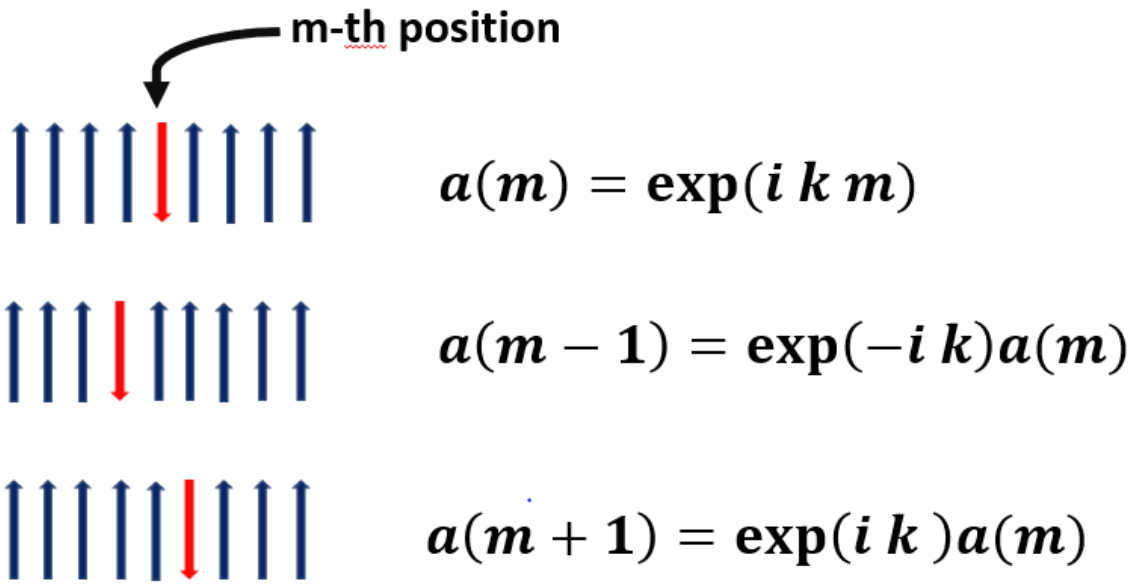



**Fig 1**: N-atom linear chain with only one opposite spin at m-th place

For r = 2, we have two distinguished cases, either the two right-spins are separate from each other in which case the same calculation gives

$$-2\epsilon a(m_1 m_2) = a(m_1 + 1, m_2) + a(m_1 - 1, m_2) + a(m_1, m_2 + 1) + a(m1, m_2 - 1) - 4a(m_1, m_2) \quad (3)$$

If they are nearest neighbors, we have

$$-2\epsilon a(m_1, m_1+1) = a(m_1-1, m_1+1) + a(m_1, m_1+2) - 2a(m_1, m_1+1) \qquad (4)$$

Using constants $c_1, c_2, f_1, f_2$ we have,

$$a(m_1 m_2) = c_1\, e^{i(f_1 m_1 + f_2 m_2)} + c_2\, e^{i(f_2 m_1 + f_1 m_2)}$$

$$\epsilon = 2 - \cos f_1 - \cos f_2 \qquad (5)$$

Setting $c_1 = e^{\frac{i\varphi}{2}}, c_2 = e^{-\frac{i\varphi}{2}}$ and using the same periodic boundary condition, we have

$$N f_1 - \varphi = 2\pi\lambda_1$$

$$N f_2 + \varphi = 2\pi\lambda_2$$

Where $0 \le \lambda_1, \lambda_2 \le N-1$ and we have $k = f_1 + f_2 = \frac{2\pi}{N}(\lambda_1 + \lambda_2)$. But this method does not yield sufficiently many solutions, contrary to Bloch's suggestion. If the wave numbers $f_1, f_2$ are complex conjugate to each other the there can be N-1 solutions. Let $f_1 = u - i\,v, f_2 = u + i\,v$. Then we have also $\varphi = \psi + i\chi$ where $\psi = \pi(\lambda_2 - \lambda_1)$ and $\chi = Nv$.

From first approximation we have, $e^{-v} = \cos u$ and $\epsilon = \frac{1}{2}(1 - \cos 2u)$ (6)

From second approximation, $v = v_0 + \epsilon$ and $\epsilon = \tan^2 u e^{-\chi + i\psi}$ (7)

In the end we have, $\epsilon = \pm \tan^2 u e^{-(N v_0)}$ (8)

If $u \ll 1$, then $\cos u \sim 1$, $v_0 \ll 1$ and $v_0 = \frac{1}{2}u^2$

But if $u \sim 0\left(\frac{1}{\sqrt{N}}\right)$, then $N v_0$ is finite and $v = v_0 + \epsilon < 0$ and the scheme diverges. As a result, there is no solution with two complex conjugate wave numbers.

To obtain this solution, in the same scheme where for small k, $f_1$ does not increase, we get some additional solution with real or complex wave numbers.

$$a(m_1, m_2) = \begin{cases} 0, & m_2 \neq m_1 + 1 \\ (-1)^{m_1}, & m_2 = m_1 + 1 \end{cases} \qquad (9)$$

Here, all the eigenvalues $\epsilon$ with two complex conjugate wave numbers are smaller than all eigenvalues with the same wave number k and real wave numbers. The corresponding energy to first order lies deeper than all solutions with real wave numbers in ferromagnetic case and higher in antiferromagnetic case.

For the generalized case, with r spins in right direction, we assume

$$a(m_1, \dots, m_r) = \sum_{P=1}^{r!} \exp(i \sum_{k=1}^{r} f_{Pk} m_k + \frac{1}{2} \sum_{k<l}^{r} \varphi_{Pk,Pl}) \qquad (10)$$

$$\epsilon = \sum_{k=1}^{r} (1 - \cos(f_k)$$

P is some permutation of numbers 1, 2, …, r and Pk denotes the number that this permutation puts n place of k. Proceeding with this scheme, we find the number of solutions with real $f_i$ is found to be $\binom{N-r+1}{r}$ which is much smaller than the required number of solutions $\binom{N}{r}$.

As a resolution to tackle this problem we assume that there are two wave complexes with n and p (>n) where $p = r - n$. Hence, we investigate what number of solutions can be obtained this way. Then phase $\varphi$ becomes very important. If we go ahead with this assumption and do the calculations as we did for all the aforementioned cases, we find the total number of solutions to be,

$$z(N, r) = \frac{N-2r+1}{N-r+1} \binom{N}{r} \qquad (11)$$

As we see that this indeed gives all the solutions of the problem.

# Applications and Developments

Bethe ansatz has played a major role in many developments of modern solid-state physics. One application of it is the mean-field theory treatment of ferromagnetic Ising model. Bethe-Peierls approximation reduces the problem of computing partition functions and expectation values. It is an improvement over Bragg-Williams method. Bethe-Peiers approximation takes into account specific short-range orders, which gives more correct values of specific heat and furthermore, the critical exponents [5]. Thus, Bethe's solution has been instrumental in the rise of modern condensed matter physics. Also, from the experimental point of view, there has been many experiments involving ferromagnetism which are directly connected to Bethe's theory [6]. As I work on optics experiments at Richard Averitt's lab, my main topic of interest is light matter interaction which I probe using various time-resolved techniques such as THz time-domain spectroscopy, optical pump-THz probe, mid-IR pump-broadband plasma THz probe, high field THz pump-THz probe spectroscopies. I will report a previous THz control of magnon in antiferromagnetic NiO. In NiO, there lies a magnon mode at 1 THz which can be probed by a magneto-

optic Kerr effect (MOKE) probe. Basically, Kerr effect is the change of light polarization due to the magnetism in a material when a light pulse is passed through it [8].

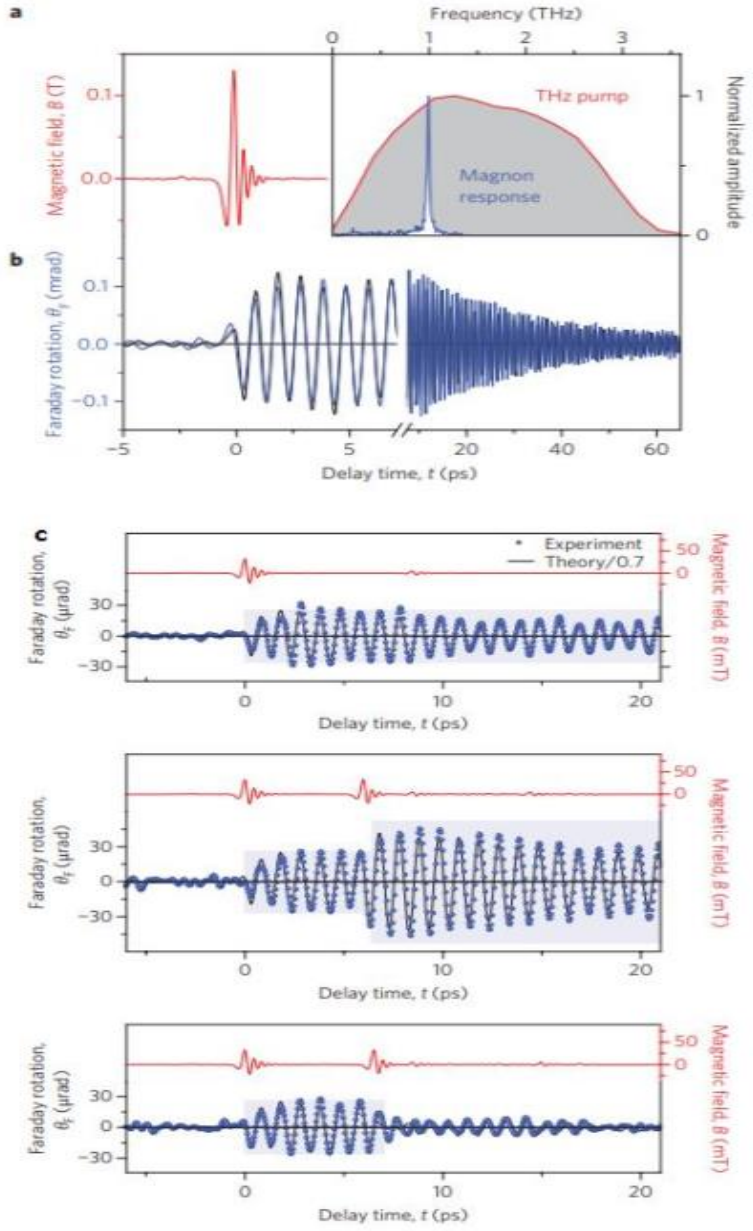
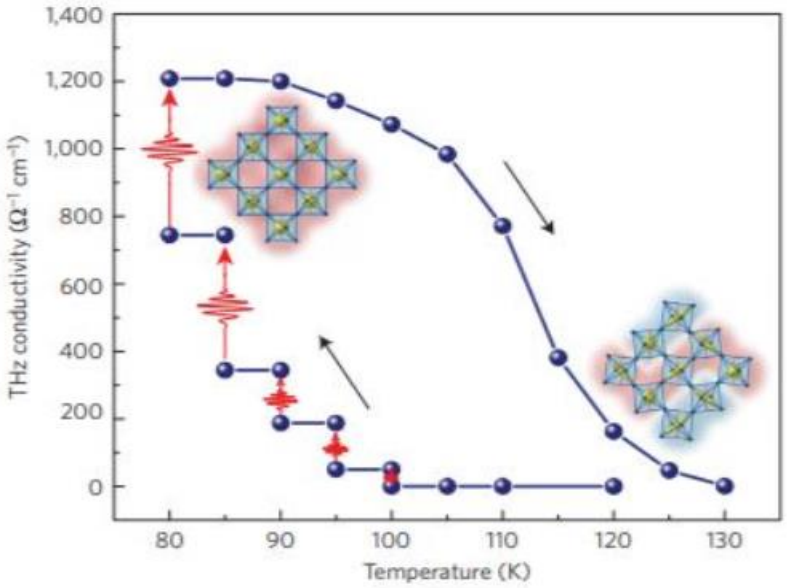



**Fig 2**: Ultrafast coherent control of magnons in NiO

In figure 2, we can see that the magnon mode is at 1 THz for a single-cycle pulse which creates the oscillation of the Faraday rotation angle $\theta_F$. $\theta_F$ denotes the change of polarization which is a signature of the magnetism in the material. Now, if we send multi-cycle pulses with a time-delay between them,

then as per the principle of constructive and destructive interference, the magnon mode can be switched on/off or enhanced/suppressed. This paves the way to the ultrafast photocontrol and switching of magnetism.

Previously, THz induced metal-insulator transition has been reported in $V_2O_3$ metamaterial [7]. Strongly correlated transition metal oxide $La_{0.67}Ca_{0.33}MnO_3$ has been reported to have shown photoinduced hidden metallic phases [9]. Here, a single-shot pulse initiates this metallic phase by activating local charge excitons that mediates magnetic-lattice couplings and this phase stabilizes the metallic phases. As a continuation of this work, in Averitt group, I am trying to explore some of the hidden photo-switchable magnetic phase in the thin-film samples of the same material. For this, I am using the resonant soft X-ray scattering facilities of Advanced Photon Source (APS) of Argonne National




Lab. Some new exciting data are on the way.

**Fig 3**: Photoinduced hidden metallic phases in LCMO. When sample is heated, the THz conductivity decreases smoothly while with decreasing temperature, the conductivity increases in a step-like fashion.

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