FINAL SCIENTIFIC REPORT

E.O.A.R. GRANT N° 63-51.

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Faculté des Sciences
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The accompanying list of publications presents a rather complete picture of the research activities of the Brussels group sponsored by the EOAR under Grant 63-51. We will refer to these publications by their numbers in the text.

The theoretical interests of the principal investigators evolved considerably in the course of the contract, from primary interest in the many body problem to primary interest in particle physics. This report will be divided into two sections : the first reviews our work on the namy body problem and the second on problems of particle physics and general relativity.

Many Body Problem.

Our first research project undertaken in the course of the contract was that of a theory of freezing and melting (1,2). The principal theoretical remark was the characterization of the solid phase in terms of a restricted ensemble of broken symmetry. The analogy with ferromagnetism makes the idea clear. The condensed phase of a ferromagnet is characterized by an order parameter which effectively limits the number of accessible states to only those which have this order parameter. For example for spin 1/2, the magnetic phase is characterized by a given value of the difference of the number of up and down spins. The question is how to characterize the solid state by an analogous order parameter. The answer is as follows. What characterizes a liquid is that the single particle density is everywhere constant

$$\langle \rho(\underset{\sim}{r}) \rangle = \text{constant}$$

whereas in a solid $\langle \rho(\underset{\sim}{r}) \rangle$ is a periodic function in the lattice

$$\langle \rho(\underset{\sim}{r}) \rangle = \sum_{\underset{\sim}{G}} \hat{\rho}_{\underset{\sim}{G}} e^{i \underset{\sim}{G} \cdot \underset{\sim}{r}} \quad ; \quad \underset{\sim}{G} = \text{set of reciprocal lattice vectors.}$$

The order parameters are $\hat{\rho}_G$ and the effective parts of many body configuration space are restricted though the conditions

$$\sum_{i=1}^{N} e^{i \underset{\sim}{q} \cdot r_i} = N \delta_{\underset{\sim}{q}, \underset{\sim}{G}} \hat{\rho}_{\underset{\sim}{G}}$$

For a liquid only $G = 0$ is admissible and $\hat{\rho}_0 = 1$. For example if $\hat{\rho}_{\underset{\sim}{G}}$ is small it is a simple matter to show that the liquid solid ratio of many body configuration space is

$$e^{-N \sum |\hat{\rho}_{\underset{\sim}{G}}|^2/2}$$

Once this remark is made it is quite easy to get a molecular field approximation for the solid phase. In fairly good approximation one gets

$$\varphi(\underset{\sim}{r}) = C \sum_{\substack{\underset{\sim}{R} \text{ on near} \\ \text{neighbors}}} e^{-\beta \int v_{att}(\underset{\sim}{r}-\underset{\sim}{r}')\, \varphi(\underset{\sim}{r}'-\underset{\sim}{R}_j)}$$

where

$$\rho(\underset{\sim}{r}) = \sum_{\underset{\sim}{R}_j} \varphi(\underset{\sim}{r}-\underset{\sim}{R}_j)$$

v_{att} is the attractive force between the particles and φ is confined to a unit cell. This equation was solved numerically in (2) and yielded a very good equation of state for the solid. However, it was subsequently found that certain thermal properties such as specific heat were not adequately approcimated in this way. Present calculations are being carried out which allow for configurations in which the cores of particles may possibly touch. These are much more complicated to evaluate, but present indications are that the required effects do indeed come about by this more refined version yielding quite an accurate estimate of the melting point. We also add, that at low temperatures, the cluster expansion of which the molecular field is the leading approximation yields the standard phonon theory. It is not yet clear how this generalizes to high temperatures.

We now turn to a discussion of (3) and (4). In the theory of superconductivity, it was pointed out by Thouless that one should expect phase transition precursor phenomenom of the same variety as observed in condensation or magnetism. This is marked by a divergent specific heat. In the magnetic and condensation cases, one also has divergent response functions, the susceptibility and compressibility respectively. In (3) it was shown that the physical response function - the diamagnetic susceptibility developsasingularity which is related to that of the specific heat. However, for dynamical reasons the diamagnetic singularity is much more mild (like [constant + $\sqrt{T-T_c}$] rather than $\sqrt{T-T_c}$). In (3) it was shown how to cast the temperature dependent BCS theory of superconductivity into a form which was identical to that of the Weiss theory of ferromagnetism. Thereupon, one could readily understand, in analogy to the magnetic case, how by going into a condensed phase the system accommodates itself to the singularities discussed above. The parallel formalisms of band ferromagnetism and superconductivity are set out clearly in paper 3.

In 4, we turned to more general considerations, related to what is called the Goldstone theorem. In all phase transitions, some symmetry principle characteristic of the hamiltonian is broken in the condensed phase though the establishment of an order parameter. When the group of symmetry operations is continuous, a collective mode, whose frequency goes to zero as its wave length goes to infinity, is established. These are the phonons in solids (group of translations), spin waves in magnets (group of rotations), Anderson modes in superconductors, etc... However it has not been generally realized that these modes are related to dynamical response functions and sum rules, in different ways according to the nature of the group in question. In 4, it is shown that, whereas in a ferromagnet with isotropic exchange coupling, the nature of the collective modes is completely determined by symmetry alone, the same is not true in a superconductor. This is because the latter obeys a much more restricted set of symmetry operations. Gauge invariance is the group that is broken in the superconductor and this corresponds in the ferromagnet to rotational invariance about one axis only. As a consequence, the nature of the collective mode arises through the interplay of both dynamical and symmetry considerations for all wave lengths but infinity.

The relationship among symmetry considerations, dynamical sum rules, and equations of motion is the essential theme of (4). A simpler and deeper understanding of the nature of the Anderson modes in a superconductor emerges.

As a result of research on phase transitions and ferromagnetism over the past few years, a certain point of view emerged. Because of our steady inclination towards a change in research interests, it was deemed appropriate to the moment to set out this point of view in review form before retiring, at least momentarily, from the field. These reviews are in (5), (6), (7) and (9).

In reference 8, the band theory of ferromagnetism was developed. In particular the nature of spin waves is explored taking into account the Bloch nature of the single particle states. In the limit of infinitely heavy effective mass, it was shown how the Heisenberg model spin waves are recovered. However, a very difficult problem still remains which concerns the complete theory of how a heavy mass band does indeed become localized. If the band picture is essentially correct, then the results of (8) apply. In particular, it was shown that there are two contributions to the spin wave frequency, one from the effective mass of the band and the other from overlap of Wannier functions. In the limit of heavy mass, the latter dominates. There is still much work remaining in this difficult subject and we are contemplating a return to it some time in the future. Metallic ferromagnetism is a long way from being understood.

Reference (10) provides an interpretation of a remarkable experiment of Känzig et. al. A solution .01% to .1% KOH in KCl causes a shift in dielectric constant from 4 to 10 in a temperature range from about 1°K to 10°K. The dielectric constant shows a marked peak in this range at a temperature proportional to the concentration. It was observed by us that an analogous phenomenom occurs in the inverse susceptibility function of dilute transition paramagnetic metallic ions dissolved in Cu, Ag, Au. In the latter class of substances, the interpretation was given in terms of an exchange force due to indirect exchange through the condition electrons. Because this force oscillates, one gets a kind of random antiferromagnetic transition. A correlation zone is established in which a few spins are antiferromagnetically correlated to a given spin. It was suggested that because there is an oscillatory behavior of the dipole-dipole force in angle the OH^- system in KCl behaves quite ana[illegible]ously, giving rise to a random antiferroelectric transition. Preliminary optical experiments of Lüty are in accord with this interpretation, as well as order of magnitude estimates of the temperature of the peak in dielectric constant. This problem has since attracted a deal of attention in the literature and it will be of interest to watch its development.

In reference (11), it was shown that if the sound velocity of a metal has as its primary contribution, the bulk modulus due to core repulsion then the BCS one phonon exchange mechanism effectively reverses in sign and superconductivity is not possible. The bulk modulus of a metal has two components. One is that due of the conduction electrons. As the ions move the electrons follow adiabatically so as to maintain local charge neutrality. This movement is resisted by the zero point compressibility of a Fermi gas. It is thought that this is the primary

mechanism of the bulk modulus in alkali and other open metals such as Al. The other contribution is due to the cores of the ions which repel each other when the core wave functions overlap due to Pauli exclusion principle. This contribution to the bulk modulus dominates in the noble metals, Cu, Ag, Au.
How does this affect superconductivity ? The normal phonon mechanism is that as an electron travels through the lattice it polarizes the ions creating a positive polarization cloud to which another electron is attracted. This cloud lasts for the period of a lattice vibration time. However if there is a core the atoms touch and rebound creating a negative polarization cloud over the second part of the cycle. Clearly, if the repulsion is great it is the second part which dominates and causes an effective repulsion. These ideas were put into the mathematical machinery of the dynamical BCS theory along with a dielectric constant containing all the required effects. It was estimated that if 60% the bulk modulus is due to core effects, superconductivity is suppressed. An interesting confirmation has recently come to light. Among the rare earths only La and Lu are not paramagnetic and hence are available for superconductivity. La is a superconductor (it has no 4f electrons) and Lu is not (it has a filled 4f shell). It is estimated experimentally that the velocity of sound is three times greater in Lu than in La and hence a factor of ten in bulk modulus. Since the crystal structures as well as external electronic structures are identical, the difference can only be in core moduli. Therefore Lu has at least 90% of its bulk modulus due to the core. By our estimates, we then expect Lu not to be a superconductor, as is indeed the case.

In (12) the formal expansion for an N boson gas was derived. This is a very subtle problem because in the Bose Einstein condensed phase, the occupation of the ground state N_o is macroscopic. It is shown however that this problem can be met when the theory is expressed in terms of the fluctuations of N_o. These are all $O(N_o)$ and when incorporated into graphs, allow for a linked cluster expansion of the free energy in which each graph is $O(N)$. An immediate bonus is an extremely compact form which allows one to derive the theory of the Bogoliubov phonon in a straight forward random phase approximation. The Hugenholtz Pines theorem on the inevitable existence of a phonon also drops out straight forwardly.

It was pointed out in (13) that the specific heat of the many boson gas changes its order of singularity from 3rd order in the ideal gas to 2nd order in a Hartree Fock approximation for the real gas. However, the numerical estimates when applied to liquid helium were much too high. Therefore, it was decided to screen out the Hartree Fock estimate by developing a random phase approximation on the high temperature side of the transition temperature (14). Much to our delight, not only did the effect get screened out, but a minimum developed in the specific heat above the critical point in a manner completely reminiscent of experiment. The reason for the minimum can be traced to that part of the dynamical screening which gives rise to the phonon below the transition point. This is an extremely interesting connection which had not hitherto been appreciated. With a choice of parameters which are not unreasonable, it is possible to fit the experimental specific heat above the critical temperature. However, in the immediate critical region, the observed logarithmic singularity cannot be accounted for in the present approximation.

Field Theory and Particle Physics.

Reference 15 is a remark which arose in our study of the rôle of Mach's principle in general relativity. Mach's principle has been interpreted by Sciama and by Weisskopf in terms of an active interpretation of covariance. An acceleration in a terrestial frame is interpreted as an acceleration of the distant stars with respect to us. As a result of this acceleration, gravitational waves are emitted [in Weisskopf's version] and we feel an effective force ma. Newton's equation is that the sum of the forces vanishes. Thus $F - ma = 0$ where F is the local force and ma the force from the distant stars. In order to make the term ma have coefficient unity a condition is placed on the gravitational constant, $K \simeq [\sigma R^2]^{-1}$ where σ is the density of matter in the universe and R its visible radius. That this equation is approximately true is regarded as support for the theory. In his early work Einstein hinted that such ideas could be valid, basing his intuition on the calculations of Thirring of the induced Coriolis and centrifugal forces within a rotating sphere of matter. Later, Einstein retracted this point of view.

In (15) we took this theory to task. In effect the sources of a gravitational field due to accelerating bodies can only be calculated directly in terms of contravariant quantities (the instantaneous velocities). To find the field one must have covariant quantities. This requires knowledge of the space time metric and hence the solution of the problem. Therefore the problem is a self consistent one. When one sets up the mathematical theory, one sees that the resulting equations are simply an expression of general covariance. No condition can possibly arise. The reason why Thirring's calculation is valid, is that his sphere was already imbedded in a (Euclidean) universe. The sense of his calculation is that the perturbation of this metric caused by a rotating massy sphere can be handled in linear fashion since the main contribution to the metric is from the distant stars which always maintain it almost Euclidean. Thus the zeroth order Euclidean metric may be used as an index lowerer in linear approximation. The existence of a local Euclidean metric is presumably the principal content of Mach's principle.

In (16), we have taken advantage of the general covariance of the interaction of a given field interacting with gravity. As a consequence of this covariance, a Ward identity arises. This identity relates the gravitational interaction of a particle to its self energy. This is deeply analogous to the Ward identity and gauge covariance of electrodynamics, where the central point concerns the local conservation of electric current. In the present case, the conservation law is that of energy and momentum. Upon further inquiry as to the physical interpretation of this identity, it turned out to reduce to the principle of equivalence for particles on the mass shell. Thus the Einstein argument is turned around. He argued that the observed principle of equivalence implies general covariance and we prove the converse. In so doing we generalize the principle of equivalence to propagation off the mass shell.

In (17) and (18), we embarked on a program of the study of broken symmetry in field theoretic situations which are characterized by the presence of gauge vector mesons. Two known examples of gauge vector mesons are the photon and the graviton. In these cases the symmetries which are ensured by these mesons (gauge invariance and Lorentz covariance respectively) are not broken. However, in strong interactions, there exists a set of vector mesons which are coupled to conserved currents (or approximately conserved currents). These mesons were in fact predicted by Sakurai using previous theoretical ideas of Yang and Mills and various experimental indications. The difficulty is that these mesons have mass and their theoretical introduction in the light of gauge theories requires zero mass. On the other hand the symmetry of strong interactions is not strict. We therefore directed our attention to the question as to how this breakdown of symmetry affects the masses of the vector mesons. The principal result of our investigation is that some of the vector mesons acquire mass in the presence of broken symmetry. Those which do not acquire mass are coupled to the currents which generate the additive quantum numbers of the Lie group in question. Thus in SU_3 with broken symmetry along the hypercharge axis, the ρ and ω do not acquire mass whereas the K^* does. If this point of view is correct, it is necessary that another mechanism causes the ρ and ω to be massy. One such theory is due to Schwinger. If this turned out to be correct, the utility of our approach would be to obtain mass splitting. Therefore, we would predict that the ρ and ω be degenerate which is indeed the case.

At the present time we are not placing much faith in this idea primarily because of the successes of SU_6 which groups all pseudoscalar and vector mesons together in a supermultiplet. This finds its dynamical counterpart in bootstrap dynamics and it is more in this direction that we are presently leaning. However these vector meson ideas may eventually come into play in the theory of weak interactions where the ever nebulous intermediate vector meson remain an unsolved enigma.

In (19) a mathematical argument was presented which attempts to explain why only those representations of SU_3 which occur naturally are those of its adjoint group ("the eight fold way"). It is postulated that the fundamental group is U_3 and at the same time baryon conservation occurs as a superselection rule. The consequence of the latter requirement is that a gauge angle factorizes in the matrix representations of U_3. The only such representations are also representations of the product group $U(1) \times (SU_3/Z)$. $U(1)$ is the gauge group and (SU_3/Z) is the adjoint group of SU_3, Z being the center. This argument, as all pure group theoretic arguments, is obviously pure phenomenology. Our ultimate understanding must lie in dynamics.

In (20), we have begun to formulate a dynamics of particles. This is based on the bootstrap idea of Chew. It is appropriate that our report finish on this paper since it is this work which is expected to dominate our attention through the next contract period.

Our principal notion is to express all interesting quantities in terms of vacuum fluctuations. These fluctuations generate other fluctuations as well as themselves through self consistent equations. In a certain approximation [ladder approximation], these equations resemble strongly the bootstrap equations with the very important difference that they now converge. A further mutilation can be affected to make the equations identical to those of the N/D method, but this is neither physically well motivated, nor justified.

We outline the method on a simple example. Suppose there exists a two body bootstrap. By this we mean a bound state of two particles arises through a meson exchange which bound state has the same quantum numbers as the meson which exchanges. Then the bound state can do the exchanging as well. Our bootstrap effectively equates the propagator of the bound state to that of the meson. In ladder approximation, the equation takes the form

$$K_2 - SS = \int SS\left[S^{-1}S^{-1}(K_2 - SS)S^{-1}S^{-1}\right]K_2 \qquad 1)$$

where S is the single particle propagator, assumed given, and K_2 the two body propagator. One solution is $K_2 = SS$ or no interaction. In order for a non trivial solution to arise one needs a bound state. Then $K_2 - SS$ has singular behavior

$$K_2 - SS = \frac{S\Gamma(p)S \; S\Gamma(p')S}{P^2 - M^2} \qquad 2)$$

where p and p' are the relative incoming and outgoing momenta. P is the total momentum and M the mass of the bound state. In this way 1) becomes

$$\Gamma(p) = \int d^4k \; \frac{\Gamma(P+p+k)\,\Gamma(P-p-k)}{(p-k)^2 - M^2}\, S(P+k)\,S(P-k)\,\Gamma(k)$$

In the approximation $\Gamma(p)$ = constant, this equation, plus a residue condition (normalization of the bound state wave function), recovers the usual bootstrap theory. It has a logarithmic divergence. In our version, convergence is assured and we have a preliminary estimate that asymptotically $\Gamma(p) \to [\log p]^{-1}$

We have generalized this procedure and presented a variational principle from which the equations may be derived.

At the present time, we are trying to enhance our fundamental understanding of the theory while at the same time we are proceeding with applications. Among these are :

a) an attempt to produce a reasonable solution

b) the expression of the reciprocal bootstrap in this new language

c) group theoretical implications

d) connections with field theory, in particular a discussion of the dilemma posed by Haag's theorem and ghost states.

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