Further experimental results and a theoretical discussion will be published at a later time.

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Unified Theory of Interacting Bosons

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(Received January 25, 1957)

RECENT work has contributed to the understanding of properties of helium II. Yet there is room for a unified theoretical approach to the problem of interacting bosons for both solid and liquid states. In particular the liquid is like the solid as regards cohesive energy and packing. One is interested in computing these from first principles, as well as in the connection between the vibration spectrum of the solid and the excitation spectrum of the liquid, the elucidation of the liquid solid transition under pressure, scattering of excitations, etc. The treatment of these diverse phenomena requires construction of wave functions for the system of interacting bosons, which are reasonably accurate and simple, from a unified point of view. In the following we report on one such unified approach, based on an elementary physical picture. The procedure is an outgrowth of the small-oscillation theory of the interaction of a particle and a scalar field.[1]

The Hamiltonian for a system of bosons of mass M with the two-body interaction potential V (thus neglecting the detailed electronic structure of the atoms) will be written in the formalism of second quantization:

$$H=\frac{\hbar^2}{2M}\int\nabla\psi^\dagger\cdot\nabla\psi d^3x+\tfrac{1}{2}\int\int\psi^\dagger(\mathbf{x})\psi^\dagger(\mathbf{x}')\times V(\mathbf{x}-\mathbf{x}')\psi(\mathbf{x})\psi(\mathbf{x}')d^3xd^3x',$$

where $\psi(\mathbf{x})$, $\psi^\dagger(\mathbf{x})$ are operators satisfying the Bose-Einstein commutation rules such as $[\psi(\mathbf{x}),\psi^\dagger(\mathbf{x}')]=\delta(\mathbf{x}-\mathbf{x}')$. Associated with H are the Heisenberg equations of motion for the time-dependent operators $\psi(\mathbf{x},t)$ and $\psi^\dagger(\mathbf{x},t)$:

$$\frac{\partial\psi}{\partial t}=\frac{i}{\hbar}[H,\psi];\quad\frac{\partial\psi^\dagger}{\partial t}=\frac{i}{\hbar}[H,\psi^\dagger].$$

We may consider H as governing the motion of a nonlinear, three-dimensional classical wave field. The commutation rule for the canonically conjugate variables,

$$q(\mathbf{x})=(\psi+\psi^\dagger)(\hbar/2)^{\frac{1}{2}}\quad\text{and}\quad p(\mathbf{x})=(\psi-\psi^\dagger)(\hbar/2)^{\frac{1}{2}}i,$$

is replaced by the Poisson-bracket relation. $\hbar$ is retained insofar as it enters in the kinetic energy of the field, describing the DeBroglie wave character of the associated particles. The classical equation of motion has special, exact, separable solutions of the form $\psi=f(\mathbf{x})\times\exp(-iEt/\hbar)$, where $f(\mathbf{x})$ and E are obtained from the nonlinear eigenvalue problem

$$Ef=-\frac{\hbar^2}{2M}\nabla^2f+\int V(\mathbf{x}-\mathbf{x}')|f(\mathbf{x}')|^2d^3x'\cdot f(\mathbf{x}),$$

$$\int|f|^2d^3x=N.$$

We note that there is always a solution of uniform density, namely,

$$f(x)=\left(\frac{N}{L^3}\right)^{\frac{1}{2}},\quad E=\frac{N}{L^3}\int V(\mathbf{x})d^3x.$$

But if $V(\mathbf{x})$ is negative in some region of space, there may be other solutions, such as a periodic solution with E lower than for the uniform solution. In the classical theory there are solutions in the vicinity of each exact solution in which the field carries out small oscillations. Writing $Q=(\varphi+\varphi^\dagger)(\hbar/2)^{\frac{1}{2}}$, $\psi=e^{-iEt/\hbar}[f(\mathbf{x})+\varphi(\mathbf{x},t)]$ and linearizing the equation of motion, we obtain

$$+\hbar^2\ddot{Q}=+\frac{\hbar^2}{2M}\left(\nabla^2-\frac{\nabla^2f}{f}\right)\left\{-\frac{\hbar^2}{2M}\left(\nabla^2-\frac{\nabla^2f}{f}\right)Q(\mathbf{x},t)+2f\int V(\mathbf{x}-\mathbf{x}')f(\mathbf{x}')Q(\mathbf{x}')\cdot d^3x'\right\}.$$

The character of the oscillation spectrum depends on $V(\mathbf{x})$ and on the underlying solution $f(\mathbf{x})$. For the uniform solution one obtains Bogolyubov's[2] spectrum yielding phonons for long wavelengths, free-particle behavior for short wavelengths.

The classical analysis may be used to find eigenfunctions by noting that three elementary canonical transformations are involved; a time-dependent one introducing a phase, a linear shift $\psi\rightarrow f+\psi$, and a normal-mode transformation. These are then simple unitary transformations in the quantum theory, the first adding a term to H. We are thus led to the set of approximate eigenfunctions,

$$\Phi=\exp(S_2)\cdot\exp(S_3)\Phi_0(\cdots N_\mathbf{k}\cdots).$$

Φ_0 are eigenfunctions of the number operators $N_\mathbf{k}=\psi_\mathbf{k}^\dagger\psi_\mathbf{k}$. [$\psi_\mathbf{k}$ is a Fourier component of $\psi(\mathbf{x})$.]

$$S_2=\int\{f(\mathbf{x})\psi^\dagger(\mathbf{x})-f^*(\mathbf{x})\psi\}d^3x,$$

and S_3 is a quadratic form in ψ, $\psi^\dagger$. From the set we construct eigenfunctions of the total number and

momentum operators by applying projection operators and we form an orthogonal set. For the uniform solution,

$$S_3=i\sum_{k_z>0}(L_k\psi_k^\dagger\psi_{-k}^\dagger+\text{cc}).$$

Noting that the method has a variational aspect, L_k need not be taken from the small-oscillation analysis but may be freely chosen to describe average large-amplitude effects. We obtain improved ground-state energy and single- and multiple-excitation spectra.

For the solid-like solution, $f(\mathbf{x})$ is periodic. We expand $\psi=\sum a_k^\alpha\varphi_k^\alpha(\mathbf{x})$, where $[a_k^\alpha,a_l^{\dagger\beta}]=\delta_{\alpha,\beta}\delta_{k,l}$. Here φ_k^α are a complete set of Bloch tight-binding orbitals for which $\mathbf{k}$ takes on values in the first zone; α labels the zones. For $\mathbf{k}=0$ the φ_k^α are periodic; for $\mathbf{k}\neq0$ they have a modulating factor. Thus if the linear shift is performed only for the a_0^α, the ground-state expectation values of physical quantities are periodic. If shifts for $\mathbf{k}\neq0$ are required, the expectation value of the correlation operator ceases to be periodic.

The connection between the two solutions is seen by referring to the quantum problem of a particle in a well with several minima (or stationary points). Because of the tunnel effect, good approximate wave functions are superpositions of functions appropriate to the classical separate regions. By analogy, we take

$$\Psi=\mathcal{P}(N)\mathcal{P}(\mathbf{P})\int G(R)\exp S_2(R)\cdot\exp S_3(R)\Phi(\cdots N_k\cdots)dR.$$

The coefficients of the linear and quadratic forms depend on R; the integral over R includes a discrete sum; $\mathcal{P}(N)$ and $\mathcal{P}(\mathbf{P})$ are projection operators of total number of particles N with total momentum $\mathbf{P}$. Detailed calculations of properties of liquid and solid helium based on the present approach are in progress.

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Microscopic Theory of Superconductivity*

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(Received February 18, 1957)

SINCE the discovery of the isotope effect, it has been known that superconductivity arises from the interaction between electrons and lattice vibrations, but it has proved difficult to construct an adequate theory based on this concept. As has been shown by Fröhlich,[1] and in a more complete analysis by Bardeen and Pines[2] in which Coulomb effects were included, interactions between electrons and the phonon field lead to an interaction between electrons which may be expressed in the form

$$H_I=\sum_{k,k',s,s'}\frac{\hbar\omega|M_\kappa|^2}{(E_k-E_{k'})^2-(\hbar\omega)^2}\times c^*_{k'-\kappa,s'}c_{k',s'}c^*_{k+\kappa,s}c_{k,s}+H_{\text{Coul}},\quad(1)$$

where $|M_\kappa|^2$ is the matrix element for the electron-phonon interaction for the phonon wave vector κ, calculated for the zero-point amplitude of the vibrations, the c's are creation and destruction operators for the electrons in the Bloch states specified by the wave vector $\mathbf{k}$ and spin s, and H_{Coul} represents the screened Coulomb interaction.

Early attempts[3] to construct a theory were based essentially on the self-energy of the electrons, although it was recognized that a true interaction between electrons probably played an essential role. These theories gave the isotope effect, but contained various difficulties, one of which was that the calculated energy difference between what was thought to represent normal and superconducting states was far too large. It is now believed that the self-energy occurs in the normal state, and results in a slight shift of the energies of the Bloch states and a renormalization of the matrix elements.

The present theory is based on the fact that the phonon interaction is negative for $|E_k-E_{k'}|<\hbar\omega$. We believe that the criterion for superconductivity is essentially that this negative interaction dominate over the matrix element of the Coulomb interaction, which for free electrons in a volume Ω is $2\pi e^2/\Omega\kappa^2$. In the Bohm-Pines[4] theory, the minimum value of κ is κ_c, somewhat less than the radius of the Fermi surface. This criterion may be expressed in the form

$$-V=\langle-(|M_\kappa|^2/\hbar\omega)+(4\pi e^2/\Omega\kappa^2)\rangle_{\text{Av}}<0.\quad(2)$$

Although based on a different principle, this criterion is almost identical with the one given by Fröhlich.[1,3]

If one has a Hamiltonian matrix with predominantly negative off-diagonal matrix elements, the ground state, $\Psi=\sum\alpha_j\varphi_j$, is a linear combination of the original basic states with coefficients predominantly of one sign. A particularly simple example is one for which the original states are degenerate and each state is connected to n other states by the same matrix element $-V$. The ground state, a sum of the original set with equal coefficients, is lowered in energy by $-nV$. One of the authors made use of this principle to construct a wave function for a single pair of electrons excited above the Fermi surface and found that for a negative interaction a bound state is formed no matter how weak the interaction.[5]

Because of the Fermi-Dirac statistics, difficulties are encountered if one tries to apply this principle directly to (1). Matrix elements of H_I between states specified by occupation numbers (Slater determinants) in general may be of either sign. We want to pick out