PHYSICAL REVIEW B VOLUME 40, NUMBER 5 15 AUGUST 1989-I

Nonanalytic behavior in the band theory of semiconductors

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(Received 5 May 1989)

The nonanalytic behavior of the ground state of a two-band semiconductor as a function of the Coulomb coupling constant e^2 is demonstrated. A power series in e^2 is shown to be, at best, an asymptotic expansion. This casts serious doubt on the application of the perturbative many-body technique to semiconductor physics.

In relativistic quantum electrodynamics it is well known that the perturbation series expansion in powers of the coupling constant e^2, on which the Feynman diagram technique is based, is only an asymptotic series. As first pointed out by Dyson,[1] there is a singularity lurking in the series, making its damaging influence felt, however, only in very high orders $N \gtrsim 1/\alpha = 137$. In the physics of the electron gas in a metal, Pendry[2,3] was the first one to mention that, in the so-called ladder diagrams involving multiple scattering of two electrons, the corresponding expansion in powers of the Coulombic e^2 had poles in the complex e^2 plane.[4] The poles move as a function of energy E and the emergence of each pole at a negative energy signifies a bound state. Only for $|E| > 0.5$ Ry associated with a reduced mass of 0.5 m would all the poles lie outside the circle $e^2 = e_0^2$, e_0^2 being the physical value of the Coulomb coupling constant, leading then to the convergence of the series. This result constitutes the starting point from which a new treatment of electron correlation at metallic densities is developed.[2]

In this Rapid Communication we would like to point out that, in the band theory of the semiconductor, a singularity in the e^2 power series may also exist. This singularity, similar in nature to Dyson's, renders the power series an asymptotic one, and is, in a way, related to the formation of excitons as bound electron-hole pairs.

Let H_0 represent the Hamiltonian of an electron interacting with the lattice, leading as usual to the single-particle Bloch states in various energy bands. In a simple two-band model, the ground state of a semiconductor consists of a filled valence band and an empty conduction band, the two bands being separated by a band gap, E_{gap}.

The question now facing us is, what becomes of this ground state of H_0 when the Coulombic coupling $e^2 \equiv Z$ among the electrons is turned on? Does a convergent power series in Z exist? If $Z > 0$, as is the physical case, the production of an electron-hole pair by exciting an electron from the valence band to the conduction band would cost at least E_{gap} in energy. This is partly compensated, however, by the attraction between the electron lifted to the conduction band and the hole that is left behind in the valence band. The resulting bound electron-hole pair called the exciton has an energy of order $-Z/a_0$ below the bottom of the conduction band, where $a_0 = \hbar^2\varepsilon/m^*|e^2|$ is the effective Bohr radius of the exciton. The production of N such excitons would lead to a gain of approximately $-NZ/a_0$ in energy, this being linearly proportional to N since there is saturation of forces among the electrons and holes due to their mutual screening (i.e., the forces are effectively short ranged). Hence, as long as $-Z/a_0 + E_{\text{gap}} > 0$, the ground state is stable against the creation of electron-hole pairs.

Following Dyson,[1] we consider now the opposite case where $Z < 0$, corresponding to a situation in which like charges would attract one another and opposite charges would repel each other. While the lifting of N electrons into the conduction band from the valence band or the production of N electron-hole pairs still cost NE_{gap} in energy, each of these pairs will split up and eventually form two clusters, one consisting purely of the N mutually attracting electrons, the other purely of N holes, also mutually attracting each other. On the other hand, the two clusters, being repulsive to one another, would be well separated in space. In the Thomas-Fermi theory,[5] each cluster can be viewed as a collection of identical fermions in a self-consistent central field, as is usually done for a collection of nucleons in, say, the shell model of nuclear physics. The energy of each cluster with a force center of charge Ne can then be shown to be[6]

$$E(N) = -0.7687 N^{7/3} |Z| / a_0 , \quad (1)$$

which grows as $N^{7/3}$ rather than linearly. Let the critical number N_c be defined by

$$2E(N_c) + N_c E_{\text{gap}} = 0 . \quad (2)$$

When $N > N_c$, the ground state of H_0 would become unstable against the excitation of N electron-hole pairs.

If a power series in the Coulomb coupling constant Z $(= e^2)$ is convergent for some positive value of Z, it must have a circle of convergence of radius $\geq |Z|$ centered around the origin in the complex Z plane. This series must therefore also converge on some interval of the negative real axis, i.e., for $Z < 0$. However, as we have just shown, the ground state is unstable for $Z < 0$ while it is stable for $Z > 0$. There must be a singularity at $Z = e^2 = 0$. The effect of pair creation for $Z < 0$ would become more and more prominent as N increases beyond N_c. This means the higher-order terms in the power-series expansion become more and more important, since it takes an Nth-order term to create N pairs. Consequently, the true ground state of the interacting system cannot be an analytic function of e^2 near $e^2=0$ and the power series in e^2 can therefore, at best, only be an asymptotic expansion. The divergence of the series will become noticeable at the perturbation orders $N \sim N_c$. Since N_c as given by (2), or

$$N_c = [0.65 E_{\text{gap}}/(e^2/a_0)]^{3/4}, \tag{3}$$

is a number $\lesssim 10$ for many semiconductors,[7] it is much smaller than the corresponding critical order for quantum electrodynamics where[1] $N_c \sim 137$, making the divergence trouble much more serious.

In conclusion, we have demonstrated in a semiquantitative way the nonanalytic behavior of the semiconductor ground state as a function of the Coulombic coupling constant e^2 and that a power series in e^2 is, at best, an asymptotic expansion. This casts a dark shadow of doubt on the application of the perturbative many-body theory to semiconductor physics. It would be extremely interesting to explore all its theoretical and experimental implications.

The author would like to express his sincere thanks to Professor Hung Cheng of Massachusetts Institute of Technology for the citation of Ref. 1 and other helpful discussions.

[1]F. J. Dyson, Phys. Rev. **85**, 631 (1952).
[2]J. B. Pendry, J. Phys. C **3**, 1711 (1970).
[3]J. B. Pendry, J. Phys. C **6**, 1909 (1973).
[4]S. Weinberg, Phys. Rev. **130**, 776 (1963); **131**, 440 (1963).
[5]See, for example, N. H. March, in *Theory of the Inhomogeneous Electron Gas,* edited by S. Lundqvist and N. H. March (Plenum, New York, 1983), Chap. 1.
[6]E. A. Milne, Proc. Cambridge Philos. Soc. **23**, 794 (1927).
[7]For example, $N_c \approx 4$ for GaAs; $N_c \approx 3$ for InSb.