per bound to the energy in the large r_s limit of $-3.66/r_s$. Unreasonable because for large values of r_s the electron gas forms a crystal with energy[3]

$$\langle H_{\text{true}} \rangle = -1.792/r_s + 3/r_s^{3/2} + \cdots .$$

The true ground state in this limit has a trivial translational degeneracy owing to the crystal structure and it is undoubtedly the assumption of the nondegeneracy of the extended ground state which is in error. However, it is obvious from this trivial counterexample that the extended Hamiltonian is not an upper bound to the true Hamiltonian.

[1]D. Bohm, K. Huang, and D. Pines, Phys. Rev. 107, 71 (1957).

[2]D. Bohm and D. Pines, Phys. Rev. 92, 609 (1953).
[3]E. P. Wigner, Trans. Faraday Soc. 34, 678 (1938).

"Extended Electron-Gas Hamiltonian" — an Author's Comment

David Pines
Department of Physics, University of Illinois, Urbana, Illinois 61801
(Received 21 November 1969)

In the course of developing a collective description of the electron gas, Bohm and Pines[1] (BP) found it convenient to introduce an extended Hamiltonian for the system of electrons in a uniform background of positive charge. Subsequently, Bohm, Huang, and Pines[2] (BHP) showed that if the ground state of this extended system (which contained N' additional field coordinates) is nondegenerate, the energy eigenvalues for the extended system Hamiltonian would lie above those of the true Hamiltonian. In the above paper, Coldwell[3] has shown by means of an explicit example that incautious use of the extended Hamiltonian can lead to incorrect results in the limit of very low electron densities; he has suggested that the origin of this difficulty lies in the fact that in this limit the true ground state is crystalline, and hence is no longer nondegenerate. In the present paper, it is shown that the density at which the extended Hamiltonian fails to provide an upper bound is just that at which a dielectric instability appears, signaling the onset of the transition from the liquid to the crystalline state of the electronic system. Thus, as emphasized by BHP, so long as the ground state of the electrons (plus the uniform background of positive charge) is nondegenerate (e. g., spatially homogeneous), the BP extended Hamiltonian can be relied upon in a calculation of the ground-state energy.

The extended system under consideration is described by the Hamiltonian

$$H_{\text{ext}} = H_{\text{elec}} + \sum_{k<k_c}\left[\frac{\pi_k^\dagger \pi_k}{2} - \left(\frac{4\pi e^2}{k^2}\right)^{1/2}\pi_k^\dagger \rho_k\right], \qquad (1)$$

where H_{elec} is the true Hamiltonian for the system of electrons in a uniform background of positive charge and the added terms describe a "c" number field coupled to the electronic density fluctuations. Since we are at liberty to fix the strength of this field, let us assume that each π_k represents a comparatively gentle probe of system behavior such that the electron system responds linearly; a given π_k then acts to induce a density fluctuation

$$\langle \rho_k \rangle = -(4\pi e^2/k^2)^{1/2}\chi(k,0)\pi_k, \qquad (2)$$

where $\chi(k, 0)$ is the electronic static density-density correlation function for the true system H_{elec}.[4] On making use of the well-known relation between χ and the static dielectric function $\epsilon(k, 0)$,

$$1/\epsilon(k,0) = 1 + (4\pi e^2/k^2)\chi(k,0), \qquad (3)$$

one readily finds that the net result of the added terms in the Hamiltonian (1) is to produce a change in the system energy which is

$$\frac{1}{2}\sum_{k<k_c}\frac{\pi_k^\dagger \pi_k}{\epsilon(k,0)} . \qquad (4)$$

The energy eigenvalues of the extended Hamiltonian will thus lie above those for the true Hamiltonian so long as $\epsilon(k, 0) > 0$ for all the wave vectors under consideration $(k < k_c)$. What happens if the density is such that $\epsilon(k, 0) < 0$ for some k? Nozières and the writer have discussed this possibility elsewhere,[5] and have shown that under these circumstances the positive background will be unstable against the development of spontaneous density fluctuations of the corresponding wave vector. Put in other words, a dielectric instability

develops [corresponding to the appearance of a spatially varying density (or charge) wave], and one gets a transition from a spatially homogeneous to a crystalline state.[6]

The above discussion serves to make explicit one of the central arguments given in BHP – that the ground state of H_{ext} would become degenerate only if the added field-particle interaction pushed down some excited states of H_{elec} to the ground state.

They noted that "this would be highly implausible except possibly for pathological systems. There seems to be a general theorem in physics, so far unproved, which states that *when an external* (static) *field is applied to a physical system the reaction of the system will never completely cancel it.*" The electron liquid, at a density such that a charge wave develops spontaneously, represents just such a pathological system.

[1]D. Bohm and D. Pines, Phys. Rev. 92, 609 (1953).
[2]D. Bohm, K. Huang, and D. Pines, Phys. Rev. 107, 71 (1957).
[3]R. L. Coldwell, previous paper, Phys. Rev. B 2, 1423 (1970).

[4]See, for example, D. Pines and P. Nozières, *Theory of Quantum Liquids* (Benjamin, New York, 1966), pp. 95–99.
[5]See Ref. 4, pp. 206–209.
[6]See also P. C. Martin, Phys. Rev. 161, 143 (1967).

Positronium Decay in Condensed Matter

Werner Brandt and James H. Fahs

Department of Physics, New York University, New York, New York 10003
(Received 11 March 1970)

In earlier papers [Phys. Rev. 120, 1289 (1960); 142, 231 (1966)] the pickoff annihilation rate of positronium was calculated in a cell approximation for various cell geometries. The rate can be expressed in terms of two functions $F(S, v^*)$ and $\xi(S, v^*)$ that depend on a cell potential parameter S and the reduced cell volume v^*. These functions are rederived and previous errors corrected. Extensive numerical tabulations are made available and analytical approximations presented.

The decay of positronium (Ps) in matter can be influenced strongly by electron pickoff. In this process the positron, bound to an electron as P_s annihilates with an electron bound in the medium. The pickoff annihilation rate is proportional to the overlap of the positron wave function with the electron wave function of the medium.

The pickoff annihilation rate Γ_p was derived for a simple cell model of condensed matter,[1,2] with the result

$$\Gamma_p(S, v^*, T)$$

$$= \Gamma_{0p} \frac{1 + G\{\exp[2\xi^2(S, v^*)\langle u^2(T)\rangle/r_0^2] - 1\}}{1 + F(S, v^*)} . \quad (1)$$

In Eq. (1), $\Gamma_{0p} = \pi r_e^2 c\rho_0$ is a constant proportional to the electron density ρ_0 in the domain of wave-function overlap; $S = (4m/\hbar^2) U_0 r_0^2$ is a dimensionless parameter proportional to the cell potential U_0 and the radius r_0 of the cell core; $v^* = v_1/v_0$ is the cell volume v_1 reduced by the volume v_0 of the cell core. The factor G varies between $\frac{1}{2}$ and 1, ap-

proximately as

$$G \simeq 1 - \tfrac{1}{2}\tanh[(\mu - 1)/\xi(S, v^*)] , \quad (2)$$

where $\mu = 1$, 2, 3 for planar, cylindrical, and spherical cell symmetry, respectively. The dependence on temperature T of the reduced mean-square amplitude $\langle u^2\rangle/r_0^2$ of the core vibration can be expressed as

$$\langle u^2\rangle/r_0^2 = v^{*2/\mu} \gamma_M T/T_M , \quad T_D < T \le T_M , \quad (3)$$

where γ_M is the critical value of $\langle u^2\rangle/r_0^2 \, v^{*2/\mu}$ for which melting occurs; T_D is the Debye temperature, and T_M the melting temperature. In the liquid, we set

$$\langle u^2\rangle/r_0^2 \simeq v^{*2/\mu} \gamma_M, \quad T > T_M . \quad (4)$$

At temperatures $T < T_D$, $\langle u^2\rangle$ becomes a constant, and Γ_p depends only on S and v^*.

The formulas for the functions $F(S, v^*)$ and $\xi(S, v^*)$ are given in Table I for the three geometries, together with the auxiliary compatibility