COMMENTS AND ADDENDA

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Extended Electron-Gas Hamiltonian

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This is a comment on a paper by Bohm, Huang, and Pines[1] in which they gave a formal proof that the extended Hamiltonian's eigenvalues were above the ground state of the true Hamiltonian.

An extended Hamiltonian for the electron gas system was introduced by Pines in the early fifties. In a rather formal paper, Bohm *et al.*[1] rigorously prove that if the ground state of the extended Hamiltonian is nondegenerate, the expectation value of the H_{ext} for a trial function is greater than the ground-state energy of the true Hamiltonian. Bohm and Pines[2] add the following to the basic Hamiltonian of an electron gas:

$$H_{\text{add}}(k_c) = \tfrac{1}{2} \sum_{k<k_c}{}' \left(\pi_k^* \pi_k - 2\pi_k \rho_k \sqrt{v_k}\right) ,$$

$$H_{\text{ext}}(k_c) = H_{\text{true}} + H_{\text{add}}(k_c) .$$

The new operators π_k are defined as commuting with all particle variables, having canonical conjugates q_k, and having transformation properties such that the extended Hamiltonian shares the invariance properties of the true Hamiltonian. In particular, invariance under the translation operator $U(\Delta x)$ gives

$$U^{-1} \overset{*}{\pi}_k \rho_k U = \overset{*}{\pi}_k \rho_k = U^{-1} \pi_k U = \pi_k e^{ik\cdot\Delta x} .$$

The proof which they give rests on the assumption that the ground state of the extended Hamiltonian is nondegenerate: Let E be a nondegenerate eigenvalue of H_{ext} and Φ its eigenstate. Φ is unique. Since π_k and U both commute with H_{ext}, we have

$$H_{\text{ext}}\Phi = E\Phi, \quad \pi_k\Phi = \beta_k\Phi, \quad U(\Delta x)\Phi = \omega\Phi ,$$

$$U\pi_k\Phi = \alpha\beta_k\Phi = U\pi_k U^{-1} U\Phi = \alpha\beta_k e^{ik\cdot\Delta x}\Phi .$$

Since Δx is arbitrary, it follows that

$$\beta_k = 0 .$$

Thus, for the lowest state of H_{ext}, if that state is nondegenerate, it follows that $H_{\text{add}}(k_c) = 0$, and thus $\langle H_{\text{add}}\rangle = 0$. This implies that for an arbitrary trial function ψ,

$$\psi\langle\psi| H_{\text{ext}} |\psi\rangle \geq \langle \text{gs} | H_{\text{true}} | \text{gs}\rangle .$$

Now if we use a trial function

$$\psi = \psi_0^{\text{osc}} \chi_0 ,$$

where $\psi_0^{\text{osc}} = \prod_{k<k_c} \exp(-i v_k^{1/2} \pi_k q_k)$

and χ_o is a Slater determinant of plane waves in transformed electron particle coordinates, it can be shown that the expectation value of the extended Hamiltonian is[2]

$$\langle\psi| H_{\text{ext}} |\psi\rangle = \frac{2.21}{r_s^2} + \frac{0.866}{r_s^{3/2}} - \frac{0.916}{r_s}\left(1 + \frac{\beta^2}{2} - \frac{\beta^4}{48}\right) ,$$

or in the limit of large r_s,

$$\frac{0.916}{r_s}\left(1 + \tfrac{1}{2}\beta^2 - \tfrac{1}{48}\beta^4\right) .$$

β is k_c/k_f and is a free parameter in the proof, thus to find the minimum we differentiate. This gives $\beta_{\min} = \sqrt{(12)}$ and leads to the unreasonable upper 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]

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

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).

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

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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

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

where $H_{\rm elec}$ 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 $H_{\rm elec}$.[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

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

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