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Electron-hole liquid in many-band systems. II. Ge and Si †

P. Bhattacharyya,* V. Massida, and K. S. Singwi
Physics Department, Northwestern University, Evanston, Illinois 60201

P. Vashishta
Argonne National Laboratory, Argonne, Illinois 60439

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Calculations are presented for the ground-state energy and enhancement factors for the electron-hole liquid in germanium and silicon both in the Hubbard and the self-consistent particle-hole approximations for two simplified models of the actual band structure. It is shown that the inclusion of multiple electron-hole scatterings lowers the ground-state energy by about 3 K for germanium and by about 18 K for silicon, while it raises the enhancement factors by about 20% and 50%, respectively. A detailed comparison of the experimental data with theoretical calculations is carried out and it is argued that including electron-electron and hole-hole short-range correlations would substantially improve agreement between theory and experiment.

I. INTRODUCTION

Detailed ground-state energy calculations of the electron-hole liquid (EHL) in Ge and Si have been reported by Brinkman *et al.*[1] (BRAC), Combescot and Nozières[2] (CN), and by Brinkman and Rice[3] (BR). BRAC have introduced a model in which the actual complicated band structure of the two-hole bands is approximated by two bands each having a mass corresponding to the optically averaged mass of the light and heavy holes. In the same spirit, they have replaced the anisotropic conduction bands by spherical bands corresponding to a mass which is optically averaged over the transverse and longitudinal directions. Using the Hubbard approximation, these authors have obtained for the binding energy Φ of the EHL in Ge a value of 17.9 K, corresponding to an equilibrium density $n_c \simeq 2.0\times10^{17}$ cm^{-3}.

Combescot and Nozières, on the other hand, make no such approximation. They take into account in the correlation energy all the complications associated with valence-band coupling and conduction-band anisotropy. Using the Nozières-Pines (NP) interpolation scheme,[4] these authors calculate the binding energy to be 29.0 K at an equilibrium density of 2.0×10^{17} cm^{-3}. The experimental situation regarding the binding energy is still somewhat confusing, although the most recent careful spectroscopic measurement of Thomas *et al.*[5] has established the range $18 \leq \Phi \leq 23$ K. Present thermodynamic measurements of Φ are in the range $14 \leq \Phi \leq 19$ K.[6,7]

Although the calculations of BR for the ground-state energy are in better agreement with experiment than those of CN, this must be considered a coincidence since the calculations of CN are definitely more realistic and moreover involve an approximation (NP) which is somewhat better than the Hubbard approximation. It must, however, be pointed out that in a multicomponent plasma the effect of the Hubbard approximation (and for that matter of NP) is considerably weakened, and therefore in effect, one is still doing an RPA (random-phase approximation) calculation. The situation can be summarized by saying that, at present, there exists a discrepancy between theory (CN) and experiment of definitely about 20% of the correlation energy. This discrepancy is larger than one would normally have expected in the densities of interest ($r_s < 1$). What, then, is the cause of this discrepancy? And is it possible to resolve it?

Of the four approximations discussed in the preceding paper,[8] hereafter referred to as I, the most satisfactory is the fully-self-consistent approximation (FSC). We have seen that in the simplest case of two-band systems, the FSC scheme involves a numerical solution of three coupled nonlinear integral equations for the partial structure factors. For EHL in normal Ge and Si, this scheme would involve the simultaneous solution of seven such equations, making the whole numerical procedure extremely time consuming even on the fastest digital computor. To remedy this situation, we tried in I what was called the self-consistent particle-hole (SPH) approximation It consists in using the Hubbard approximation within the same band and takes into account electron-hole multiple scatterings in the spirit of the FSC approximation. It was also shown in I by explicit numerical calculation that, at least in the case of two-band systems, the difference between the FSC and SPH approximations is about 2% of the correlation energy in the range of plasma density $r_s \leq 1$. This condition is satisfied in the case of normal

Ge and Si, and hence SPH should hopefully be fairly good.

It is known from experience gained from the electron-gas problem that RPA, because of its neglect of short-range correlations, always overestimates the correlation energy. In contrast to the electron-gas problem, the correlation energy of the EHL in Ge is nearly 70% of the ground-state energy. It is very important therefore to use a theory which takes short-range correlations between electrons and electrons, between holes and holes, and between electrons and holes into account.

The purpose of this paper is to present calculations of the ground-state energy of the electron-hole liquid and the enhancement factor ρ within the Hubbard and SPH approximations and compare our results with those of previous authors. We adopt here the same units as those used by BRAC and CN. We avoid any detailed exposition of the formal aspects of the problem, since the extension of the two-component plasma formalism (described in detail in I) to a multi-component case is straightforward, although somewhat laborious. Emphasis will rather be laid on those aspects which are peculiar to Ge and Si.

II. MODELS FOR Ge AND Si

The band structures of both Ge and Si are similar in nature. The minima in the conduction bands are ellipsoidal in shape and are located at the L points of the Brillouin zone for Ge, while in Si they are centered at the set of points obtained from $(0.85, 0, 0)2\pi/a$, the main difference being that whereas there are four equivalent ellipsoids in Ge, there are six such ellipsoids in Si. The valence band structure in both consists of two bands which are degenerate Γ_8 levels at the center of the zone but are split into heavy and light hole bands away from the center of the zone. The detailed form of the energy eigenvalue is

$$E^{\pm}(k) = Ak^2 \pm [B^2k^4 + C^2(k_x^2k_y^2 + k_y^2k_z^2 + k_z^2k_x^2)]^{1/2}, \quad (1)$$

where the constants A, B, and C are given in Table I for Ge and Si. They are exactly the same as those used by BRAC, which were taken from the latest cyclotron resonance work of Hensel and Suzuki.[9]

The degeneracy of the valence bands at $k=0$ has a subtle effect on the plasma frequency, the hole exchange energies, etc. It also leads to various complications in the evaluation of the correlation energy even within the RPA. For a detailed discussion we refer to the work of Combescot and Nozières.[2] Consequently, in the calculations presented here we shall neglect the effect of valence band coupling only as far as the calculation of the correlation energy is concerned and replace the actual valence band structure by two decoupled bands. We consider two models. In model I we replace two-hole bands with masses m_{lh} (light hole) and m_{hh} (heavy hole) by two bands each having the same mass, corresponding to the optically averaged mass m_{oh} defined by

$$m_{oh}^{-1} = \tfrac{1}{2}(m_{lh}^{-1} + m_{hh}^{-1}). \quad (2)$$

This is also the model employed by Brinkman and Rice.[1,3] In the second model, model II, we have taken the actual hole masses given in Table I. In both models, the anisotropic structure of the conduction bands is replaced by an isotropic structure corresponding to the optical mass m_{oe}, defined by

$$m_{oe}^{-1} = \tfrac{1}{3}(2m_{et}^{-1} + m_{el}^{-1}), \quad (3)$$

m_{et} and m_{el} being, respectively, the transverse and longitudinal masses of the electrons. Let us reiterate that these approximations only serve to simplify the calculation of the correlation energy. The Hartree-Fock (HF) energy is calculated exactly, including all the complications due to anisotropy and valence band coupling. Effect of the valence band warping, which is $\simeq 0.01$ Ry, is neglected in the exchange energy.[2,3]

III. GROUND-STATE ENERGY

Hartree-Fock energy: The total energy of the system is the sum of the (a) kinetic, (b) exchange, and (c) correlation contributions. Throughout this paper as in I, the energy is measured in units of excitonic rydbergs ($\mu e^4/2\kappa^2\hbar^2$), with $\mu^{-1} = m_{oe}^{-1} + m_{oh}^{-1}$. Density is measured in terms of dimensionless parameter r_s given by $n^{-1} = \frac{4}{3}\pi r_s^3 a_x^3$, with $a_x = \kappa\hbar^2/\mu e^2$. The kinetic energy per electron-hole pair is

TABLE I. List of band parameters used in the calculations. Masses are given in units of the bare electron mass.

	m_{el}	m_{et}	m_{oe}	m_{de}	A	B	C	m_{lh}	m_{hh}	κ	E_x (meV)
Ge	1.58	0.082	0.120	0.22	13.38	8.48	13.15	0.042	0.347	15.36	2.65
Si	0.9163	0.1905	0.2588	0.32	4.28	0.75	4.85	0.154	0.523	11.4	12.85

$$\epsilon_K = \frac{2.2099}{r_s^2}\frac{\mu}{\nu^{2/3}m_{de}} + \frac{\mu}{m_{hh}}\left(\frac{1}{1+(m_{lh}/m_{hh})^{3/2}}\right)^{2/3}\text{Ry}, \tag{4}$$

where ν is the number of conduction bands and m_{de} is the density-of-states mass for the electron, given by $m_{de}=(m_{et}^2 m_{el})^{1/3}$.

The calculation of the exchange energy is complicated for two reasons. First, although the exchange energy does not depend directly on the electron mass, it does depend weakly on the shape of the Fermi surface. Second, as a result of the valence band degeneracy, there are nonzero matrix elements of the Coulomb interaction between the heavy and light hole bands. Taking these factors into account the exchange energy per e-h pair can be written[2]

$$\epsilon_{ex} = -(0.9163/r_s)[\Phi(\rho_e)/\nu^{1/3} + \psi(\rho_h)], \tag{5}$$

where $\rho_e = m_{et}/m_{el}$ and $\rho_h = m_{lh}/m_{hh}$,

$$\Phi(\rho) = \rho^{1/6}[\sin^{-1}(1-\rho)^{1/2}]/(1-\rho)^{1/2}, \quad \rho<1, \tag{6}$$

and

$$\psi(\rho) = \frac{1}{(1+\rho^{3/2})^{4/3}}\left[-\tfrac{3}{16}(1-\rho)^2\ln\frac{1+\rho^{1/2}}{1-\rho^{1/2}} + \frac{\rho^2+3\rho^{3/2}+3\rho^{1/2}+1}{4} + \tfrac{3}{16}(1-\rho^2)\int_{\sqrt{\rho}}^1\frac{dx}{x}\ln\left(\frac{1+x}{1-x}\right)\right]. \tag{7}$$

Substituting the pertinent parameters for Ge and Si, we may write the HF energy per e-h pair as

$$\epsilon_{HF} = 0.4697/r_s^2 - 1.1503/r_s \text{ Ry (Ge)} \tag{8a}$$

and

$$\epsilon_{HF} = 0.7326/r_s^2 - 1.1665/r_s \text{ Ry (Si)}. \tag{8b}$$

Correlation energy. For the sake of completeness, we shall rewrite the expression for the correlation energy per e-h pair derived in I [see Eq. (44)]. It is

$$\epsilon_{corr} = -\frac{4}{\pi\alpha}\frac{1}{r_s^2}\int_0^{r_s}\bar{\gamma}(r_s')\,dr_s' - \epsilon_{ex}\text{ Ry}, \quad \alpha=(\tfrac{9}{4}\pi)^{-1/3}, \tag{9}$$

where

$$\bar{\gamma}(r_s') = -\frac{1}{2q_F}\int_0^\infty \gamma(q)dq \tag{10}$$

and

$$\gamma(\vec{q}) = \sum_{ij}\xi_i\xi_j\bar{n}_i\bar{n}_j\gamma_{ij}(\vec{q}). \tag{11}$$

In Eq. (11), $\bar{n}_i = n_i/n$ and $\xi_i = +1$ if the ith component is a hole and -1 if it is an electron. $\gamma_{ij}(\vec{q})$ is the Fourier transform of the pair distribution function $g_{ij}(\vec{r})-1$ as defined by Eq. (14) of I.

The problem of calculating the correlation energy is therefore reduced to the calculation of $\gamma_{ij}(\vec{q})$, which in the present scheme should be calculated in a self-consistent manner.

Since $\gamma_{ij}(\vec{q})$ can, in turn, be calculated from the fluctuation-dissipation theorem [Eq. (15) of I] provided the partial polarizabilities are known, we first address ourselves to the task of evaluating them. This can be easily done by generalizing Eqs. (2) and (3) of I for many components. For the case of ν-electron and two-hole bands, defining the local field correction $G_{ij}(\vec{q})$ through

$$\psi_{ij}(\vec{q}) = \xi_i\xi_j\phi(\vec{q})[1-G_{ij}(\vec{q})], \quad \phi(\vec{q}) = 4\pi e^2/\kappa q^2, \tag{12}$$

we get for the polarizabilities the expressions

$$\phi(\vec{q})\chi_{11}(\vec{q},\omega) = -[Q_0^1(\vec{q},\omega)/H_1(\vec{q},\omega)\Delta(\vec{q},\omega)] \times(\{1+[F_1(q)+\nu-2]Q_0^1(\vec{q},\omega)\}\{1+F_{\nu+1}(q)Q_0^{\nu+1}(\vec{q},\omega)+F_{\nu+2}(q)Q_0^{\nu+2}(\vec{q},\omega) + [F_{\nu+1}(q)F_{\nu+2}(q)-1]Q_0^{\nu+1}(\vec{q},\omega)Q_0^{\nu+2}(\vec{q},\omega)\} - (\nu-1)[1-G(\vec{q})]^2Q_0^1(\vec{q},\omega)\{Q_0^{\nu+1}(\vec{q},\omega)+Q_0^{\nu+2}(\vec{q},\omega)+[F_{\nu+1}(q)+F_{\nu+2}(q)-2]Q_0^{\nu+1}(\vec{q},\omega)Q_0^{\nu+2}(\vec{q},\omega)\}), \tag{13a}$$

$$\phi(\vec{q})\chi_{12}(\vec{q},\omega) = \{[Q_0^1(\vec{q},\omega)]^2/H_1(\vec{q},\omega)\Delta(\vec{q},\omega)\} \times(\{1+F_{\nu+1}(q)Q_0^{\nu+1}(\vec{q},\omega)+F_{\nu+2}(q)Q_0^{\nu+2}(\vec{q},\omega)+[F_{\nu+1}(q)F_{\nu+2}(q)-1]Q_0^{\nu+1}(\vec{q},\omega)Q_0^{\nu+2}(\vec{q},\omega)\} - [1-G(\vec{q})]^2\{Q_0^{\nu+1}(\vec{q},\omega)+Q_0^{\nu+2}(\vec{q},\omega)+[F_{\nu+1}(q)+F_{\nu+2}(q)-2]Q_0^{\nu+1}(\vec{q},\omega)Q_0^{\nu+2}(\vec{q},\omega)\}), \tag{13b}$$

$$\phi(\vec{q})\chi_{1,\nu+1}(\vec{q},\omega) = -[Q_0^1(\vec{q},\omega)Q_0^{\nu+1}(\vec{q},\omega)/\Delta(\vec{q},\omega)]\{1+[F_{\nu+2}(q)-1]Q_0^{\nu+2}(\vec{q},\omega)\}[1-G(\vec{q})], \tag{13c}$$

$$\phi(\vec{q})\chi_{1,\nu+2}(\vec{q},\omega) = -[Q_0^1(\vec{q},\omega)Q_0^{\nu+2}(\vec{q},\omega)/\Delta(\vec{q},\omega)]\{1+[F_{\nu+1}(q)-1]Q_0^{\nu+1}(\vec{q},\omega)\}[1-G(\vec{q})], \tag{13d}$$

$$\phi(\vec{q})\chi_{\nu+1,\nu+1}(\vec{q},\omega) = -[Q_0^{\nu+1}(\vec{q},\omega)/\Delta(\vec{q},\omega)]\{\{1+[F_1(q)+\nu-1]Q_0^1(\vec{q},\omega)\}[1+F_{\nu+2}(q)Q_0^{\nu+2}(\vec{q},\omega)] - \nu[1-G(\vec{q})]^2 Q_0^1(\vec{q},\omega)Q_0^{\nu+2}(\vec{q},\omega)\}, \quad (13e)$$

$$\phi(\vec{q})\chi_{\nu+1,\nu+2}(\vec{q},\omega) = [Q_0^{\nu+1}(\vec{q},\omega)Q_0^{\nu+2}(\vec{q},\omega)/\Delta(\vec{q},\omega)]\{\{1+[F_1(q)+\nu-1]Q_0^1(\vec{q},\omega)\} - \nu[1-G(\vec{q})]^2 Q_0^1(\vec{q},\omega)\}, \quad (13f)$$

$$\phi(\vec{q})\chi_{\nu+2,\nu+2}(\vec{q},\omega) = -[Q_0^{\nu+2}(\vec{q},\omega)/\Delta(\vec{q},\omega)]\{\{1+[F_1(q)+\nu-1]Q_0^1(\vec{q},\omega)\}[1+F_{\nu+1}(q)]Q_0^{\nu+1}(\vec{q},\omega) - \nu[1-G(\vec{q})]^2 Q_0^1(\vec{q},\omega)Q_0^{\nu+1}(\vec{q},\omega)\}, \quad (13g)$$

where

$$H_1(\vec{q},\omega) = \{1+[F_1(q)-1]\}Q_0^1(\vec{q},\omega), \quad (14)$$

$$F_i(q) = 1 - \tfrac{1}{2}q^2/(q^2+q_{Fi}^2), \quad q_{Fi}^3 = 3\pi^2 n_i, \quad (15)$$

$$\Delta(\vec{q},\omega) = \{1+[F_1(q)+\nu-1]Q_0^1(\vec{q},\omega)\}\{1+F_{\nu+1}(q)Q_0^{\nu+1}(\vec{q},\omega) + F_{\nu+2}(q)Q_0^{\nu+2}(\vec{q},\omega)+[F_{\nu+1}(q)+F_{\nu+2}(q)-2]Q_0^{\nu+1}(\vec{q},\omega)Q_0^{\nu+2}(\vec{q},\omega)\}, \quad (16)$$

and $Q_0^i(\vec{q},\omega) = -(4\pi e^2/\kappa q^2)\chi_0^i(\vec{q},\omega)$, which are evaluated in Eqs. (48) and (49) of I.

These expressions have been written down under the following assumptions: (i) For particles of like charges, we have used the Hubbard approximation if they are within the same band and the RPA otherwise (ii) the two electron-hole local-field corrections have been taken to be equal, i.e.,

$$G(\vec{q}) = G_{1,\nu+1}(\vec{q}) = G_{1,\nu+2}(\vec{q}). \quad (17)$$

Such an approximation can hardly have too much of an effect on the final energy, since, as we shall see later, the effect of multiple scatterings itself is quite small. (iii) We have used the Hubbard approximation to evaluate $\Delta(\vec{q},\omega)$ by setting $G_{1,\nu+1}(\vec{q}) = G_{1,\nu+2}(\vec{q}) = 0$. This approximation saves computer time by more than a factor of 10. It should also be a good approximation for the correlation energy insofar as our experience in the positron case has been that the use of different dielectric functions to screen the bare positron-electron interaction has a small effect on the enhancement factor, which is a far more sensitive quantity.

Let us now follow Sjölander and Stott[10] and use for the local field the expression

$$G_{1,\nu+1}(\vec{q}) = -\frac{1}{n}\int \frac{\vec{q}\cdot\vec{q}'}{q'^2}\gamma_{1,\nu+1}(\vec{q}-\vec{q}')\frac{d\vec{q}'}{(2\pi)^3}, \quad (18)$$

where n is the number of electrons in a unit volume. If we now use the fluctuation-dissipation theorem [Eq. (15) in I]

$$n_i\left(\delta_{ij} + \frac{n_j}{n}\gamma_{ij}(\vec{q})\right) = -\frac{\hbar}{\pi}\int_0^\infty d\omega\, \mathrm{Im}\chi_{ij}(\vec{q},\omega), \quad (19)$$

for the case $i=1$ and $j=\nu+1$, it immediately leads to the linear integral equation

$$\gamma_{1,\nu+1}(\vec{q}) = f(\vec{q})\left(1+\frac{1}{n}\int \frac{\vec{q}\cdot\vec{q}'}{q'^2}\gamma_{1,\nu+1}(\vec{q}-\vec{q}')\frac{d\vec{q}'}{(2\pi)^3}\right), \quad (20)$$

where

$$f(\vec{q}) = \frac{\hbar q^2}{4\pi^2 n \tilde{n}_1 \tilde{n}_{\nu+1} e^2} \times \int_0^\infty d\omega\, \mathrm{Im}([Q_0^1(\vec{q},\omega)Q_0^{\nu+1}(\vec{q},\omega)/\Delta(\vec{q},\omega)] \times\{1+[F_{\nu+2}(q)-1]Q_0^{\nu+2}(\vec{q},\omega)\}). \quad (21)$$

Equation (20) now has to be solved numerically and the solutions are used to calculate the partial-pair-correlation functions and correlation energies, as indicated earlier.

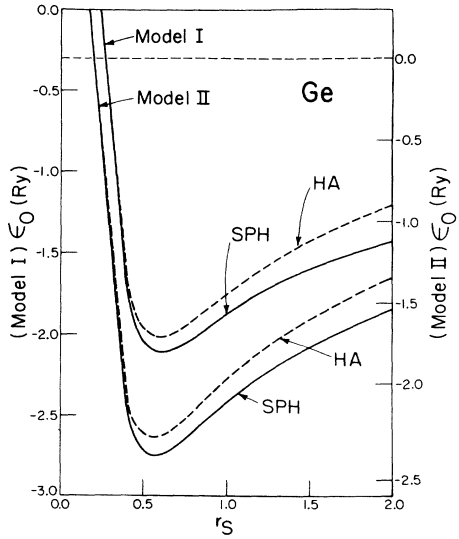

FIG. 1. Ground-state energy of the electron-hole liquid in Ge plotted against r_s in Hubbard (dashed line) and SPH (solid line) approximations with isotropic electron bands for models I and II.

IV. RESULTS AND DISCUSSIONS

A. Germanium

The results for the ground-state energy of the electron-hole liquid per pair, ϵ_0, in both models and in both approximations are plotted in Fig. 1. For model I in the Hubbard approximation, we get a ground-state energy minimum of −2.02 Ry at $r_s \cong 0.6$. This corresponds to a binding energy Φ of 20.4 K, corresponding to an equilibrium density $n_c = 2.0 \times 10^{17}$ cm^{-3}. However, when e-h multiple scattering is included, the minimum of the energy drops to −2.11 Ry corresponding to $\Phi = 23.0$ K at the same value of n_c.

For model II, however, our results for ϵ_0 are much lower. In the Hubbard approximation, the minimum of ϵ_0 is −2.33 Ry at $r_s \cong 0.6$, corresponding to a binding energy $\Phi = 29.9$ and $n_c = 2.0 \times 10^{17}$ cm^{-3}. This is very close to the binding energy of 29.0 K obtained by the more sophisticated treatment of Combescot and Nozières, indicating that model II is a reasonable approximation to the actual band structure. With the inclusion of e-h multiple scattering, Φ is 33.4 K at the same value of n_c. Throughout the above discussion the excitonic binding energy is taken to be equal to 3.6 meV.[2,3]

The experimental situation regarding the binding energy of the metallic phase in Ge is still somewhat confusing. The spectroscopic measurements presently yield values of 23 K,[11] 18–23 K,[5] and 30 K,[12] although the last value is somewhat uncertain since the excitonic line shape does not seem to have been fitted properly.

The enhancement factor ρ in model I is 1.8 in Hubbard approximation and 2.2 with electron-hole multiple scattering. In model II, ρ already has a value 2.3 in the absence of multiple scattering, which increases to 2.8 on its inclusion. These values are, however, much lower than an estimate by Benoît à la Guillaume and Voos of $\rho \sim 12$.[13]

Improved accuracy in the determination of Φ will result once this line shape is understood in detail. The work function has so far yielded values which are somewhat lower than these obtained spectroscopically. The best estimates of Φ are 17 K,[12] 14–19 K,[6] and 17.9 ± 0.4 K.[7] The reason for this descrepancy does not seem to be properly understood at present. From the theoretical point of view, a more disturbing feature is the magnitude of the discrepancy with the results of model II. We shall comment on this point later.

B. Silicon

We have plotted the ground-state energy of the electron-hole liquid in Si for both models in two different approximations in Fig. 2.

For model I, the minimum of ϵ_0 has a value of −1.58 Ry at $r_s \cong 0.85$, corresponding to $\Phi = 67$ K at a critical density $n_c \cong 3.4 \times 10^{18}$ cm^{-3}. This compares very well with the values obtained by Brinkman and Rice (see Table III for a detailed comparison). When e-h multiple scattering is included, the binding energy at $n_c = 2.9 \times 10^{18}$ cm^{-3} drops to a value $\Phi = 83$ K. For model II in the Hubbard approximation, we get a ground-state energy minimum of −1.66 Ry at $r_s \cong 0.85$, corresponding to a binding energy of $\Phi = 77$ K at $n_c = 3.4 \times 10^{18}$ cm^{-3}. As in the case of Ge, we see that model II in the Hubbard approximation yields results very close to those obtained by the more exact treatment of CN, who obtained a binding energy of 73 K at $n_c = 3.4 \times 10^{18}$ cm^{-3}. In model II, with the inclusion of multiple scattering, the binding energy drops to 95 K at the same critical density.

The enhancement factor for model I in the Hubbard approximation is 2.2. When multiple scattering is taken into account, ρ becomes 3.5. As in Ge, ρ is typically larger in model II. Thus, in the Hubbard approximation, ρ is already 2.5 becoming 3.7 when multiple scattering is taken into account.

The experimental data on Si is far more scanty than that available for Ge. The experimental data of Haynes[14] indicates a binding energy of around 80 K at $n_c = 3.7 \times 10^{18}$ cm^{-3}; the optical luminescence studies of Pokrovskii *et al.*[15] also give nearly the same results as those of Haynes. However, the latest experiments of Benoît à la Guillaume and Voos[11] give $\Phi = 65$ K.

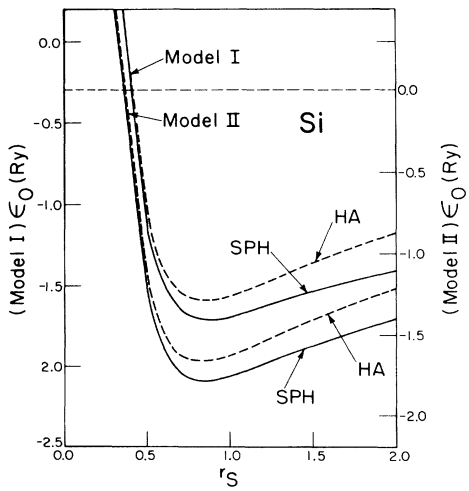

FIG. 2. Ground-state energy of the electron-hole liquid in Si plotted against r_s in Hubbard (dashed line) and SPH (solid line) approximations with isotropic electron bands for models I and II.

TABLE II. Correlation energy for Si and Ge in the Hubbard (HA) and self-consistent particle-hole (SPH) approximations with isotropic electron bands for models I and II.

	ϵ_{corr} (Ry) Si				ϵ_{corr} (Ry) Ge			
	Model I		Model II		Model I		Model II	
r_s	HA	SPH	HA	SPH	HA	SPH	HA	SPH
0.1	−3.811	−3.842	−4.101	−4.143	−3.492	−3.519	−4.424	−4.466
0.2	−2.595	−2.646	−2.779	−2.844	−2.405	−2.452	−3.009	−3.083
0.3	−2.114	−2.174	−2.256	−2.335	−1.975	−2.034	−2.447	−2.537
0.4	−1.832	−1.908	−1.950	−2.040	−1.721	−1.791	−2.119	−2.219
0.5	−1.635	−1.721	−1.738	−1.856	−1.542	−1.622	−1.890	−1.998
0.6	−1.487	−1.582	−1.579	−1.685	−1.407	−1.496	−1.718	−1.833
0.7	−1.369	−1.472	−1.459	−1.565	−1.299	−1.396	−1.580	−1.703
0.8	−1.273	−1.384	−1.349	−1.468	−1.210	−1.315	−1.468	−1.598
0.9	−1.192	−1.312	−1.263	−1.388	−1.136	−1.249	−1.375	−1.511
1.0	−1.125	−1.253	−1.191	−1.322	−1.074	−1.195	−1.297	−1.440
1.1	−1.068	−1.204	−1.130	−1.267	−1.020	−1.150	−1.230	−1.380
1.2	−1.019	−1.164	−1.077	−1.220	−0.975	−1.113	−1.174	−1.329
1.3	−0.976	−1.130	−1.032	−1.180	−0.935	−1.082	−1.124	−1.286
1.4	−0.939	−1.103	−0.992	−1.146	−0.901	−1.057	−1.082	−1.250
1.5	−0.906	−1.080	−0.957	−1.117	−0.870	−1.036	−1.044	−1.217
1.6	−0.876	−1.061	−0.925	−1.090	−0.842	−1.018	−1.009	−1.188
1.7	−0.849	−1.045	−0.896	−1.067	−0.817	−1.003	−0.978	−1.162
1.8	−0.823	−1.030	−0.868	−1.045	−0.792	−0.990	−0.947	−1.137
1.9	−0.798	−1.018	−0.842	−1.025	−0.769	−0.978	−0.919	−1.113
2.0	−0.774	−1.006	−0.817	−1.005	−0.747	−0.968	−0.891	−1.089

Since it is useful to know the density dependence, we give in Table II the variation of correlation energy ϵ_{corr} as a function of r_s in the Hubbard and SPH approximations with isotropic conduction bands for models I and II for Ge and Si. The numerical accuracy of the correlation energy in Table II is better than 1%.

V. CRITIQUE

It is the purpose of this section to sum up the results of the theoretical calculations and discuss them critically in the light of the latest experimental data, which are available with some certitude for EHL in Ge and less so for EHL in Si (see Table III).

It is fair to say that of the various models adopted, the one considered by Combescot and Nozières approaches closest to incorporating all the subtle band-structure effects. Their calculation of the correlation energy is basically one within the Hubbard approximation, but includes effects due to anisotropy and valence band coupling. We have

TABLE III. Summary of available theoretical and experimental data on the electron-hole liquid in Ge and Si. The anisotropy of the conduction bands is not included in Brinkman *et al*. and our calculations of ϵ_{corr}.

		Brinkman *et al*.[a]	Model I Hubbard	Model I SPH	Combescot and Nozières[b]	Model II Hubbard	Model II SPH	Experiment
Ge	$-\epsilon_g$ (meV)	5.3	5.36	5.59	6.1	6.18	6.48	
	$\Phi(K)$[i]	19.7	20.4	23.0	29.0	29.9	33.4	30,[c] 23,[d] 18–23[e]
	n_c ($\times 10^{17}$ cm^{-3})	1.8	2.0	2.0	2.0	2.0	2.0	17,[c] 14–19,[f] 17.9[g]
	$\rho \equiv g_{eh}(0)$		1.8	2.2		2.3	2.8	$\cong$2.4[e]
Si	$-\epsilon_g$ (meV)	20.4	20.4	21.8	21	21.3	22.9	
	$\Phi(K)$[i]	67	67	83	73	77	95	~80,[h] 65[d]
	n_c ($\times 10^{18}$ cm^{-3})	3.4	3.4	2.9	3.4	3.4	3.4	$\simeq$3.7
	$\rho \equiv g_{eh}(0)$		2.2	3.5		2.5	3.7	

[a] Reference 1.
[b] Reference 2.
[c] Reference 12.
[d] Reference 11.
[e] Reference 5.
[f] Reference 6.
[g] Reference 7.
[h] Reference 14.
[i] $|\Phi| = \epsilon_g - \epsilon_{exciton}$, where following BR and CN we have taken $\epsilon_{exciton}$ equal to 3.6 meV for Ge and 14.7 meV for Si.

seen that our calculations based on a simplified model, model II, gives results in the Hubbard approximation which are very close to those obtained by CN. The advantage of this simplified model is that it is possible, in principle, to do a fully-self-consistent calculation, although we have so far not done so.

We have seen, however, that within the limitations of our partially self-consistent scheme the value of Φ is higher than the range of values for which such a lot of experimental evidence has accumulated. What, then, is the reason for this discrepancy? Before commenting on this question, let us examine the Hubbard approximation. In a one-component plasma, say the electron gas, the exchange contribution to the correlation energy cancels half the RPA diagrams at short wavelengths. In a six-component plasma, however, the cancellation is only about $\frac{1}{12}$ of the RPA contribution. In other words, the effect of Hubbard approximation is considerably reduced and we are effectively doing a RPA calculation. If we now compare the correlation energies of the equal-mass model system (introduced in I) in the RPA and FSC approximation, we note that the RPA overestimates by about 7% or so at $r_s = 0.6$. Strictly for the purpose of an order-of-magnitude estimate, if we assume that the same figures carry over for EHL in Ge, it would imply that the FSC scheme would yield a $\Phi \sim 23$ K. The same procedure applied to Si gives $\Phi \sim 67$ K. In our view, therefore, the self-consistent scheme would go a long way toward removing the apparent discrepancy that remains between theory and experiment. These complications have their basics in the circumstance that electron-electron and hole-hole scatterings are as important as electron-hole scatterings in the densities of interest.

On the experimental side, a way should be found to determine the enhancement factors, which, as we have seen, are quite different in the RPA and the SPH approximation. On the other hand, the difference between the ground-state energies calculated in different approximations is not so marked and hence does not constitute as sensitive a test of the theory.

Note added in proof. Recently, P. Vashishta, S. G. Das, and K. S. Singwi [Phys. Rev. Lett. 33, 911 (1974)] have calculated the thermodynamics of the electron-hole liquid for five systems: Ge, Si, and Ge under large $\langle 111 \rangle$ uniaxial stress, Ge[111], Si under large $\langle 100 \rangle$ uniaxial stress Si[100], and GaAs which is a direct band-gap semiconductor. Important effects of (e,e), (h,h), and (e,h) multiple scatterings and the anisotropy of the bands are included in the calculation of the correlation energy (FSC approximation with the effect of the anisotropy taken into account). For Ge, the ground-state energy, enhancement factor, compressibility, critical temperature, critical density, temperature dependence of Fermi energy, chemical potential, and equilibrium density are in good agreement with experiments. Predictions are made for other systems.

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†Present address: Dept. of Physics, University of Illinois, Urbana, Ill. 61801.

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