# Effective mass of self-trapped electrons in gases

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The effective mass  $m^*$  of self-trapped electrons in gases is calculated, and used to estimate the translational contribution  $-(3/2) kT \ln(m^*/m)$  to the free-energy difference between self-trapped and free states for electrons in helium gas. When added to the free-energy difference between stationary self-trapped and free states this translational contribution has the effect of converting metastable stationary self-trapped states into stable moving self-trapped states.

# I. INTRODUCTION

An electron in thermal equilibrium with a disordered condensed system with which it repulsively interacts can form a quantum-mechanical localized state. In this state, the electron, by pushing away atoms of the condensed system, effectively digs its own well, falls into it, and becomes self-trapped.

Necessary conditions on temperature, density, and electron-atom interaction strength for having such self-trapped states in gases have been calculated by many authors,<sup>1-8</sup> in various approximations. A common feature of these treatments is that free energies are calculated for a stationary self-trapped state, i.e., in its center-of-mass frame of reference, thereby omitting contributions from translational motion to free energies. The density of translational states depends on the particle mass, and the effective mass  $m^*$ of the moving self-trapped state, which receives contributions from the inertia of the gas atoms it sets in motion, is expected to be considerably larger than the free-electron mass m. The difference in free energies between self-trapped and free states due to translational motion is  $-\frac{3}{2}kT\ln(m^*/m)$ , favoring the formation of the trapped state beyond those considerations involved for stationary states. So the necessary conditions on temperature, density, and interaction strength for having self-trapped states in gases are modified by including translational motion. In this work, we estimate the effective mass  $m^*$  for self-trapped states, and find that inclusion of the term  $-\frac{3}{2}kT\ln(m^*/m)$  lowers the free energy of trapped states relative to free states, by an amount sufficient to convert a region of density and temperature in which stationary self-trapped states were previously found to be metastable into a stable region for moving self-trapped states states.

## II. CALCULATION OF m\*

The Helmholtz free energy for the formation of the stationary (V = 0) trapped state of lowest energy in an ideal, noninteracting gas is<sup>8</sup>

$$F_{t}^{0} = \int d^{3}r[(\hbar^{2}/2m)|\nabla\psi_{0}(\mathbf{\ddot{r}})|^{2} + g\rho_{0}(\mathbf{\ddot{r}})\psi_{0}^{2}(\mathbf{\ddot{r}}) + kT\rho_{0}(\mathbf{\ddot{r}})\ln\rho_{0}(\mathbf{\ddot{r}})/\rho]$$
(1)

with *m* the electron mass, *g* an interaction strength (dimensions of energy-volume,  $g = 2\pi a \hbar^2 / m$  for electron-atom *s*-wave scattering). The fluid density  $\rho_0(\mathbf{\bar{r}})$  and the electron wave function  $\psi_0(\mathbf{\bar{r}})$ , determined by extremizing  $F_i^0$  are, with  $\beta = 1/kT$ 

$$\rho_{0}(\mathbf{\tilde{r}}) = \rho \ e^{-\beta_{g}\psi_{0}^{2}(\mathbf{\tilde{r}})},\tag{2}$$

$$-(\hbar^2/2m)\nabla^2\psi_0(\mathbf{\vec{r}}) + \rho g e^{-\beta g \psi_0^2(\mathbf{\vec{r}})}\psi_0(\mathbf{\vec{r}}) = E\psi_0(\mathbf{\vec{r}}).$$
(3)

Exact numerical solutions to Eqs. (2) and (3) have been obtained in Ref. 8, leading to values for  $F_t^0$  to be compared with  $F_f^0 = \rho g$  for a free electron, to determine conditions under which  $(F_t^0 \leq F_f^0)$  the self-trapped state is stable. Since  $\rho_0(\mathbf{\hat{r}})$  and  $\psi_0(\mathbf{\hat{r}})$  do not depend on time, the trapped state is stationary in these calculations.

In this paper, we impose a uniform velocity  $\overline{\mathbf{V}}$ on the self-trapped state, and find the new Helmholtz free energy  $F_t$  in the form  $F_t = F_t^0 + \frac{1}{2}m^*V^2$ , defining the effective mass  $m^*$ . This effective mass  $m^*$  will be found to be connected with a dissipative phenomenon via the gas diffusion constant D [see Eq. (31)]. Therefore it is clear that to maintain the velocity V constant, a steady electric field is necessary to provide the energy necessary to maintain the diffusion, and we assume such a field to be present.

First the electron ground-state wave function  $\psi_0(\mathbf{\tilde{r}})$  is replaced by  $\psi(\mathbf{\tilde{r}} - \mathbf{\tilde{v}}t)$ , representing a uniform center-of-mass velocity  $\mathbf{\tilde{V}}$  for the self-

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trapped state. This uniform velocity alters the gas density from  $\rho_{\rm 0}(r)$  to a new function, which we write

$$\rho(\mathbf{\vec{r}},t) = \rho(\mathbf{\vec{r}} - \mathbf{\vec{v}}t) + \delta\rho(\mathbf{\vec{r}},t) .$$
(4)

The first term in Eq. (4) represents the adiabatic, thermodynamic equilibrium response of the gas to the motion of the electron, while  $\delta\rho(\mathbf{\bar{r}}, t)$  is the dynamic response influenced by thermal diffusion processes. We will find the trapped state free energy  $F_t$  to depend quadratically on  $\delta\rho$ , so that if we calculate  $\delta\rho$  from linear response theory to terms linear in velocity  $\mathbf{V}$ , we will get the dependence of  $F_t$  on  $V^2$ , and hence find the effective mass. Making the replacements

$$\psi_0(\mathbf{r}) \rightarrow \psi(\mathbf{r} - \mathbf{V}t)$$

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and

$$\rho_0(\mathbf{r}) \rightarrow \rho(\mathbf{r} - \mathbf{V}t) + \delta\rho(\mathbf{r}, t)$$

in Eq. (1),  $F_t$  up to terms quadratic in  $\delta \rho$  is given by

$$F_{t} = \int d^{3}r [(\hbar^{2}/2m)|\Delta\psi(\vec{\mathbf{r}} - \vec{\mathbf{V}}t)|^{2} + g\rho(\vec{\mathbf{r}} - \vec{\mathbf{V}}t)\psi^{2}(\vec{\mathbf{r}} - \vec{\mathbf{V}}t) + kT\rho(\vec{\mathbf{r}} - \vec{\mathbf{V}}t)\ln\rho(\vec{\mathbf{r}} - \vec{\mathbf{V}}t)/\rho] + \int d^{3}r \,\delta\rho(\vec{\mathbf{r}}, t) [g\psi^{2}(\vec{\mathbf{r}} - \vec{\mathbf{V}}t) + kT\ln\rho(\vec{\mathbf{r}} - \vec{\mathbf{V}}t)/\rho] + \int d^{3}r [\delta\rho(\vec{\mathbf{r}}, t)]^{2}/\rho(\vec{\mathbf{r}} - \vec{\mathbf{V}}t).$$
(5)

Since  $\rho(\vec{r} - \vec{V}t)$  represents the adiabatic response to the moving self-trapped state, it satisfies an equation similar to Eq. (2)

$$\rho(\vec{\mathbf{r}} - \vec{\mathbf{V}}t) = \rho e^{-\beta g \psi^2 (\vec{\mathbf{r}} - \vec{\mathbf{V}}t)}, \qquad (6)$$

so that the term linear in  $\delta\rho$  in Eq. (5) disappears,

$$F_{t} = \int d^{3}r [(\hbar^{2}/2m)|\nabla\psi(\mathbf{\tilde{r}} - \mathbf{\tilde{V}}t)|^{2} +g\rho(\mathbf{\tilde{r}} - \mathbf{\tilde{V}}t)\psi^{2}(\mathbf{\tilde{r}} - \mathbf{\tilde{V}}t) +kT\rho(\mathbf{\tilde{r}} - \mathbf{\tilde{V}}t)\ln\rho(\mathbf{\tilde{r}} - \mathbf{\tilde{V}}t)/\rho] + \int d^{3}r [\delta\rho(\mathbf{\tilde{r}}, t)]^{2}/\rho(\mathbf{\tilde{r}} - \mathbf{\tilde{V}}t).$$
(7)

In this expression  $F_t$  is regarded as a functional of  $\psi(\mathbf{\tilde{r}} - \mathbf{V}t)$ , since  $\rho(\mathbf{\tilde{r}} - \mathbf{V}t)$  is already determined by Eq. (6) in terms of  $\psi(\mathbf{\tilde{r}} - \mathbf{V}t)$ . Left to determine is the dependence of the fluctuation part  $\delta\rho(\mathbf{\tilde{r}}, t)$  on  $\psi(\mathbf{\tilde{r}} - \mathbf{V}t)$ . This we do using linear response theory, assuming  $\delta\rho(\mathbf{\tilde{r}}, t) \ll \rho(\mathbf{\tilde{r}} - \mathbf{V}t)$ . In terms of the wave-vector-frequency transform of  $\delta\rho(\mathbf{\tilde{r}}, t)$ ,

$$\delta\rho(\vec{\mathbf{k}},\omega) = \int d^{3}r \int dt \,\delta\rho(\vec{\mathbf{r}},t) \, e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{r}}} \, e^{-i\omega t}, \qquad (8)$$

we have the first order, or linear response

$$\delta\rho(\vec{\mathbf{k}},\,\omega) = \chi(\vec{\mathbf{k}},\,\omega)V(\vec{\mathbf{k}},\,\omega) \,. \tag{9}$$

Here,  $V(\vec{k}, \omega)$  is the wave-vector, frequency dependent perturbation

$$V(\vec{k}, \omega) = \int d^{3}r \int dt g \psi^{2}(\vec{r} - \vec{\nabla}t) e^{i\vec{k}\cdot\vec{r}} e^{-i\omega t}, \quad (10)$$

which produces  $\delta\rho(\vec{k}, \omega)$ , and  $\chi(\vec{k}, \omega)$  is the generalized susceptibility, or linear response function for the gas.<sup>9</sup> To calculate the free energy  $F_t$ up to terms of order  $V^2$ , it is sufficient to expand the response function in powers of frequency:

$$\chi(\vec{\mathbf{k}},\,\omega) = \chi(\vec{\mathbf{k}},\,0) + [d\chi(\vec{\mathbf{k}},\,\omega)/d\,\omega]_0 \omega + \cdots .$$
(11)

Taking into consideration that the real part of  $\chi$  is even in  $\omega$ , while the imaginary part of  $\chi$  is odd in  $\omega$ , we see that, in Eq. (11), the first term is real, while the second term is imaginary, representing energy dissipation in the gas. The first term,  $\chi(\vec{k}, 0)$ , simply corresponds to the first-order approximation to the static response of the gas to the moving electron, which is already contained in the term  $\rho(\vec{r} - \vec{V}t)$ . To see this, calculate  $\delta\rho(\vec{k}, \omega)$  using just this term,

$$\delta\rho(\mathbf{k},\,\omega) = \chi(\mathbf{k},\,0)V(\mathbf{k},\,\omega)\,,\tag{12}$$

which gives the space-time density fluctuation,

$$\delta\rho(\mathbf{\vec{r}},t) = (2\pi)^{-3}g \int d^{3}k \int d^{3}r' \chi(\mathbf{\vec{k}},0)\psi^{2}(\mathbf{\vec{r}}'-\mathbf{\vec{V}}t) \\ \times e^{i\mathbf{\vec{k}}\cdot(\mathbf{\vec{r}}-\mathbf{\vec{r}}')}.$$
(13)

For a fluid, the behavior of  $\chi(\vec{k}, 0)$  for small wave vectors  $\vec{k}$  is known to be<sup>10</sup>

$$\lim_{k\to 0} \chi(\mathbf{k}, 0) = -\rho/mc^2,$$

where c is the isothermal sound velocity. For the ideal gas,  $c^2 = kT/m$ ,  $\chi(\mathbf{k}, 0) - -\rho\beta$ , and Eq. (13) gives

$$\delta\rho(\vec{\mathbf{r}},t) = -\rho\beta g \psi^2(\vec{\mathbf{r}}-\vec{\nabla}t). \tag{14}$$

Comparing this with the relation

$$\rho(\mathbf{\vec{r}}-\mathbf{\vec{V}}t)=e^{-\beta_g\psi^2(\mathbf{\vec{r}}-\mathbf{\vec{V}}t)}=1-\rho\beta_g\psi^2(\mathbf{\vec{r}}-\mathbf{\vec{V}}t)+\cdots,$$

we see that the term  $\chi(\vec{k}, 0)$ , which yields the static response to the moving electron in linear response theory has already been included in  $\rho(\vec{r} - \vec{V}t)$ . Proceeding to the next term in Eq. (11),

$$\delta\rho(\vec{\mathbf{k}},\omega) = [d\chi(\vec{\mathbf{k}},\omega)/d\omega]_0 \omega V(\vec{\mathbf{k}},\omega)$$
(15)

and writing  $\chi(k, \omega)$  in terms of real and imaginary parts,  $\chi = \chi' + i\chi''$ , we have, as previously remarked

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$$\left(\frac{d\chi}{d\omega}\right)_{0} = i \left(\frac{d\chi''}{d\omega}\right)_{0}$$
$$= i C_{k}.$$
(16)

The imaginary part  $\chi''$  is obtainable from  $S(k, \omega)$ , the dynamic structure factor for the gas,<sup>10</sup>

$$\chi^{\prime\prime}(\vec{k},\,\omega) = -\pi(1 - e^{-\beta\,\omega})S(\vec{k},\,\omega) \tag{17}$$

so that

$$C_{k} = \pi \beta \rho S(\vec{k}, 0) . \tag{18}$$

Then the space-time density fluctuation from this term is

$$\delta\rho(\mathbf{\ddot{r}},t) = i(2\pi)^{-4} \int d^{3}k \int d\omega \,\omega C_{k} V(\mathbf{\ddot{k}},\omega) \,e^{i\,\omega t} \,. \tag{19}$$

The integral over  $\omega$  in Eq. (19) may be written

as

$$\int d\omega \,\omega V(\vec{k},\,\omega) \,e^{i\,\omega\,t} = -i\,\frac{d}{dt}\int V(\vec{k},\,\omega) \,e^{i\,\omega\,t}d\,\omega \quad (20)$$

and, expressing  $V(\mathbf{k}, \omega)$  in the form given by Eq. (10),

$$d\omega \,\omega V(\vec{\mathbf{k}},\,\omega) \,e^{i\,\omega\,t}$$

$$= -2\pi i g \,\frac{d}{dt} \int d^{3}r' \,e^{i\,\vec{\mathbf{k}}\cdot\vec{\mathbf{r}}\cdot} \,\psi^{2}(\vec{\mathbf{r}}'-\vec{\nabla}t)$$

$$= 2\pi i g \int d^{3}r' \,e^{i\,\vec{\mathbf{k}}\cdot\vec{\mathbf{r}}\cdot} \,\vec{\nabla}\cdot\vec{\nabla}'\psi^{2}(\vec{\mathbf{r}}'-\vec{\nabla}t) \,, \quad (21)$$

in which the gradient operator is taken with respect to  $\vec{r}' - \vec{V}t$ . Inserting Eq. (21) into Eq. (19), and replacing  $\vec{r}' - \vec{V}t$  by  $\vec{r}''$ ,

$$\begin{split} \delta\rho(\mathbf{\vec{r}},t) &= \delta\rho(\mathbf{\vec{r}}-\mathbf{\vec{\nabla}}t) \\ &= -(2\pi)^{-3}g \int d^{3}r^{\prime\prime} [\mathbf{\vec{\nabla}}\cdot\mathbf{\vec{\nabla}}\psi^{2}(r^{\prime\prime})] \int d^{3}k \, C_{k} \exp[-i\mathbf{\vec{k}}\cdot(\mathbf{\vec{r}}-\mathbf{\vec{\nabla}}t-\mathbf{\vec{r}}^{\prime\prime})] \,, \end{split}$$

(22)

so that the density fluctuation  $\delta \rho$  is stationary in the coordinate system which moves with the selftrapped state. Equation (22) provides the desired connection between  $\delta \rho$  and  $\psi$ , and when inserted in the last term of Eq. (7) gives the free energy  $F_t$  as a functional of the electron wave function  $\psi$ . Minimization of  $F_t$  with respect to  $\psi$  then produces the Schrödinger wave function for the moving electron. Comparison of Eq. (1) for the free energy  $F_t^0$  of the stationary electron with Eq. (7) giving  $F_t$  for the moving electron indicates that  $\psi_0(\vec{\mathbf{r}})$  and  $\psi(\vec{\mathbf{r}}-\vec{\mathbf{V}}t)$  satisfy different Schrödinger equations, because of the added fluctuation term in Eq. (7). Were this term not present,  $\psi(\vec{\mathbf{r}} - \vec{\mathbf{V}}t)$  would satisfy the same Schrödinger equation as  $\psi_0(\mathbf{r})$ , Eq. (3), indicating  $\psi(\mathbf{r} - \mathbf{V}t)$  $=\psi_0(\vec{r}-\vec{V}t)$ , and the shape of the self-trapped state would remain undistorted as it moves through the gas. We now argue that such shape distortions can be safely neglected for sufficiently small velocities V, when the last term in Eq. (7) is small. Since this term may then be regarded as a perturbation, and since it depends on  $V^2$ , we will have  $\psi(\mathbf{\tilde{r}} - \mathbf{V}t) = \psi_0(\mathbf{\tilde{r}} - \mathbf{V}t) + O(V^2)$ . Now  $F_t$  is an extremum for  $\psi = \psi_0$  (in the absence of the

fluctuation term), so changes in  $\psi$  of the order  $\delta \psi = \psi - \psi_0$  will produce changes in  $F_t$  of the order  $(\delta \psi)^2$ . Including fluctuations produces a  $\delta \psi$  proportional to  $V^2$ , and a  $\delta F_t$  proportional to  $V^4$ , and hence negligible for small V. Therefore the wave function for the moving trapped state  $\psi(\vec{\mathbf{r}} - \vec{\nabla}t)$  can be taken as the (known) displaced wave function  $\psi(\vec{\mathbf{r}} - \vec{\nabla}t) = \psi_0(\vec{\mathbf{r}} - \vec{\nabla}t)$  for the stationary trapped state in Eq. (7) for  $F_t$  and as well in Eq. (22) for  $\delta \rho(r, t)$ . It then remains to characterize the gas response function  $C_k$  in Eq. (22). The dynamic structure factor  $S(k, \omega)$  for a gas in the small  $\vec{k}$ ,  $\omega$  regime is known to be a Lorentzian representing thermal diffusion<sup>10</sup>:

$$S(k, \omega) = \frac{1}{\pi} \frac{Dk^2}{\omega^2 + (Dk^2)^2},$$
 (23)

where D, the diffusion constant depends on the interactions between gas atoms. It may at first glance appear unjustified to have earlier treated the gas atoms as noninteracting in calculating free energy  $F_t$ , and now to use a response function characterized by these previously neglected interactions. However, this merely reflects the circumstance that although these interactions

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make only very small corrections to equilibrium properties, they are nonetheless important in determining the thermal diffusion. From Eqs. (23) and (18) follows

$$C_{k} = \beta \rho / Dk^{2} , \qquad (24)$$

and the integral over  $C_k$  in Eq. (22) is

$$\int d^{3}k C_{k} \exp[-ik \cdot (\vec{\mathbf{r}} - \vec{\nabla}t - \vec{\mathbf{r}}^{\prime\prime})] = \frac{4\pi\beta\rho}{D|\vec{\mathbf{r}} - \vec{\nabla}t - \vec{\mathbf{r}}^{\prime\prime}|} ,$$
(25)

resulting in the following expression for the fluctuation  $\delta \rho$ :

$$\delta\rho(\mathbf{\ddot{r}}-\mathbf{\vec{V}}t) = \frac{-\beta\rho g}{2\pi^2 D} \int d^3 r^{\prime\prime} \frac{\mathbf{\vec{V}}\cdot\mathbf{\vec{\nabla}}\psi^2(\mathbf{\ddot{r}}^{\prime\prime})}{|\mathbf{\ddot{r}}-\mathbf{\vec{V}}t-\mathbf{\ddot{r}}^{\prime\prime}|}.$$
 (26)

This gives the density fluctuations in the gas outside of the moving self-trapped state. It carries the same restrictions for validity as the Lorentzian form for  $S(k, \omega)$  in Eq. (23), namely the distance  $|\mathbf{\tilde{r}} - \mathbf{\tilde{V}}t|$  should be outside of the trapped state by at least a mean free path for atom-atom collisions. For smaller distances, the gas atoms respond more like free particles, and a simple calculation enforces the expectation that the contribution to  $\delta \rho$  from this free-particle region is negligible. However, because of this rather illdefined lower limit on  $|\vec{\mathbf{r}} - \vec{\mathbf{V}}t|$  as well as the ambiguity involved in defining the boundary of the self-trapped state when the density profile around the electron is by no means sharp, we can only estimate the size of  $\delta \rho$ . Consistent with these constraints, we assume  $|\vec{r} - \vec{V}t| \gg |\vec{r}''|$ ; approximate the denominator in Eq. (26) by

$$\left|\mathbf{\ddot{r}} - \mathbf{\vec{\nabla}}t - \mathbf{\ddot{r}}^{\prime\prime}\right| \cong \left|\mathbf{\ddot{r}} - \mathbf{\vec{\nabla}}t\right|^{-1} \left(1 + \frac{\mathbf{\ddot{r}}^{\prime\prime} \cdot (\mathbf{\ddot{r}} - \mathbf{\vec{\nabla}}t)}{|\mathbf{\ddot{r}} - \mathbf{\vec{\nabla}}t|^2}\right), \qquad (27)$$

integrate over polar angles of  $\mathbf{\tilde{r}}''$ , and obtain

$$\delta\rho(\vec{\mathbf{r}} - \vec{\mathbf{V}}t) \cong \frac{-2\beta\rho g}{3\pi D} \frac{\vec{\mathbf{V}} \cdot (\vec{\mathbf{r}} - \vec{\mathbf{V}}t)}{|\vec{\mathbf{r}} - \vec{\mathbf{V}}t|^3} \\ \times \int_0^\infty r''^3 \frac{d}{dr''} \psi_0^2(r'') dr'' \,. \tag{28}$$

Integration by parts then gives

$$\delta\rho(\vec{\mathbf{r}} - \vec{\mathbf{V}}t) \cong \frac{\beta\rho g}{2\pi^2 D} \frac{\vec{\mathbf{V}} \cdot (\vec{\mathbf{r}} - \vec{\mathbf{V}}t)}{|\vec{\mathbf{r}} - \vec{\mathbf{V}}t|^3}.$$
(29)

The difference in free energies between a moving and a stationary self-trapped state, from Eqs. (1) and (7) is

$$F_{t} - F_{t}^{0} = \beta^{-1} \int d^{3}r \frac{[\delta\rho(\vec{\mathbf{r}}, t)]^{2}}{\rho_{0}(\vec{\mathbf{r}} - \vec{\nabla}t)}$$
$$= \frac{1}{2}m^{*}V^{2}. \qquad (30)$$

Here we can safely replace  $\rho_0(\vec{r} - \vec{V}t)$  by the

uniform density  $\rho$  for the restricted range of distances for which Eq. (29) is valid,  $|\vec{\mathbf{r}} - \vec{\mathbf{V}}t| > R$ . Then integration yields the result

$$m^* = \frac{2}{3\pi^3} \frac{\beta \rho}{R} \left(\frac{g}{D}\right)^2.$$
(31)

Accounting for the translational motion of the electron, the difference in free energy of self-trapped and free-electron states will be given by  $-\frac{3}{2}kT\ln(m^*/m)$ .

#### **III. NUMERICAL ESTIMATES**

Numerical estimates are now made of these results for self-trapped electrons in helium gas, along the stable limit line, and summarized in Table I. In Ref. 8, values of gas density  $\rho$  and temperature T at which the self-trapped state becomes stable  $(F_t^0 = F_f^0 = \rho g)$  were shown to be given by (Eq. 4.33 of Ref. 8)

$$(4\pi k)^{-1}g^{5/2}(2m/\hbar^2)^{3/2}\rho^{3/2}/T = 11.605.$$
 (32)

For application to helium gas we use a scattering length a in  $g = 2\pi a\hbar^2/m$  corrected for multiple scattering by a Wigner-Seitz method<sup>11</sup> ( $a \rightarrow 0.62$  Å as  $\rho \rightarrow 0$ ). To calculate an effective radius  $R_0$  for the self-trapped state, we define  $R_0$  as the classical turning point for a gas atom in the repulsive potential  $g\psi_0^2(R)$ ,  $g\psi_0^2(R_0) = \frac{3}{2}kT$ . Since the density profile around the electron is  $\rho(R)$  $=\rho \exp[-\beta g \psi_0^2(R)]$ , this definition of  $R_0$  requires  $\rho(R_0) = \rho e^{-3/2}$ . Figure 5 of Ref. 8 gives the density profile along the stable limit line as a function of a dimensionless length  $z = (2m\rho g/\hbar^2)^{1/2}R$ , and indicates that  $\rho(z_0) = \rho e^{-3/2}$  corresponds to  $z_0 = 1.7$ , or  $R_0 = 19.3/\sqrt{\rho}$  Å, where  $\rho$  is the gas density in units of 10<sup>21</sup> cm<sup>3</sup>. As previously remarked, the distance R appearing in Eq. (31) is to be taken equal to  $R_0$  increased by a mean free path l, for which we use<sup>12</sup>  $l = (\frac{1}{2}\pi)^{1/2}(1/4\rho\sigma)$  $\approx 10.45/\rho$  Å for a He-He cross section  $\sigma \approx 30$  Å<sup>2</sup>.<sup>13</sup> This leads to the values of R given in the third column of Table I for four values of  $\rho$  and T along the stable limit line. Values of the diffusion constant D for helium gas at these densities and temperatures, obtained from experimental measurements of viscosity  $\eta_{1}^{14}$  using the approximate relation  $D \cong \eta/M\rho$ , are given in the fourth column of Table I. As a check on the self-consistency of using the linear response theory to calculate  $\delta \rho$ , which requires  $\delta \rho / \rho \ll 1$ , we calculate the maximum value for this ratio, which, according to Eq. (29) occurs for  $\vec{r} - \vec{\nabla}t = \vec{R}$ , and in the direction of  $\vec{\mathbf{V}}$ . Results are given in the fifth column of Table I, with V measured in cm/sec, and indicate a satisfactory smallness of  $\delta \rho / \rho$  for speeds V up to thermal velocities of helium gas

<i>T</i> (°K)	$ ho \ (10^{21} \ { m cm}^{-3})$	$D \ (10^{-3} \ {\rm cm}^2/{\rm sec})$	R (Å)	$\frac{10^5 \ (\delta \rho)_{\max}}{\rho}$	$\frac{m^*}{M}$	$-\frac{3}{2}\frac{KT}{\rho g}\ln\frac{m^*}{m}$
10	2.0	1.64	18.8	3.0V	20.8	-0.26
20	2.9	1.86	14.9	2.1V	14.8	-0.35
30	3.6	1.89	12.9	1.8V	13.9	-0.41
40	4.3	1.93	11.6	1.7V	13.2	-0.46
50	4.8	2.03	11.0	1.4V	11.2	-0.51

TABLE I. Estimates of effective mass  $m^*$  and related parameters for four sets of  $\rho$ , T values along the stable limit line for stationary self-trapped electrons.

atoms,  $V \cong 10^4$  cm/sec. The sixth column of Table I gives values for the effective mass  $m^*$ as fractions of helium mass M, obtained from Eq. (31). These values are somewhat smaller (by ~20%) than the hydrodynamic estimate of onehalf the mass of atoms excluded by the trapped state.

We now estimate the contribution to the difference in free energies between self-trapped and free states, due to translational motion in the absence of an external electric field. Because of the dissipation, the average velocity Vof the self-trapped state now decays with time to zero, starting from any assumed initial value,



FIG. 1. Solid line is the density-temperature curve for the transition to the self-trapped electron state in fluid helium, obtained from Eq. (32), using the numerical factor 9.49 in place of 11.6. The triangles represent experimental points denoting isothermal measurements (Refs. 2, 4, 15) of mobilities of  $10^{-1}$  of the semiclassical value for electrons in plane-wave states (see Ref. 7).

but according to equilibrium statistical mechanics, due to random fluctuation forces, the meansquare instantaneous velocity  $\langle v^2(t) \rangle$  goes to its equipartition value  $\langle v^2(t) \rangle - 3kT/m^*$ . Assuming that  $m^*$  in this equilibrium result is the same as that we calculated under steady state conditions, we get the values of  $-\frac{3}{2}(kT/\rho g)\ln(m^*/m)$  given in the last column of Table I, representing the translational contribution to the difference in free energy of self-trapped and free states, in units of  $\rho g$ . Although the numerical estimates involved in obtaining  $m^*$  are rather crude, the insensitivity of the factor  $\ln(m^*/m)$  to these uncertainties implies that these free energy estimates should be correct at least in regards to order of magnitude. Previous calculations, which omitted the translational contribution indicated a metastable region for self-trapped states, where  $F_t^0$  had a local minimum, but with minimum value larger than  $F_f^0 = \rho g$  for a free state, by about  $0.04\rho g$ . (See Fig. 7 of Ref. 8.) From the values in Table I for the translational contribution to the free energy, it is clear that these previously found metastable states are now stable. The effect is to increase the region in the  $\rho$ , T plane where self-trapped states are favored to include the previously designated metastable region. As shown in Ref. 8 this amounts to replacing the numerical factor 11.605 in Eq. (32) by 9.4905, thus increasing the maximum temperature T at which self-trapped states exist, for a fixed density  $\rho$ , by about 22%. In Fig. 1, the temperature-density curve for the transition to the selftrapped state is compared with isothermal measurements of the density at which the electron drift mobility sharply drops.<sup>2,4,15</sup> The quoted increase in theoretical maximum temperatures for self-trapped states upon including translational motion is seen to result in a good fit between theory and experiment.

Finally we note that the effective mass m \* appearing in the equipartition result  $\langle v^2(t) \rangle = 3kT/m^*$  has been measured in <sup>4</sup>He at T = 4.2 K and  $\rho \cong 2 \times 10^{21}$  cm<sup>-3</sup> to be in the range  $3M \le m^* \le 5M$ , where M is the mass of a <sup>4</sup>He atom.<sup>16</sup> These values appear to be about  $\frac{1}{5}$  of the estimates of  $m^*$  given in Table I, which will tolerate some reduction (for example by increasing the distance l in  $R = R_0 + l$  to  $R = R_0 + 2l$ , say), but nothing like a factor of  $\frac{1}{5}$ . It appears possible that the correct value for  $m^*$  in the equilibrium free energy may be substantially less than the value for  $m^*$  calculated for a steady average velocity V. Namely, the mass  $m^*$  appearing in the equipartition result  $\langle v^2 \rangle = 3kT/m^*$  should be determined by the inertial

- <sup>1</sup>I. M. Lifshitz, Usp. Fiz. Nauk <u>83</u>, 617 (1964) [Sov. Phys. Usp. <u>7</u>, 549 (1965)]; Sov. Phys. JETP <u>26</u>, 462 (1968).
- <sup>2</sup>J. L. Levine and T. M. Sanders, Jr., Phys. Rev. <u>154</u>, 138 (1967).
- <sup>3</sup>M. A. Krivoglaz, Sov. Phys. Solid State <u>12</u>, 2840 (1971); Usp. Fiz. Nauk <u>111</u>, 617 (1973) [Sov. Phys. Usp. 16, 856 (1974)].
- <sup>4</sup>H. R. Harrison and B. E. Springett, Phys. Lett. A <u>35</u>, 73 (1971).
- <sup>5</sup>A. G. Khrapak and I. T. Yakubov, Zh. Eksp. Teor. Fig. <u>69</u>, 2042 (1975) [Sov. Phys. JETP <u>42</u>, 1036 (1976)].
- <sup>6</sup>V. B. Shikin, Usp. Fiz. Nauk <u>121</u>, 457 (1977) [Sov. Phys. Usp. 20, 226 (1977)].
- <sup>7</sup>J. P. Hernandez, Phys. Rev. A <u>7</u>, 1755 (1973); Phys. Rev. B <u>11</u>, 1289 (1975).

response of the self-trapped state to random collisions with the gas atoms, and these may occur too rapidly for the full steady state diffusive flow to be set up around it, implying a reduced value for the equipartition  $m^*$ .

However, even a severe reduction of the values of  $m^*$  appearing in the term  $-\frac{3}{2}kT\ln(m^*/m)$  by as much as  $\frac{1}{5}$  of the values quoted in Table I does not alter the conclusion that metastable selftrapped states are converted into stable states upon including translational free energy contributions.

- <sup>8</sup>R. L. Moore, C. L. Cleveland, and H. A. Gersch, Phys. Rev. B 18, 1183 (1978).
- <sup>9</sup>L. D. Landau and I. M. Lifshitz, *Statistical Physics* (Addison-Wesley, Reading, Mass., 1958).
- <sup>10</sup>D. Pines and P. Nozières, *Theory of Quantum Liquids* (Benjamin, New York, 1966).
- <sup>11</sup>See for example, T. P. Eggarter, Phys. Rev. A <u>5</u>, 2496 (1972).
- <sup>12</sup>K. Huang, Statistical Mechanics (Wiley, New York, 1963).
- <sup>13</sup>R. Feltgen, H. Pauly, F. Torello, and H. Vehmeyer, Phys. Rev. Lett. 30, 820 (1973).
- <sup>14</sup>As given by W. E. Keller, Phys. Rev. <u>105</u>, 41 (1957).
   <sup>15</sup>J. A. Janke, M. Silver, and J. P. Hernandez, Phys. Rev. B 12, 3420 (1975).
- <sup>16</sup>J. Howell and M. Silver, Phys. Rev. Lett. <u>34</u>, 921 (1975).