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$$\frac{P_s^{\max}(\hbar\omega_+^0)}{P_s^{\max}(\hbar\omega_-^0)} \simeq \frac{\omega_t}{\omega_l} = \left(\frac{\epsilon_\infty}{\epsilon_0}\right)^{1/2} .$$

In the present case, however, the situation is quite different at small $k_\perp$, where the above maxima take place, because for $k_\perp \ll k_s$ the terms in $\cos(\omega a/v)$ in (43) are larger than the terms in $\sin(\omega a/v)$ by the factor $k_s^2/k_\perp^2 \gg 1$, so that now the above-mentioned approximation is valid over the entire frequency range of interest.

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Electron Localization in Disordered Systems

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The general features of the electronic structure of disordered materials are investigated using Edwards's model of an electron in the presence of dense weak random scatterers. This model is equivalent to that of Zittartz and Langer which considers an electron in a Gaussian random potential. A self-consistent-field (SCF) formulation, which generalizes and clarifies that of earlier works, is used to demonstrate the presence of a mobility edge, a transition between localized and extended states at energy E_c. Particular emphasis is placed upon the symmetry and analytic structure of the SCF and upon how the SCF theory introduces the symmetry breaking which leads the localized states. In particular, the localization probability, the probability density that an electron with energy E returns to its initial position after infinite time, is found to vary as $|E-E_c|^{13/6}$ for $E \le E_c$ and to vanish for $E > E_c$. Below the mobility edge the size of the localized states is found to vary as $|E-E_c|^{-2/3}$. Although questions concerning electron localization can rigorously be answered from a consideration of quantities which are the averages of a product of two Green's functions, such as the localization probability, the SCF theory obtained from the average Green's function alone gives rise to the same analytic structure as the SCF theory which is based upon the localization probability. This indicates that it may generally be possible to extract information concerning electron localization from the simpler average Green's function. The SCF theory is also generalized to consider quantities which are related to electron mobility. Although the mathematical difficulties encountered in this case resemble those of the general three-body problem, a proof is given that the low-lying states do, in fact, give a vanishing mobility. In addition, the SCF is used to derive the model which Mott employs to show that the mobility due to electrons in localized states vanishes as $\omega^2 \ln\omega$ as the frequency ω tends to zero.

I. INTRODUCTION

Because of the periodic arrangement of atoms or molecules in crystalline materials, the universal features of their electronic structure are easily deduced; corresponding universal features of the electronic structure of disordered materials are currently being sought.[1] But the lack of periodicity in disordered materials leads to the loss of simplification that is provided by the Bloch-Floquet theorem, and only very simple model Hamiltonian have been employed in the study of the electronic structure of these materials. However, if there are indeed universal characteristics of this electronic structure, the models employed should be adequate to qualitatively represent these generic properties.[1]

Since the pioneering work of Anderson concerning the absence of diffusion in certain random lattices,[2] interest has been focused upon two questions: (i) Are the electronic states in disordered systems localized or extended, and (ii) which features of the model Hamiltonian determine electronic localization as the electron's energy is varied?[1–25] This concern with the question of electron localization has been heightened by the use of the Mott-Cohen-Fritzsche-Ovshinsky (CFO) model[3–5,15] to explain the general properties of the electronic structure of amorphous semiconductors.[26] This model, which is based upon some (assumed) general features of the electronic structure in disordered materials, requires the existence of localized electronic states in the band tails and extended ones for energies in the center of the band. Thus, the region of energy in the neighborhood of the energy E_c where the electronic states change from localized to extended is of central importance. This energy is termed the mobility edge, since by definition the localized states have a vanishing mobility at 0 °K.

The mobility edge must bear some mathematical analogies to critical points (and/or phase transitions) in fluid and magnets.[9–11,13,22,23] It is clear from the use of classical analyses such as percolation theory[13] that for energies near E_c the long-range potential fluctuations determine whether the electron is localized.[22] This analogy between electron localization and critical points (or phase transitions) reinforces the belief that simple models are both useful and necessary in the study of the electronic structure of disordered systems. (Compare the simplicity, yet generality, of the Ising model.)

A number of different models and methods have been used to study electronic structure in random systems. Some of these, deriving from Anderson's original work, consider the probabilistic convergence or divergence of the renormalized perturbation series for the electron's self-energy (a one-electron model).[2,17–20] While this approach can provide criteria for the determination of E_c, it gives little information, if any, concerning the nature of the electronic states themselves or about the mobility in the region of E_c. Just as mean-field theories are useful in the description of phase changes (except near critical points), so are they in the study of the electronic structure of disordered materials. The coherent-potential approximation (CPA),[27] which is just of this mean-field variety, adequately describes the electronic structure of disordered systems in the energy regions where there are extended states. As expected from the analogy with phase changes, the CPA fails in the region near E_c; it predicts only extended states. Cluster-theory generalizations of the CPA can provide the requisite band tails of localized states,[23,28,29] but they too must fail in the region near E_c because of the neglect of long-range potential fluctuations.[23] Despite what has been learned from classical and semiclassical models, a fully quantum-mechanical framework is clearly needed.

The present work employs the same model (an electron in the presence of a system of dense weak random scatterers) as used by Edwards and Gulyaev to discuss the density of states of a heavily doped semiconductor.[8] This model was subsequently used by Zittartz and Langer to consider the low-lying levels in a random potential[7] in a reformulation of the work of Halperin and Lax.[6] Zittartz and Langer[7] considered a self-consistent-field formulation which had been used earlier by Edwards in a discussion of the mathematically isomorphic problem of polymer-excluded volume (self-avoiding random walks).[30,31] A number of the approximations employed by Zittartz and Langer are clearly only valid for the low-lying states, while some of those used by Edwards in the polymer problem still require further clarification. Thus, in this paper it is necessary to review this self-consistent-field theory, to exhibit its fundamental aspects and shortcomings, and to present some generalizations thereof. This clarified self-consistent-field (SCF) theory is then used to demonstrate the presence of a mobility edge at E_c. That is, it is shown that for energies less than E_c the electronic states are localized, while for energies greater than E_c they are extended. The localization criterion implied is chosen to be the absence of diffusion. Thus, if $a_0(t, E)$ represents the probability amplitude that an electron with energy E which is initially at the origin returns to the origin at time t, then $p_0(E) = \lim\langle |a_0(t, E)|^2\rangle$ as $t \to \infty$ represents the ensemble-averaged probability (over all configurations of the disordered system) that the electron can return to its starting point as $t \to \infty$.[1,2,17,23] Thus we show that within this model $p_0(E) \equiv 0$ for $E > E_c$, but $p_0(E) \neq 0$ for $E < E_c$. The nature of the electronic structure is manifest, and it is shown that the range of the localized states varies as $R_0 \propto [-(E - E_0)]^{-2/3}$ and that the localization probability is $p_0(E) \propto [-(E - E_c)]^{13/6}$ in the region near the mobility edge (for $E < E_c$).[23] The present theory also allows the evaluation of the mobility. Although the mathematical complexities expected in this case are not unlike those encountered in the three-body problem, it is still possible to demonstrate the absence of mobility (at 0 °K) in the region of a finite density of states. These results lead to the model used by Mott to show that the conductivity due to electrons in localized states varies as $\omega^2 \ln \omega$ as the frequency $\omega \to 0$.[3]

II. MODEL AND PATH-INTEGRAL REPRESENTATION

Consider a single electron in the presence of a set of N scatterers, where the scatterers have a density $\rho = N/\Omega$, and Ω is the volume of the system. If $v(\vec{r} - \vec{R}_l)$ is the electron-scatterer interaction, the one-electron Hamiltonian is

$$H(\{\vec{R}_j\}) = \frac{\hbar^2}{2m} \nabla_{\vec{r}}^2 + \sum_{j=1}^{N} v(\vec{r} - \vec{R}_j) , \tag{2.1}$$

where m is the electron mass. The Hamiltonian (2.1) obviously depends parametrically on the positions of the stationary scatterers. Because of the mathematical complexities of the problem at hand, it is imperative to consider the simplest case at each stage in order to eliminate the need for extraneous mathematical approximations. Thus the scattering centers are taken to be distributed randomly with the probability density

$$P(\{\vec{R}_j\}) = \Omega^{-N} . \tag{2.2}$$

As noted in earlier works, the use of (2.2) is satisfactory in the consideration of heavily doped semiconductors with short-range electron-scatterer interactions (where the correlations between scatterers can safely be ignored).[7,8]

For a given configuration of the scatterers the one-electron causal Green's function obeys the Schrödinger equation

$$\left(i\hbar \frac{\partial}{\partial t} - H(\{\vec{R}_j\}) \right) \mathcal{G}(\vec{r}\,\vec{r}\,'; t \,|\, \{\vec{R}_j\}) = \delta(\vec{r} - \vec{r}\,')\,\delta(t). \tag{2.3}$$

We are generally concerned with properties which are averages over different replicas of the identically prepared system. Furthermore, measured properties are also averages over the many different environments in a single sample. Thus, it is only necessary to consider properties which are averages over all configurations of the scatterers. The average Green's function is defined by

$$G(\vec{r}\,\vec{r}\,'; t) = \Omega^{-N} \int \cdots \int \prod_{j=1}^{N} d\vec{R}_j \, \mathcal{G}(\vec{r}\,\vec{r}\,'; t \,|\, \{\vec{R}_k\}) \equiv \langle \mathcal{G} \rangle . \tag{2.4}$$

Equation (2.4) implies that $G(\vec{r}\vec{r}\,'; t)$ has the usual properties of Green's functions; e.g., it satisfies the initial condition

$$G(\vec{r}\vec{r}\,'; t) \to (i\hbar)^{-1} \delta(\vec{r} - \vec{r}\,') \quad \text{as } t \to 0^+ . \tag{2.5}$$

Thus G of (2.4) can be considered to describe the propagation of a particle, even though it does not correspond to a "real" electron in a specific configuration of the random system. Approximation techniques which are useful in calculating one-electron Green's functions will also be useful for G in (2.4). We therefore speak of G as describing the motion of a fictitious "average electron" which moves in the "averaged system." As usual, the average Green's function in energy space is the Fourier transform of (2.4),

$$G(\vec{r}\vec{r}\,'; E + i\epsilon) = \int_0^\infty dt \, e^{-i(E+i\epsilon)t/\hbar} \, G(\vec{r}\vec{r}\,'; t) , \tag{2.6}$$

and the average density of states is

$$\rho(E) = -(1/\pi) \operatorname{Im} \operatorname{Tr} G(\vec{r}\vec{r}\,'; E + i\epsilon) . \tag{2.7}$$

Before explicitly introducing the path-integral representation of G, we can give simple physical insight into its form. The "average system" is translationally invariant. Since the "average electron" cannot in general be a free electron, the only possible interaction can be an electron-electron self-interaction. That is, upon averaging out the positions of the scatterers, there is nothing else left for the electron to interact with but itself. Although a completely quantum-mechanical theory is employed in this paper, it is convenient to first describe the electron classically. Then, if $\vec{r}(t)$ describes the average electron's trajectory, the self-potential is of the symbolic form

$$V_{\text{eff}} = V[\vec{r}(t) - \vec{r}(t')] + (\text{three time terms}) + \cdots . \tag{2.8}$$

The general case of (2.8) is of enormous mathematical complexity, and it is therefore imperative to consider the simplest possible case where only the two-time term $V[\vec{r}(t) - \vec{r}(t')]$ is retained. This term is the only one that survives (see below) in the convenient mathematical limit,

$$\lim_{\rho v^2} \equiv \lim(\rho \to \infty, \; v \to 0, \; \rho v^2 \to \text{finite}), \tag{2.9}$$

where the density of scatterers is large, but the electron-scatterer interaction is weak. This limit is appropriate to some cases of heavily doped semiconductors. More importantly, however, if there are universal features of electronic structure in disordered systems, this simplest model is all that is necessary to exhibit them.

It is amusing to pause to compare (2.9) with the familiar long-time ($t \to \infty$) weak-coupling ($v \to 0$, but $v^2 t \to$ finite) limit in ordinary classical statistical mechanics. In the statistical-mechanical case, this limit provides an essential simplification. However, in the limit (2.9), the present problem is reduced to one that is still mathematically intractable, as it is isomorphic to the polymer-excluded volume problem,[1,9-11,23] that is, the problem of the description of self-avoiding random walks. This mathematical analogy is reason enough for ignoring the higher terms in (2.8).

In the limit (2.9), Hamilton's principal function for the classical average electron is of the form

$$S[\vec{r}(\tau)] = \int_0^t d\tau \, \tfrac{1}{2} m \, [\dot{\vec{r}}(\tau)]^2$$

$$-\int_0^t d\tau \int_0^t d\tau' \, V[\vec{r}(\tau)-\vec{r}(\tau')] \,. \tag{2.10}$$

We, of course, are interested in the quantum-mechanical description of this average electron. However, the passage from (2.10) to the usual Hamiltonian quantum mechanics is not convenient, since there is no conserved, or nearly conserved, Hamiltonian. Thus, it is necessary to consider instead the Lagrangian-Feynman path-integral formulation of quantum mechanics where every trajectory $r(\tau)$ going from $\vec{r}(0)=\vec{r}'$ to $\vec{r}(t)=\vec{r}$ is given the "weight" $\exp\{iS[r(\tau)]/\hbar\}$.

We briefly review the introduction of the path-integral representation[32] of G in order to introduce the requisite notation and concepts. The mathematical details necessary to obtain the localization probability $p_0(E)$ are very similar to those used to obtain G. The one-electron Green's function defined by (2.3) has the usual path-integral representation

$$\mathcal{G}(\vec{r}\vec{r}\,';\, t\,|\{\vec{R}_j\}) = \theta(t)\int_{\vec{r}(0)=\vec{r}'}^{\vec{r}(t)=\vec{r}} \mathcal{D}[\vec{r}(\tau)] \times \exp\left[\frac{i}{\hbar}\int_0^t d\tau\left(\frac{m}{2}\,[\dot{\vec{r}}(\tau)]^2 - \sum_{j=1}^{N} v[\vec{r}(\tau)-\vec{R}_j]\right)\right], \tag{2.11}$$

where $\mathcal{D}[\vec{r}(\tau)]$ is the usual Feynman measure, $\dot{\vec{r}}(\tau)\equiv d\vec{r}(\tau)/d\tau$, and $\theta(t)$ is the Heaviside step function which makes G a causal Green's function. [The $\theta(t)$ will often be omitted for convenience.] As Edwards and Gulyaev note, the average (2.11), namely, (2.4), can be explicitly obtained because the $\{\vec{R}_j\}$ and therefore the $\{v[\vec{r}(\tau)-\vec{R}_j]\}$ are independent random variables.[8,21] The result is

$$G(\vec{r}\vec{r}\,';\, t) = \int_{\vec{r}(0)=\vec{r}'}^{\vec{r}(t)=\vec{r}} \mathcal{D}[\vec{r}(\tau)] \exp\left\{\frac{i}{\hbar}\,\frac{m}{2}\int_0^t d\tau[\dot{\vec{r}}(\tau)]^2 + \rho\int d\vec{R}\left[\exp\left(-\frac{i}{\hbar}\int_0^t d\tau\, v[\vec{r}(\tau)-\vec{R}]\right)-1\right]\right\}. \tag{2.12}$$

If the exponential in v in (2.12) is expanded in a power series in v, the result is just that introduced heuristically in (2.8). Equation (2.12) clearly describes a Green's function G which is translationally invariant. For, if we consider instead $G(\vec{r}+\vec{a},\, \vec{r}\,'+\vec{a};\, t)$, the change in variables $\rho(t)=\vec{r}(t)+\vec{a}$, $\vec{R}' = \vec{R}+\vec{a}$ on the right-hand side of (2.12) shows that $G(\vec{r}+\vec{a},\, \vec{r}\,'+\vec{a};\, t) = G(\vec{r},\, \vec{r}\,';\, t) = G(\vec{r}-\vec{r}\,',\, \vec{0};\, t)$.

The average potential is defined by

$$\overline{V} = \rho\int d\vec{R}\, v[\vec{r}(\tau)-\vec{R}] = \rho\int d\vec{R}\, v(\vec{R}) \tag{2.13}$$

and can be taken to be zero, thereby establishing the origin in energy. The limit (2.9) is now easily applied to (2.12). In the expansion of the exponential of v only the quadratic term survives, giving[1,8–11,21,23]

$$-\frac{\rho}{2\hbar^2}\int d\vec{R}\int_0^t d\tau\int_0^t d\tau'\, v[\vec{r}(\tau)-\vec{R}]\, v[\vec{r}(\tau')-\vec{R}] = \frac{-\rho}{2\hbar^2}\int_0^t d\tau\int_0^t d\tau'\, W[\vec{r}(\tau)-\vec{r}(\tau')] \,, \tag{2.14}$$

where

$$W(\vec{r}) = \int \frac{d^3k}{(2\pi)^3}\, e^{i\vec{k}\cdot\vec{r}}\, |v_{\vec{k}}|^2 \tag{2.15}$$

and $v_{\vec{k}}$ is the Fourier transform of $v(\vec{r})$. The final result is thus[1,8–11,21,23]

$$G(\vec{r}\vec{r}\,';\, t) = \int_{\vec{r}(0)=\vec{r}'}^{\vec{r}(t)=\vec{r}} \mathcal{D}[\vec{r}(\tau)] \exp\left(\frac{i}{\hbar}\,\frac{m}{2}\int_0^t d\tau\,[\dot{\vec{r}}(\tau)]^2 - \frac{\rho}{2\hbar^2}\int_0^t d\tau'\int_0^t W[\vec{r}(\tau)-\vec{r}(\tau')]\right), \tag{2.16}$$

as heuristically introduced from (2.10). [$W(r)$ can be easily generalized to include the pair correlation function, but there is no point in including the added complications.]

Note that, again making the analogy with polymer statistics, for imaginary times (2.16) is the distribution function for the end-to-end vector distribution for a continuous polymer chain with the segment-segment interaction $-\rho W$.

Having reviewed the model and the path-integral representation of G, consideration is now given to those quantities which are necessary to establish electron localization.

III. LOCALIZATION CRITERIA

The criterion for electron localization is, in this paper, chosen to be the absence of diffusion in disordered systems.[1,2,17,23] Let

$$c_0(t\,|\{\vec{R}_j\}) = \mathcal{G}(\vec{0}\vec{0};\, t\,|\{\vec{R}_j\}) \tag{3.1}$$

be the probability amplitude that an electron, which is moving in a given configuration of the random system and which is initially at the origin, returns to the origin at time t. The ensemble-averaged probability that the electron return to its starting point for long times is then

$$p_0 \equiv \lim_{t\to\infty} \Omega^{-N}\int\cdots\int \prod_{j=1}^{N} d\vec{R}_j\, |c_0(t\,|\{\vec{R}_k\})|^2 \equiv \lim_{t\to\infty} \langle |c_0(t\,|\{\vec{R}_k\})\rangle \,. \tag{3.2}$$

If $p_0\equiv 0$, all electronic states are extended, while if $p_0\neq 0$, the electron has a finite probability of returning, and some states must be localized.[1,2,17,23] Rather than considering p_0, it is more revealing to investigate the dependence of electron localization upon the energy of the electron. Let $\mathcal{G}(\vec{r}\vec{r}\,';\, E|\{\vec{R}_j\})$

be the time-independent Green's function. Using the general properties of Fourier transforms, it can be shown that in general,[1,17,23]

$$\lim_{t\to\infty} |\mathcal{G}(\vec{0}\vec{0};\, t\,|\{\vec{R}_j\})|^2 \equiv \int dE\, p_0(E\,|\{\vec{R}_j\}), \tag{3.3}$$

where

$$p_0(E\,|\{\vec{R}_j\}) \equiv \lim_{\epsilon\to 0^+} [(\epsilon/\pi)\, \mathcal{G}_0(E+i\epsilon\,|\{\vec{R}_j\}) \times \mathcal{G}_0(E-i\epsilon\,|\{\vec{R}_j\})] \tag{3.4}$$

and $\mathcal{G}_0(z\,|\{\vec{R}_j\})$ is shorthand for $\mathcal{G}(\overrightarrow{00};\, z\,|\{\vec{R}_i\})$. Taking averages of (3.3) over the random distribution of scatterer positions leads to

$$p_0 \equiv \int_{-\infty}^{\infty} dE\, p_0(E)\ , \tag{3.5}$$

where

$$p_0(E) = \Omega^{-N} \int\cdots\int \prod_{j=1}^{N} d\vec{R}_j\, p_0(E\,|\{\vec{R}_k\}) \equiv \langle p_0(E\,|\{\vec{R}_k\})\rangle\ . \tag{3.6}$$

$p_0(E)$ is therefore the probability density in energy space that an average electron with energy E can return to its initial position after an infinite time. Hence, if $p_0(E)\neq 0$, electronic states at energy E are localized; otherwise they are extended.

This criterion for electron localization, in effect, is equivalent to Mott's.[3-5] Mott defines localized states as those which do not contribute to the dc conductivity. If an average electron with energy E could contribute to the dc conductivity, given infinite time the probability distribution for the position of the electron would spread out roughly uniformly over the *accessible part* of the system. For a system with infinite volume, the probability that such an average electron returns to its initial position after infinite time must vanish. Using the same arguments for the case of a localized electron, it is clear that $p_0(E)$ must be proportional to the density of states at E per unit volume and inversely proportional to some measure of the volume of the localized state.

The evaluation of $p_0(E)$ requires the evaluation of the average of the product of two Green's functions just as in the case of the conductivity. The average of the product of $\mathcal{G}(E)\,\mathcal{G}(E')$ can be obtained from that of $\mathcal{G}(t)\,\mathcal{G}(t')$ by Fourier transformation, so we can consider the path-integral representation of the latter.[1,10] Squaring (2.11), averaging with (2.2), and taking the limit (2.9) simply leads to the path integral

$$\begin{aligned}\lim_{\rho v^2} \langle \mathcal{G}\mathcal{G}\rangle = &\int_{\vec{r}(0)=\vec{r}\,'}^{\vec{r}(t)=\vec{r}} \mathfrak{D}[\vec{r}(\tau)] \exp\left(\frac{i}{\hbar}\frac{m}{2}\int_0^t d\tau\,[\dot{\vec{r}}(\tau)]^2\right) \int_{\vec{\rho}(0)=\vec{\rho}\,'}^{\vec{\rho}(t')=\vec{\rho}} \mathfrak{D}[\vec{\rho}(\tau')] \exp\left(\frac{i}{\hbar}\frac{m}{2}\int_0^{t'} d\tau'[\dot{\vec{\rho}}(\tau')]^2\right.\\ &- \frac{\rho}{2\hbar^2}\int_0^t d\tau_1\int_0^t d\tau_2\ W[\vec{r}(\tau_1)-\vec{r}(\tau_2)] - \frac{\rho}{2\hbar^2}\int_0^{t'} d\tau_1'\int_0^{t'} d\tau_2'\ W[\vec{\rho}(\tau_1')-\vec{\rho}(\tau_2')]\\ &\left. - \frac{\rho}{2\hbar^2}\int_0^t d\tau\int_0^{t'} d\tau'\ W[\vec{r}(\tau)-\vec{\rho}(\tau')]\right)\ ,\end{aligned} \tag{3.7}$$

with W given by (2.15). Again the polymer-statistics analogy is revealing: For imaginary times (3.7) represents the end-vector distribution for a pair of interacting polymer chains.

IV. INTRODUCTION OF RANDOM FIELDS

The identity

$$\exp\left(-\frac{\rho}{\hbar^2}\int_0^t d\tau\int_0^t d\tau'\ W[\vec{r}(\tau)-\vec{r}(\tau')]\right) = \mathfrak{N}\int\delta\phi\ \exp\left(-\frac{i}{\hbar}\int_0^t \phi[\vec{r}(\tau)]d\tau - \frac{1}{2\rho}\int d\vec{r}\int d\vec{r}\,'\ \phi(\vec{r})\ W^{-1}(\vec{r}-\vec{r}\,')\,\phi(\vec{r}\,')\right)\ , \tag{4.1}$$

with

$$\mathfrak{N}^{-1} = \int\delta\phi\ \exp\left(-\frac{1}{2\rho}\int d\vec{r}\int d\vec{r}\,'\ \phi(\vec{r}) \times W^{-1}(\vec{r}-\vec{r}\,')\,\phi(\vec{r}\,')\right)\ , \tag{4.2}$$

has been introduced earlier in both the contexts of the polymer[30,31] and electron localization problems.[1,10,33] Here $W^{-1}(\vec{r}-\vec{r}\,')$ is the functional inverse of $W(\vec{r}-\vec{r}\,')$,

$$\int W(\vec{r}-\vec{r}\,'')\,W^{-1}(\vec{r}\,''-\vec{r}\,')\,d\vec{r}\,'' = \delta(\vec{r}-\vec{r}\,')\ . \tag{4.3}$$

If we interpret

$$P[\phi]\,\delta\phi = \mathfrak{N}\ \exp\left(-\frac{1}{2\rho}\int d\vec{r}\int d\vec{r}\,'\ \phi(\vec{r}) \times W^{-1}(\vec{r}-\vec{r}\,')\,\phi(\vec{r}\,')\right) \tag{4.4}$$

as the probability that the function ϕ has the particular value in function space between $\phi(\vec{r})$ and $\phi(\vec{r})+\delta\phi(\vec{r})$, then ϕ is a Gaussian random variable. In particular, it has zero mean and the variance is $W(\vec{r}-\vec{r}\,')$:

$$\langle\phi(\vec{r})\rangle_\Phi \equiv \int \phi(\vec{r})P[\phi]\delta\phi = 0 \,, \tag{4.5}$$

$$\langle\phi(\vec{r})\,\phi(\vec{r})\rangle_\Phi = W(\vec{r}-\vec{r}\,') \,. \tag{4.6}$$

[The functional integrals in (4.2) and (4.5) and (4.6) can be thought to be a regular integration over all the generalized Fourier coefficents of the expansion of $\phi(\vec{r})$ in any complete set of functions.] The identity (4.1) is easily verified by using the transformation

$$\phi(\vec{r}) = \phi'(\vec{r}) + \frac{i\rho}{\hbar}\int_0^t d\tau\, W[\vec{r}-\vec{r}(\tau)], \quad \delta\phi \equiv \delta\phi' \tag{4.7}$$

on the right-hand side of (4.1). Substituting (4.1) into (2.16) gives

$$G(\vec{r}\vec{r}\,';\, t) \equiv \langle G(\vec{r}\vec{r}\,';\, t;\, [\phi])\rangle_\Phi \,, \tag{4.8}$$

where

$$G(\vec{r}\vec{r}\,';\, t;\, [\phi]) = \int_{\vec{r}(0)=\vec{r}\,'}^{\vec{r}(t)=\vec{r}} \mathfrak{D}[\vec{r}(\tau)] \times \exp\left(\frac{i}{\hbar}\,\frac{m}{2}\int_0^t d\tau[\dot{\vec{r}}(\tau)]^2 - \frac{i}{\hbar}\int_0^t \phi[\vec{r}(\tau)]d\tau\right) . \tag{4.9}$$

But (4.9) just describes the Green's function for a single particle in the potential $\phi(\vec{r})$; thus it satisfies the simple Schrödinger equation

$$\left(i\hbar\,\frac{\partial}{\partial t} + \frac{\hbar^2}{2m}\,\nabla_{\vec{r}}^2 - \phi(\vec{r})\right) G(\vec{r}\vec{r}\,';\, t;\, [\phi]) = \delta(\vec{r}-\vec{r}\,')\,\delta(t) \,. \tag{4.10}$$

The Fourier transform of (4.8) can easily be performed formally to give

$$G(\vec{r}\vec{r}\,';\, E) \equiv \langle G(\vec{r}\vec{r}\,';\, E;\, [\phi])\rangle_\Phi \,, \tag{4.11}$$

where $G(E;\,[\phi])$ is just the corresponding time-independent Green's function defined by

$$\left(E + \frac{\hbar^2}{2m}\,\nabla_{\vec{r}}^2 - \phi(\vec{r})\right) G(\vec{r}\vec{r}\,';\, E;\, [\phi]) = \delta(\vec{r}-\vec{r}\,') \,. \tag{4.12}$$

We note that (4.11) and (4.12) along with the definition of the ϕ averaging [(4.4)–(4.6)] represents the starting point of the calculations of Zittartz and Langer.[7] The derivation is presented here because most of the above equations are to be used further. In particular, we can immediately express $\langle \mathcal{G}\mathcal{G}\rangle$ in terms of this ϕ average.[1,10,23] The result can be shown to be

$$\langle \mathcal{G}\mathcal{G}\rangle \rightarrow \langle G(\vec{r}\vec{r}\,';\, t;\, [\phi])\,G(\vec{\rho}\vec{\rho}\,';\, t';\, [\phi])\rangle_\Phi \,, \tag{4.13}$$

which is easily Fourier transformed to

$$\langle \mathcal{G}(E)\,\mathcal{G}(E')\rangle \rightarrow \langle G(\vec{r}\vec{r}\,';\, E;\, [\phi])\,G(\vec{\rho}\vec{\rho}\,';\, E';\, [\phi])\rangle_\Phi \,. \tag{4.14}$$

The $G(t;\,[\phi])$ and $G(E;\,[\phi])$ are, of course, the Green's functions defined in (4.10) and (4.12). Thus, from (3.6) the localization probability density is

$$p_0(E) \equiv \langle p_0(E;\,[\phi])\rangle_\Phi \equiv \lim_{\epsilon\to 0^+}\left(\frac{\epsilon}{\pi}\,\langle G_0(E+i\epsilon;\,[\phi])\,G_0(E-i\epsilon;\,[\phi])\rangle_\Phi\right), \tag{4.15}$$

where $G(z;[\phi])$ is shorthand for $G(\vec{0}\vec{0};\, z;\, [\phi])$. It is clear from the similarity of (4.15) to the expression for the average density of states at the original (and final) position of the electron,

$$n_0(E) = -\frac{1}{\pi}\lim_{\epsilon\to 0^+} \mathrm{Im}\langle G_0(E+i\epsilon;\,[\phi])\rangle_\Phi \,, \tag{4.16}$$

that approximation techniques which are useful in evaluating (4.16) will also be of value in obtaining (4.15). We therefore consider a generalization of the self-consistent-field theory of Edwards[30,31] and Zittartz and Langer.[7] Application is first made to $\langle c_0(t\,|\{\vec{R}_j\})\rangle$ and $n_0(E)$ where the approximations are physically more transparent. Then they can be applied to $p_0(E)$ and a preliminary discussion of mobilities can also be given.

V. SELF-CONSISTENT FIELD (SCF)

As noted following (2.12), the average Green's function G is translationally invariant. Since localized states are not translationally invariant, in order to obtain localized states symmetry must somehow be broken.[10] There are many ways in which this may be accomplished. Halperin and Lax[6] and Zittartz and Langer[7] break symmetry in the simplest possible manner. They assume that potential fluctuations are possible which give rise to localized states which are deep traps. Thus, they break symmetry by focusing attention upon a particular configuration of the random potential $\phi(r)$ and by assuming that there are in fact localized states. They do not prove that these low-lying states are localized, since the localized states they considered may be infinitely degenerate with other such states which are centered at other places in the system, thereby leading to bands of states.

In a recent cluster theory of the electronic structure of disordered systems (using a one-band model), symmetry is broken in a similar manner[23]; however, the existence of localized states is not assumed. Here attention is focused upon a cluster of atoms with a fixed configuration of the random variables and an average is performed over the random potentials in the remainder of the system. Then the existence of localized states can be determined and their properties studied as the cluster becomes larger and/or as similar and degenerate clusters are placed elsewhere in the system. However, in the region near E_c theories based upon finite clusters cannot distinguish between extended and localized states. Thus, in this region the infinite-range potential fluctuations determine electron localization or delocalization.[23]

Using the model presented in Sec. II, Edwards introduces a mean-field theory of electron localization[1,9,10] which bears some analogy with the van der Waals theory of fluids and the Curie-Weiss theory of ferromagnetism. Edwards considers that the average electron is free to move inside a cubical potential well and then determines whether the well is of finite or infinite extent. The electron is then localized or extended, respectively.

Here we break symmetry in quite a different fashion. Employing the popular "mythology" of Green's functions, $G(\vec{r}\,\vec{r}\,'; t)$ is given the interpretation of the probability amplitude that if we "create" an average electron at the point $\vec{r}\,'$ at time $t=0$, we then can "annihilate" this average electron (there is only one here) at the point $\vec{r}$ at time t. The acts of creation and annihilation at the space-time points $(\vec{r}\,', 0)$ and $(\vec{r}, t)$, respectively, in the translationally invariant "average medium" make these points in space special; it breaks symmetry for us. It therefore provides spatial origins which can act as the potential centers in an approximate calculation of G, $\langle \mathcal{G}\mathcal{G} \rangle$, etc. This is an essential feature of the SCF theory!

This method of symmetry breaking also illustrates the origin of a self-consistent description of electron localization in disordered systems. In order to illustrate this point heuristically, it is convenient to first consider the classical motion of the average electron. Given some particular trajectory or some probability distribution for the trajectory $\vec{r}(t)$ of the average electron from $\vec{r}(0)=\vec{r}\,'$ to $\vec{r}(t)=\vec{r}$, these trajectories could be combined, in some manner, with the self-interaction to provide a self-field seen by the average electron. This self-field clearly must depend parametrically on the spatial origins $\vec{r}\,'$ and $\vec{r}$ and the transit time t. Given this self-field, the trajectory (or probability distribution thereof) of the average electron can then be determined self-consistently.

The quantum-mechanical version of the SCF approximation arises from consideration of (4.10) and (4.8). If an approximate SCF theory is in fact applicable to the problem at hand, then the SCF Green's function G_{SCF} must obey the Schrödinger equation

$$\left(i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \nabla^2_{\vec{r}} - V_{\mathrm{SCF}}(\vec{r}\,|\,\vec{r}\,'; t)\right) G_{\mathrm{SCF}}(\vec{r}\,\vec{r}\,'; t) = \delta(\vec{r}-\vec{r}\,')\,\delta(t)\,, \quad (5.1)$$

where V_{SCF} is some (as yet unknown) functional of G_{SCF}, making Eq. (5.1) a closed equation. Equation (5.1) is markedly different from (2.16) or (4.8); in these $G(\vec{r}\,\vec{r}\,'; t)$ has an equation of motion which is in terms of a three-point Green's function; i.e., it is the first member of an infinite hierarchy of equations.[31] If a SCF theory is at all a valid approximation, comparison of (5.1) with (4.8) and (4.10) immediately implies that V_{SCF} must be that field, say ϕ_0, which makes the dominant contribution to the ϕ averaging (4.8). This field has been shown to be[1]

$$\phi_0(\vec{x}\,|\,\vec{r}\,\vec{r}\,'; t) = \rho \int d\vec{r}\,''\, W(\vec{r}\,''-\vec{x}) \int_0^t d\tau\, G(\vec{r}\,\vec{r}\,''; t\tau; [\phi_0]) \times G(\vec{r}\,''\vec{r}\,'; \tau 0; [\phi_0]) / G(\vec{r}\,\vec{r}\,'; t; [\phi_0])\,, \quad (5.2)$$

where the Green's functions for part of the time interval $G(t\tau; [\phi_0])$ and $G(\tau 0; [\phi_0])$ are the solutions to a Schrödinger equation like (4.10) for the particular value ϕ_0, e.g.,

$$\left(i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \nabla^2_{\vec{r}} - \phi_0(\vec{r}\,''\,|\,\vec{r}\,\vec{r}\,'; t)\right) G(\vec{r}\,''\vec{r}\,'; \tau 0; [\phi_0]) = \delta(\vec{r}\,'-\vec{r}\,'')\,\delta(\tau)\,. \quad (5.3)$$

The SCF $\phi_0(\vec{x}\,|\,\vec{r}\,\vec{r}\,'; E)$ which gives the dominant contribution to the ϕ averaging in (4.11) for $G(E)$ is given by Zittartz and Langer,[7] who assume that it gives rise to low-lying localized states. Their result is

$$\phi_{\mathrm{SCF}}(\vec{x}) = -\int d\vec{r}\,''\, W(\vec{x}-\vec{r}\,'')\, G(\vec{r}\,\vec{r}\,''; E; [\phi_{\mathrm{SCF}}]) \times G(\vec{r}\,''\vec{r}\,'; E; [\phi_{\mathrm{SCF}}]) / G(\vec{r}\,\vec{r}\,'; E; [\phi_{\mathrm{SCF}}])\,. \quad (5.4)$$

The Green's functions on the right-hand side of (5.4) are the solutions of (4.12) for the particular value $\phi=\phi_{\mathrm{SCF}}$. [$\phi_0(t)$ and $\phi_{\mathrm{SCF}}(E)$ are clearly not Fourier transforms of each other.] Equations (5.2), (5.3), etc., represent a very complicated set of self-consistency conditions. To obtain appropriate solutions, we must know something of the general analytic structure of the SCF Green's functions $G([\phi_0])$. In the analogous polymer case of self-avoiding random walks, there is some knowledge of the analytic structure of $G(\vec{r}0; L)$, where L is the length of the walk. However, there is nothing known about the properties of the partial Green's functions in (5.2) and (5.3). From the facts that (in the polymer analogy) $G(\vec{r}0; L)$ is believed to have fractional critical-type exponents, and the partial Green's functions can only be more complicated, it is obviously very difficult to find the self-consistent solutions to (5.2), (5.3), etc. Thus, we follow Edwards and Zittartz and Langer in trying to find explicit approximations for $G([\phi])$ before determining the dominant field ϕ_0 by the use of steepest descents in function space. Zittartz and Langer evaluate $G([\phi])$ by a perturbative diagram summation. Here we follow Edwards and assume that the relevant fields ϕ are sufficiently slowly varying that the WKB approximation to $G([\phi])$, $G^{\text{WKB}}([\phi])$, is all that is required.[23,30] This approximation turns out to be satisfied in the important regions of the dominant field ϕ_0, and corrections to $G^{\text{WKB}}([\phi_0])$ could, in principle, be incorporated in the standard manner. Before introducing the WKB Green's functions, we should pause to reflect upon the fundamental symmetry of the SCF formulation.

If we wish to evaluate $n_0(E)$ of (4.16) or $\langle c_0(t|\{\vec{R}_j\})\rangle$, the SCF in (5.2) would have $\vec{r}=\vec{r}'$, which we can define as the origin $\vec{r}=\vec{0}$. Thus, if $\phi_0(\vec{x}\,|\,\vec{0}\vec{0};\,t)$ is assumed to be spherically symmetric, the Green's functions on the right-hand side of (5.2) are those for spherically symmetric potentials. Since all of them have at least one of their end points at the origin, they are only s-wave Green's functions. Taking W to also be of the form $W(|\vec{r}''-\vec{x}|)$ implies that $\phi_0(\vec{x}\,|\,\vec{0}\vec{0};\,t)$ is in fact spherically symmetric. However, when the two end points differ, $\vec{r}\neq\vec{r}'=\vec{0}$, the potential $\phi_0(\vec{x}\,|\,\vec{r}\vec{0};\,t)$ is not spherically symmetric as is assumed by Zittartz and Langer. The SCF has $D_{\infty h}$ symmetry: cylindrical symmetry about the $\vec{0}$-$\vec{r}$ axis and a plane of symmetry bisecting the $\vec{0}$-$\vec{r}$ axis. This plane of symmetry arises because of the equivalence of the two end points.[33] The above arguments also apply to $\phi_0(\vec{x}\,|\,\vec{0}\vec{0};\,E)$ and $\phi(\vec{x}\,|\,\vec{r}\vec{0};\,E)$. As shown in Sec. X, the SCF reduces to a spherically symmetric potential only for the case of deep traps, the case treated by Zittartz and Langer and by Halperin and Lax. In the case of $\vec{r}\neq\vec{r}\,'$, the evaluation of $G^{\text{WKB}}([\phi])$ requires the formal analytic solution for the classical trajectories for a particle in an arbitrary potential of $D_{\infty h}$ symmetry. This is the general classical three-body problem.

Although the above discussion has been concerned with the SCF evaluation of $\langle\mathcal{G}\rangle$, it serves to represent the fundamental aspects of the SCF method; virtually identical considerations apply in the SCF calculation of $\langle\mathcal{G}\mathcal{G}\rangle$, etc. Steepest descents in function space can be used to obtain the dominant field ϕ_1 which contributes to the averaging in (4.14), etc. In the general case of $\vec{r}\neq\vec{r}\,'\neq\vec{\rho}=\vec{\rho}\,'$ (all different), the field ϕ_1 has four origins, thereby complicating the evaluation of $G^{\text{WKB}}([\phi])$. On the other hand, when using the Kubo-Greenwood-Peierls formula to evaluate the conductivity, only the case $\vec{r}=\vec{r}\,'\neq\vec{\rho}=\vec{\rho}\,'$ of two origins is required. However, the SCF ϕ_1 is then needed for all $|\vec{r}-\vec{\rho}\,|$, and the quantities $\partial\phi_1/\partial\vec{r}$ and $\partial\phi_1/\partial\vec{\rho}$ are present in the SCF equations for ϕ_1. These equations are much more complicated than those which arise in the consideration of the mobility in Sec. X. However, in evaluating $p_0(E)$ from (4.16) all four points are the same—they can then be taken as the origin. Hence, the relevant field ϕ_1 has spherical symmetry, and it turns out to be simply related to the SCF ϕ_0 which is obtained in the approximate evaluation of $n_0(E)$.

In order to continue the calculation, it is necessary to introduce the WKB Green's functions $G^{\text{WKB}}(\vec{r}\vec{r}\,';\,t;\,[\phi])$ and/or $G^{\text{WKB}}(\vec{r}\vec{r}\,';\,E;\,[\phi])$. Recently, there has been considerable interest in the evaluation of semiclassical Green's functions in order to obtain approximate S-matrix elements for heavy-particle collisions and to find bound-state energies for nonseparable potentials. The collisional work focuses upon t space, while the bound-state studies consider E space.[34–37] The latter is clearly the more relevant here. After introducing these WKB Green's functions, we can consider the evaluation of the SCF's ϕ_0 and ϕ_1 and their interpretation.

VI. SEMICLASSICAL GREEN'S FUNCTIONS

The path-integral representation of $G(\vec{r}\vec{r}\,';\,t;[\phi])$ given in (4.9) can be used to obtain the semiclassical Green's function.[34–37] Fourier transformation then leads to $G^{\text{WKB}}(\vec{r}\vec{r}\,';\,E;\,[\phi])$ as a summation over all of the classical trajectories from $\vec{r}\,'$ to $\vec{r}$ with energy E. Even when the angular momentum is specified, the classical path with this double-ended condition, $\vec{r}$ and $\vec{r}\,'$, is not unique. The partial-wave semiclassical Green's functions can be written in simple closed forms; however, from (4.15) and (4.16) it is clear that it is only necessary to evaluate the average Green's function for electron positions at the origin both initially and finally. In the approximate SCF theory, the potentials (the SCF's) ϕ_0 and ϕ_1 are spherically symmetric about this origin. Hence, only the s-wave part of the Green's function is required. Before presenting the s-wave Green's function it is necessary to recall a few preliminary familiar facts and definitions concerning the semiclassical approximation. The s-wave Green's function $G_s^{\text{WKB}}(rr';\,E;\,[\phi])$ is a one-dimensional Green's function for radial motion, where r is non-negative. It is well known that the usual WKB wave functions have the wrong behavior for $r\to 0$, where, for instance, the s-wave function should approach a constant. This discrepancy in the radial WKB functions is rectified in the standard manner by the inclusion of the Langer correction.[38] Thus, the effective radial potential

$$V_{\text{eff}}(r)=\phi(r)+\hbar^2/8mr^2\,, \tag{6.1}$$

with the extra centrifugal barrier, is employed instead of the potential $\phi(r)$. When the WKB s-wave functions are continued into the classically forbidden region inside the inner turning point arising from this centrifugal correction, they are indeed found to have the requisite behavior as $r \to 0$. This result assumes that the values of $\phi(r)$, $\phi_0(r)$, and $\phi_1(r)$ are less singular than r^{-2} as $r \to 0$, a result which is proven quite generally in Secs. VII and VIII. It is clear that attractive potentials $\phi(r)$ may admit of bound states, while purely repulsive $\phi(r)$ cannot. It is often convenient to take the extended states to be box normalized in a radial well of length L. The limit $L \to \infty$ can then be taken in the usual manner.

Define the radial momentum

$$p(r) = \{2m\,[E - V_{\mathrm{eff}}(r)]\}^{1/2} \tag{6.2}$$

and the radial action

$$\mathcal{A}(r) = \int_{r_1}^{r} p(y)\,dy \; . \tag{6.3}$$

Here r_1 is the inner turning point, where $p(r_1) = 0$. The s-wave Green's function is then[37]

$$G_s^{\mathrm{WKB}}(rr';\, E;\, [\phi]) = (m/4\pi i\hbar rr')\,[p(r)p(r')]^{-1/2} \times (1 - e^{i\theta'})^{-1}\big(e^{i[\mathcal{A}(r)-\mathcal{A}(r')]/\hbar} + e^{i[\mathcal{A}(r)+\mathcal{A}(r')]/\hbar - i\pi/2} + e^{-[\mathcal{A}(r)+\mathcal{A}(r')]/\hbar + i\pi/2 + i\theta'} + e^{-i[\mathcal{A}(r)-\mathcal{A}(r')]/\hbar + i\theta'}\big) , \tag{6.4}$$

where

$$\theta' \equiv \theta'(E;\, [\phi]) = \oint p(r)\,dr/\hbar \, - \, \pi \, , \tag{6.5}$$

and the contour integral is to be taken over one complete period of the classical motion. Because of the box normalization, the extended states are discrete. Equation (6.4) has poles at the zeros of $1 - e^{i\theta'}$, i.e., when the Bohr-Sommerfeld quantization condition is satisfied,

$$\oint p_n(r)\,dr = (n + \tfrac{1}{2})h, \quad n = 0, 1, 2, \ldots \quad . \tag{6.6}$$

The residues at these poles are found to be

$$\frac{4m}{rr'}\,[p_n(r)\,p_n(r')]^{-1/2}\,T^{-1}(E_n)\cos\left(\int_{r_1}^{r} \frac{p_n(y)\,dy}{\hbar} - \frac{\pi}{4}\right) \times \cos\left(\int_{r_1}^{r'} \frac{p_n(y)\,dy}{\hbar} - \frac{\pi}{4}\right) , \tag{6.7}$$

where $T(E_n)$ is the period for the closed orbit,

$$T(E_n) = \oint dr\, m/p_n(r) \; . \tag{6.8}$$

Equation (6.7) is the usual bilinear product of the normalized WKB wave functions $\psi_n(r)\,\psi_n^*(r')$ for the state at energy E_n. The normalization is, of course, of an approximate nature, resulting from the substitution for $\cos^2[\int_{r_1}^{r} p_n(y)\,dy/\hbar - \frac{1}{4}\pi]$, which is rapidly oscillating in the classically accessible region, the average value of $\frac{1}{2}$. This approximation becomes poor in the vicinity of classical turning points. However, in the turning-point region the simple WKB wave functions (6.7) are divergent (although square integrable) anyhow, so the approximation is immaterial. For bound states, the normalization should contain a small correction from the classically inaccessible region. Its influence on the wave function in the classically allowed region is negligible, but it will be useful to consider this correction to extend the SCF into the classically forbidden region.

The use of the WKB Green's function (6.4) gives rise to a well-known and understood approximation to $G(E;[\phi])$ which is an explicit functional of ϕ. The corrections to this WKB Green's function can also be systematically studied. The validity of the approximation requires that

$$\left| \frac{m\hbar\,\partial V_{\mathrm{eff}}(r)}{\partial r} \right| \ll [p(r)]^3 \; , \tag{6.9}$$

a condition which is obviously violated near the classical turning point. This prohibits the determination of the SCF $\phi_1(r)$ in the immediate neighborhood of the classical turning points *if any indeed exist*. The divergence in the WKB wave function at classical turning points can, of course, easily be rectified by the use of the uniform semiclassical wave functions which asymptotically become the sinusoidal WKB functions (6.7) in the classical region and the exponentially decaying functions otherwise. The uniform semiclassical radial s-wave functions are proportional to[39]

$$r^{-1}\,[w(r)]^{1/6}[k(r)]^{-1/2}\,\mathrm{Ai}\{-[\tfrac{3}{2}w(r)]^{2/3}\} \, , \tag{6.10}$$

where Ai is the Airy function, $k(r) = p(r)/\hbar$, and $w(r) = \mathcal{A}(r)/\hbar$. Although (6.10) is finite at classical turning points, it is not analytic at these points. Thus, functional derivatives of (6.10) with respect to $\phi(R)$ do not exist at these turning points. This then precludes the determination of the SCF ϕ_1 near the turning points, but its value in these regions can be obtained by continuation through the regions. Hence, the more general semiclassical approximation (6.10) is not considered further.

Aside from our general understanding of the use of the WKB approximation (6.4), the most important aspect of its introduction lies in the fact that it provides an explicit functional of ϕ which admits of both bound (localized) and extended states. Hence, (6.4) does not contain any implicit assumption as to the presence or absence of localized states. It is an approximation which represents $G(E;[\phi])$ in the spectral expansion

$$G(rr';E;[\phi]) = \sum_n \frac{\psi_n(r;[\phi])\psi_n^*(r';[\phi])}{E - E_n[\phi]} \; , \tag{6.11}$$

where the wave functions, extended and possibly localized, ψ_n, and energies E_n are obtained from the WKB approximation with the radial potential (6.1).

Since we require the wave functions for $r \to 0$, it is convenient first to evaluate the Langer correction. Let

$$A(r) \equiv \mathcal{A}'(r) + \mathcal{A}^0(r) , \tag{6.12}$$

where

$$\mathcal{A}^0(r) = \int_{(2\kappa)^{-1}}^{r} dy \left[2m\left(E - \frac{\hbar^2}{8my^2} \right) \right]^{1/2} , \tag{6.13}$$

$$\mathcal{A}'(r) = \int_{r_1}^{r} dy \{2m[E - V_{\mathrm{eff}}(y)]\}^{1/2}$$
$$- \int_{(2\kappa)^{-1}}^{r} dy \left[2m\left(E - \frac{\hbar^2}{8my^2} \right) \right]^{1/2} , \tag{6.14}$$

and

$$\kappa = (2m|E|/\hbar^2)^{1/2} , \tag{6.15}$$

so $(2\kappa)^{-1}$ is the inner turning point when $\phi \equiv 0$. $\mathcal{A}^0(r)$ diverges logarithmically as $r \to 0$, while $\mathcal{A}'(r)$ is regular in this limit. The divergence in $\mathcal{A}^0(r)$, however, is just that which is necessary to cancel a similar incorrect divergence in the normalization, the prefactor in (6.4), in this limit to provide wave functions (and Green's functions) which approach a constant value as r (and r') $\to 0$. Thus, since $\phi(r)$ is less singular than r^{-2} as $r \to 0$, $\mathcal{A}'(r)$ can be neglected with respect to $\mathcal{A}^0(r)$ as $r \to 0$. Similarly, for $r > r_1$ the integrand in (6.14) can be approximated by $\{2m[E - \phi(y)]\}^{1/2}$. Thus, we make the further simplification by taking

$$\mathcal{A}'(r) \to A(r) = \int_0^r dy \{2m[E - \phi(y)]\}^{1/2} . \tag{6.16}$$

The results of the approximation in (6.16) are well known in the case of the Coulomb potential where it leads to the WKB eigenvalues $E_n = -e^2/2a_0(n + \frac{1}{2})^2$, with $n = 0, 1, 2, \ldots$, instead of the exact results $E_n = -e^2/2a_0n^2$, $n = 1, 2, \ldots$, which are obtained when the Langer correction is maintained. Thus, in employing the simplification (6.16), the radial quantum numbers for the bound states from ϕ_0 and ϕ_1 (if there are any) are taken to be integers instead of half odd integers. For high quantum numbers the difference is negligible anyhow. Similarly, the use of (6.13) and (6.16) gives the proper energy dependence of $|\psi_n(0)|^2$ in the Coulomb problem. The appropriate quantization condition and energy dependence of the density at the origin are the major properties in the evaluation of $p_0(E)$ and $n_0(E)$. The similarity between the final ϕ_0 and ϕ_1 and the Coulomb potential then permits the simplification (6.16).

For $r \to 0$ it is necessary to connect the sinusoidal wave functions (6.7) with the usual exponentially decaying WKB functions which are valid inside the centrifugal Langer barrier of (6.1). The leading term in the exponential is

$$\exp\left\{ -\int_r^{(2\kappa)^{-1}} dy \left[2m\left(\frac{\hbar^2}{8my^2} - E \right) \right]^{1/2} \Big/ \hbar \right\}$$
$$\to \exp(\tfrac{1}{2} \ln \kappa r) , \quad r \to 0 \tag{6.17}$$

assuring that the radial wave functions are constant as $r \to 0$. Using (6.17) in (6.13) and (6.4) can be shown to lead to

$$G_s^{\mathrm{WKB}}(E; [\phi]) = |E|^{1/2} [(2m)^{3/2}/4\pi i\hbar^3]$$
$$\times [1 - i + 2e^{i\phi}(1 - e^{i\theta})^{-1}], \tag{6.18}$$

where

$$\theta = 2\hbar A(r_2)$$
$$= \oint \{2m[E - \phi(r)]\}^{1/2} dr , \tag{6.19}$$

and r_2 is the outer turning point which is the solution to

$$\phi(r_2) = E . \tag{6.20}$$

If the approximation (6.18) is introduced into the ϕ averaging for $\langle G(E; [\phi]) \rangle_\phi$, the resultant SCF ϕ_0 is found to be complex. The general Zittartz-Langer SCF (5.4) must likewise be complex. In order to avoid such complications, it is simplest to employ manifestly real quantities and determine the SCF separately for the real and imaginary parts of $\langle \mathcal{G} \rangle$, $\langle \mathcal{G}\mathcal{G} \rangle$, etc. Thus, we use the spectral decomposition of (6.18), whereupon (6.18) and (4.16) imply that

$$n_0(E) = [(2m)^{3/2}/2\pi\hbar^2] \langle \sum_n |E_n[\phi]|^{1/2}$$
$$\times T^{-1}(E_n[\phi]; [\phi])\, \delta(E - E_n[\phi]) \rangle_\phi \tag{6.21}$$

is the density of states at the origin.

Having introduced the WKB approximation with all the requisite notation, etc., the SCF's ϕ_0 and ϕ_1 can be determined.

VII. SCF ϕ_0

The initial approximation consists in replacing $G_0(E; [\phi])$ by its WKB approximation. Given this approximation, if a further SCF approximation is valid, the SCF must again be that field which makes the dominant contribution to the ϕ averaging in (6.21), etc., for the analogous case of $p_0(E)$. Since the SCF's ϕ_0 and ϕ_1 have spherical symmetry, the SCF can still be obtained if the random fields $\phi(r)$ in (4.15) and (4.16) are limited to be spherically symmetric with the origin $\vec{0}$ representing the average electron's initial and final position. The contribution to the functional integrals (4.15) and (4.16) from any particular value of the random field, in particular, the SCF, is infinitesimal. Nontrivial results are obtained only when contributions are taken from a region of function space. In practice, this consists in evaluating the contributions from those random fields which are in the neighborhood of the SCF. Here, these fluctuation terms are limited to those which maintain the spherical symmetry of the SCF. In Sec. X we consider the difficulties involved when the random fields $\phi(\vec{r})$ are no longer spherically symmetric.

Having thus made the further approximation of limiting the ϕ averaging in (4.15), (4.16), etc., to an average over only spherically symmetric fields, some general conclusions may immediately be drawn which are independent of the use of the semiclassical approximation. For the sake of simplicity, it is convenient at this juncture to take the self-potential W as the pseudopotential[6,7,10,21,23]:

$$W(\vec{r}) \to w\,\delta(\vec{r}). \tag{7.1}$$

From (7.1) and (4.4) the measure associated with any spherically symmetric potential $\phi(R)$ is

$$\mathfrak{N} M[\phi]\,\delta\phi = \mathfrak{N} \exp\left(-\frac{4\pi}{2\rho w}\int_0^\infty R^2\phi^2(R)\,dR\right)\delta\phi. \tag{7.2}$$

If $\phi(R) \nrightarrow 0$ as $R \to \infty$, $M[\phi]$ vanishes identically, since the integral in the exponential of $M[\phi]$ then diverges. Thus, the SCF must belong to that class of spherically symmetric potentials which asymptotically vanish faster than R^{-1} as $R \to \infty$. The only place where ϕ may diverge and still lead to nonzero $M[\phi]$ is for $R = 0$. However, in order that $\int_0^\infty R^2\phi^2(R)\,dR$ be finite, ϕ cannot diverge faster than $R^{-3/2+\beta}$, for $\beta > 0$, as $R \to 0$. All spherically symmetric potentials with a stronger divergence at $R = 0$ lead to $M[\phi] \equiv 0$. The infinite potential fluctuations for $R = 0$ [values of the random field $\phi(r)$] can, in principle, be of either sign. However, both $n_0(E)$ and $p_0(E)$ contain factors of $|\psi_n(0;[\phi])|^2$ and these are negligibly small if $\phi(R) \to +\infty$ when $R \to 0$. The density of the average electron at the origin $|\psi_n(0;[\phi])|^2$ is, of course, maximal when $\phi(R) \to -\infty$ when $R \to 0$, and, not surprisingly, the SCF's ϕ_0 and ϕ_1 are shown below to have this property.

Hence, the wave functions $\psi_n(0;[\phi])$ can be taken as those appropriate to a potential well at the origin and to a potential which vanishes faster than $1/R$ as $R \to \infty$. If the potential well is sufficiently wide, it could have bound localized states for $E < 0$, with continuous extended states for $E > 0$. Restricting attention to the case of $E < 0$, there is the possibility of the existence of subsidiary wells centered about some $R \neq 0$ in the random potentials $\phi(R)$. In this case, for energies such that the potential only has one classical turning point, a simple WKB wave function is adequate. If there is more than one turning point, it is necessary to consider tunneling between the wells. The case of tunneling is considered in Sec. X; here it is assumed that only the single radial turning-point situation need be considered.

In order to evaluate (6.21) by steepest descents in ϕ space, it is convenient to represent the Dirac δ function in (6.21) as a generalized function,

$$n_0(E) = \lim_{\epsilon\to 0^+} 2[(2m)^{3/2}/h^2]\,\epsilon \textstyle\sum_n \langle |E_n[\phi]|^{1/2}$$
$$\times T^{-1}(E_n[\phi];[\phi])\{(E-E_n[\phi])^2+\epsilon^2\}^{-1}\rangle_\phi, \tag{7.3}$$

where the summation over n has been taken outside of the ϕ integration. A steepest-descents evaluation of the ϕ averaging leads to a different SCF $\phi_0(R;n)$ for each "state" n. This is just a reflection of the energy dependence of the SCF with $\phi_0(R;n) \to \phi_0(R;E)$, since only $E \approx E_n[\phi_0]$ contributes to a given term. If the summation over n is kept inside of the ϕ averaging and this whole integral is evaluated by steepest descents, the resultant equations define a single E-dependent SCF. If the spectral representation (6.11) of $G([\phi])$ is substituted into the formal Zittartz-Langer SCF in (5.4), this formal complex SCF has the same sum-over-states structure. However, for E near $E_n[\phi_{\text{SCF}}]$, the potential $\phi_{\text{SCF}}(R;E)$ is dominated by the singularities in $G([\phi])$ for $E \approx E_n[\phi_{\text{SCF}}]$, leading to a good approximation to a different SCF for each state. The use of a steepest-descents evaluation of (7.3) for each n separately just leads to this simpler SCF for each n. This procedure can likewise be applied in the evaluation of $\langle \mathcal{G}\,\mathcal{G}\rangle$, etc., where the absence of summations over all states in the SCF equations lead to considerable simplifications over the use of the formal SCF's.

The ϕ averaging in (7.3) can be written explicitly as

$$\mathfrak{N}\int \delta\phi \exp(B[\phi]) \equiv \mathfrak{N}\int \delta\phi\ \exp(\ln|E_n[\phi]|^{1/2}$$
$$-\ln T(E_n[\phi];[\phi]) - \ln\{(E-E_n[\phi])^2+\epsilon^2\}$$
$$-(4\pi/2\rho w)\int_0^\infty R^2\phi^2(R)\,dR), \tag{7.4}$$

and the SCF ϕ_0 is the solution to the equation

$$\left.\frac{\delta B[\phi]}{\delta\phi(R)}\right|_{\phi=\phi_0} = 0. \tag{7.5}$$

More explicitly, (7.5) implies that

$$\left(\frac{1}{2E_n[\phi]}\frac{\delta E_n[\phi]}{\delta\phi(R)} - \frac{\delta \ln T(E_n[\phi];[\phi])}{\delta\phi(R)}\right.$$
$$\left.+\frac{2(E-E_n[\phi])}{(E-E_n[\phi])^2+\epsilon^2}\frac{\delta E_n[\phi]}{\delta\phi(R)} - \frac{4\pi}{\rho w}R^2\phi(R)\right)_{\phi=\phi_0} = 0. \tag{7.6}$$

First we may note that because of the lim $\epsilon \to 0^+$, only $E \approx E_n[\phi]$ can contribute to (7.3). Thus, the solution to (7.6) can be obtained for $E \approx E_n[\phi_0]$.

However, this implies that

$$\frac{1}{E_n[\phi_0]} \gg \frac{E - E_n[\phi_0]}{(E - E_n[\phi_0])^2 + \epsilon^2}\,, \tag{7.7}$$

when $\epsilon \to 0^+$ and $E \approx E_n[\phi_0]$, since the right-hand side of (7.7) is the definition of the principal value $\mathcal{P}/(E - E_n[\phi_0])$ which vanishes when $E \to E_n[\phi_0]$. Consequently, in the determination of the SCF ϕ_0, the third term in (7.6) may be neglected with respect to the first one; i.e., to a good approximation ϕ_0 is the solution to

$$\left(\frac{1}{2E_n[\phi]}\,\frac{\delta E_n[\phi]}{\delta\phi(R)} - \frac{\delta \ln T(E_n[\phi];[\phi])}{\delta\phi(R)} - \frac{4\pi}{\rho w}\,R^2\phi(R)\right)_{\phi=\phi_0} = 0\,. \tag{7.8}$$

Equation (7.7), in fact, implies that in the consideration of the steepest-descents calculation of (7.3), the factor $\epsilon\{(E - E_n[\phi])^2 + \epsilon^2\}^{-1}$ is slowly enough varying that it may be evaluated at the saddle point ϕ_0 and taken outside of the functional integral. Performing this operation and taking the limit $\epsilon \to 0^+$ transforms (7.3) into

$$\begin{aligned} n_0(E) = {} & 2[(2m)^{3/2}/h^2]\textstyle\sum_n \delta(E - E_n[\phi_0])\,\mathfrak{N}\int \delta\phi \\ & \times \exp\{\ln|E_n[\phi]|^{1/2} - \ln T(E_n[\phi];[\phi]) \\ & - (4\pi/2\rho w)\textstyle\int_0^\infty R^2\phi^2(R)\,dR\}\,. \end{aligned} \tag{7.9}$$

The steepest-descents evaluation of (7.9) obviously leads to the saddle-point equation (7.8) for ϕ_0.

As noted in Sec. VI, the approximate radial WKB quantization condition

$$\oint (2m\{E_n[\phi] - \phi(R)\})^{1/2}\,dR = nh, \quad n = 1, 2, 3, \ldots \tag{7.10}$$

defines the energy $E_n[\phi]$ as a functional of ϕ and a function of the discrete index n (for box normalization). Taking the functional derivative of (7.10) with respect to $\phi(R)$ yields

$$\begin{aligned} \frac{\delta E_n[\phi]}{\delta\phi(R)} = {} & (2m)^{1/2}\,T^{-1}(E_n[\phi];[\phi]) \\ & \times \{E_n[\phi] - \phi(R)\}^{-1/2}\,\Theta(r_0, R)\,, \end{aligned} \tag{7.11}$$

where

$$\Theta(r_0, R) = \begin{cases} 1, & r_0 > R \geq 0 \\ 0, & \text{otherwise,} \end{cases} \tag{7.12}$$

and r_0 is the classical turning point (or L) for the potential ϕ. The contribution to the functional derivative from the dependence of r_0 on ϕ in (7.11) vanishes since it is just proportional to

$$2(2m\{E_n[\phi] - \phi(R)\})^{1/2}\,\delta(R - r_0)\bigg/\left(\frac{\partial\phi}{\partial r}\right)_{r_0} = 0\,.$$

Because the WKB approximation for $E_n[\phi]$ in (7.10) depends only on the potential in the classically allowed region, (7.11) is nonzero only in this region.

In order to evaluate the remaining functional derivative in (7.8), it is convenient to introduce a notation for partial functional derivatives with respect to $\phi(R)$. Let $\Delta/\Delta\phi(R)$ be defined by

$$\begin{aligned} \frac{\delta F(E[\phi];[\phi])}{\delta\phi(R)} &= \left(\frac{\partial F(E;[\phi])}{\partial E}\right)_{E=E[\phi]} \frac{\delta E[\phi]}{\delta\phi(R)} + \left(\frac{\delta F(E;[\phi])}{\delta\phi(R)}\right)_{E=E[\phi]} \\ &\equiv \frac{\partial F}{\partial E[\phi]}\,\frac{\delta E[\phi]}{\delta\phi(R)} + \frac{\Delta F}{\Delta\phi(R)}\,. \end{aligned} \tag{7.13}$$

From Sec. VI, we can write

$$\begin{aligned} T(E;[\phi]) &= \frac{\partial}{\partial E}\oint dR\{2m[E - \phi(R)]\}^{1/2} \\ &= \oint dR\{(2/m)[E - \phi(R)]\}^{-1/2}\,, \end{aligned} \tag{7.14}$$

and consequently

$$\begin{aligned} \frac{\Delta T(E;[\phi])}{\Delta\phi(R)} &= \frac{\partial}{\partial E}\left(\frac{\Delta}{\Delta\phi(R)}\oint dR\{2m[E - \phi(R)]\}^{1/2}\right) \\ &= -(m/2)^{1/2}\,\Theta(r_0, R)\,[E - \phi(R)]^{-3/2}\,, \end{aligned} \tag{7.15}$$

since the $\partial/\partial E$ and $\Delta/\Delta\phi(R)$ operations commute. Introducing the notation

$$\rho(E;[\phi]) = h^{-1}\,T(E;[\phi])\,, \tag{7.16a}$$

$$\rho'(E;[\phi]) \equiv \frac{\partial\rho(E;[\phi])}{\partial E} \tag{7.16b}$$

for reasons that will become apparent, the SCF equations can be written as

$$\frac{a(E)}{E\rho(E)[E - \phi_0(R)]^{1/2}}\left(1 + \frac{E}{2a(E)[E - \phi_0(R)]}\right)\Theta(r_0, R) = C^{-3/2}R^2\phi_0(R)\,. \tag{7.17}$$

In (7.17), E has been written for $E_n[\phi_0]$, the ϕ_0 dependence of $\rho(E)$ has not been explicitly expressed,

$$C^{-3/2} = 8\pi h/(2m)^{1/2}\,\rho\omega\,, \tag{7.18a}$$

$$a(E) = 1 - 2E\rho'(E)/\rho(E)\,, \tag{7.18b}$$

and clearly the ρ in (7.18a) refers to the scatterer density as in (2.12) and following. The quantity $\rho(E)$ must be obtained self-consistently from the solution of (7.17) with (7.16).

Equation (7.17) implicitly defines ϕ_0 only in the classically accessible region; its value in the nonclassical region(s) may be obtained from the considerations in Sec. VIII. The SCF ϕ_0 is clearly energy dependent. For $E < 0$ it is shown in Sec. VIII that $a(E) = +7/2$. Thus, for $r_0 > R$, or equivalently, $E > \phi_0(R)$, the left-hand side of (7.17) is negative so long as

$$-E/2a(E)\,[E-\phi_0(R)] < 1. \qquad (7.19)$$

When (7.19) is satisfied (see Sec. VIII), $\phi_0(R;E)$ is negative and can possibly lead to bound states. From (7.17) it follows that as $R\rightarrow 0$, $\phi_0(R)$ must diverge. The leading divergent term in this limit can be found by taking $\phi_0(R)\propto -R^{-n}$, and then (7.17) implies

$$\phi_0(R;E)\rightarrow -bR^{-4/3} \text{ as } R\rightarrow 0, \qquad (7.20)$$

where

$$[b(E)]^{-3/2}=(-E)\,\rho(E)\,C^{-3/2}\,a^{-1}(E)>0, \quad E<0. \qquad (7.21a)$$

If we write

$$\phi_0(R;E)\equiv Ef\,(R;E)\,, \qquad (7.21b)$$

(7.17) becomes

$$(f-1)^{-1/2}\{1-[2a(f-1)]^{-1}\}=(R/R_0)^2 f, \quad R<r_0 \qquad (7.22)$$

where

$$R_0=b^{3/4}\,(-E)^{-3/4} \qquad (7.23)$$

is a fundamental length in the system. From (7.22) it is directly apparent that

$$f(R;E)=f(R/R_0), \quad R<r_0 \qquad (7.24)$$

and (7.20) represents the leading term in a power-series expansion which is of the form

$$f=(R/R_0)^{-4/3}+\sum_{n=0}^{\infty} c_n\,(R/R_0)^{4n/3}, \quad R<r_0. \qquad (7.25)$$

Fortunately, the precise form of the series (7.25) is not required.

At the classical turning point the simple WKB wave function (6.7) diverges, and even the functional derivatives of the uniform semiclassical wave function (6.10) with respect to $\phi(R)$ do not exist at this point. As is well known, the WKB approximation is poor in the neighborhood of r_0, and a real solution for ϕ_0 from (7.17) ceases to exist when the condition (7.19) is violated. This occurs when R' satisfies

$$E-\phi_0(R';E)=-\tfrac{1}{7}E\,, \qquad (7.26)$$

which is near the classical turning point $E-\phi_0(r_0;E)\equiv 0$ when E is small—the region of energy of interest. The functional $E-\phi_0(R;E)$ starts out at the value $+\infty$ at $R=0$, where the WKB is valid, and becomes undefined (i.e., complex) slightly before it reaches the value 0 at the turning point. A solution cannot be obtained up to the turning point because of the errors in the WKB wave function (6.7) and its functional derivatives with respect to $\phi(R)$ for R near r_0. [As noted after (6.8), even the normalization of the wave function involves approximations which are not valid in this region.] Presumably, with the use of (6.10), ϕ_0 would be defined closer to the turning point; however, the equations are not tractable.

Although (7.17) does not describe ϕ_0 in the region of the classical turning point and in the nonclassical region, ϕ_0 must possess a turning point for $E<0$. The measure (7.2) implies that $\phi_0(R)\rightarrow 0$ faster than $1/R$ as $R\rightarrow\infty$ and (7.17) exhibits a large region for which $0>E>\phi_0(R;E)$.

For ϕ_0 in the classically allowed region, the condition (7.19) is violated when $R\approx R_0$ of (7.23). In this region $\phi_0(R;E)$ is still basically the leading term $-bR^{-4/3}$ as in (7.20). Thus, as a simplification $\phi_0(R;E)$ can be equated with (7.20) for R in the classically allowed region. This leads to the identification of R_0 as the classical turning point and hence as the localization radius, the dimensions of the localized states obtained from ϕ_0. Actually, the identification of R_0 with the localization radius follows directly from (7.22) and (7.24) if ϕ_0 is assumed to maintain the same two-parameter (E,R_0) dimensionless form for all $R\leqslant r_0$. The quantum-mechanical expectation value of the radial position $\langle R\rangle$ in the semiclassical limit becomes

$$\langle R\rangle=\int_0^{r_0}\frac{R\,dR}{[E-\phi_0(R;E)]^{1/2}}\Bigg/\int_0^{r_0}\frac{dR}{[E-\phi_0(R;E)]^{1/2}}$$

$$=(\text{const})\,R_0\,, \qquad (7.27)$$

where the second equality in (7.27) is obtained by transforming to the dimensionless variable R/R_0 and using (7.22) and (7.24). [As is shown in Sec. VIII, the asymptotic SCF for $R\rightarrow\infty$ depends upon the wave length κ^{-1} of (6.15), and hence so may ϕ_0 in the classical region. However, this weak additional dependence is ignored in obtaining (7.27).]

Because of the $R^{-4/3}$ attractive nature of the SCF ϕ_0, the WKB quantization condition (7.10) for ϕ_0 leads to an infinite number of bound states for $E<0$ with an accumulation point at $E\rightarrow 0^-$ and then a continuous distribution of states for $E>0$. In a real disordered system the average density of localized states must be a continuous function of energy. However, in the evaluation of $n_0(E)$ and $p_0(E)$, we consider those localized states which have finite residues in the vicinity of a particular point in space $(\vec{0})$. In this case the distribution of localized states near $\vec{0}$ is dense, but discrete. It is therefore permissible, especially in the region of high quantum numbers, to consider that in the averaged system described by the SCF there is a continuous distribution of discrete states. As is customary then, the summation over discrete states is converted into an integration over the continuous distribution

$$\textstyle\sum_n\rightarrow\int dE\;\rho(E;[\phi_0])\,, \qquad (7.28)$$

where $\rho(E)$ is the density of states. If the relationship (7.10) is inverted, we obtain $n(E;[\phi])$, the semiclassical approximation for the number of eigenstates with energy less than or equal to E, as

$$n(E;[\phi])\,h=\oint\{2m[E-\phi(R)]\}^{1/2}\,dR\,. \tag{7.29}$$

The semiclassical approximation for the density of states for the particular field ϕ is then the well-known result

$$\rho(E;[\phi])\equiv\frac{\partial n(E;[\phi])}{\partial E}=h^{-1}T(E;[\phi]), \tag{7.30}$$

which coincides with the quantity $\rho(E)$ which is defined in (7.16).

ϕ_0 is the SCF for the imaginary part of $\langle\mathcal{G}(\vec{0}\vec{0};\ E+i\epsilon)\rangle$. Since the latter quantity is real, ϕ_0 must be real in contrast to the complex ϕ_{SCF} which is obtained from the complex quantity $\langle\mathcal{G}(\vec{0}\vec{0};E+i\epsilon)\rangle$. We could likewise obtain a real SCF ϕ_0' for the real part of $\langle\mathcal{G}(\vec{0}\vec{0};E+i\epsilon)\rangle$. The equation for ϕ_0' would have the additional term $-\{\delta E_n[\phi]/\delta\phi(R)\}\times(E-E_n[\phi])^{-1}$ on the left-hand side of (7.6) with the condition that $E\neq E_n[\phi_0']$ because of the principal value function associated with $\mathrm{Re}\,G_0(E+i\epsilon;[\phi])$. This leads to only minor differences between $\phi_0(R;\ E)$ and $\phi_0'(R;E)$. As the real and imaginary parts of the Green's function are related by a Hilbert transform, an integral over all other values of energy, there is no necessity that ϕ_0 and ϕ_0' be identical.

The present results provide a $\phi_0(R;\ E)$ which has discrete states for $E<0$ and continuous ones for $E>0$, which is indicative of, but not proof of, localized states for $E<0$ and extended ones for $E>0$. Thus ϕ_0 suggests the existence of a mobility edge at $E=0$. An evaluation of $p_0(E)$ is required to provide a rigorous criterion for localization. However, as is demonstrated in the next section, apart from inconsequential factors of 2, ϕ_1—the SCF for $p_0(E)$—is identical to ϕ_0. Hence, the possible inferences obtained from ϕ_0 concerning electron localization are indeed correct. There then remains the general model-independent possibility that information concerning electron localization may be obtained directly from the analytic structure of $\langle\mathcal{G}\rangle$ when the general theory indicates it is necessary to consider $\langle\mathcal{G}\,\mathcal{G}\rangle$.

VIII. SELF-CONSISTENT THEORY OF LOCALIZATION: $\phi_1(R;E)$

The random fields $\phi(\vec{r})$ in (4.15) are restricted to be spherically symmetric in conformity with the symmetry of ϕ_1, the SCF for $p_0(E)$. The conclusions concerning ϕ_0 obtained from (7.2) are also valid for ϕ_1. The formal SCF may be obtained by directly evaluating (4.16) by steepest descents. The details follow just as in Sec. V, but the results are more complicated and are therefore not considered further.

In order to avoid dealing with complex SCF's, it is again convenient to consider the limit $\epsilon\to0^+$ before approximating the ϕ averaging. This limiting process introduces the spectral representation (6.11) of the s-wave Green's function $G_0(z;[\phi])$ for each value of the random field $\phi(R)$,

$$p_0(E;[\phi])\equiv\lim_{\epsilon\to0^+}\left[\frac{\epsilon}{\pi}\left(\sum_n\frac{|\psi_n(0;[\phi])|^2}{E-E_n[\phi]+i\epsilon}\right)\times\left(\sum_k\frac{|\psi_k(0;[\phi])|^2}{E-E_k[\phi]-i\epsilon}\right)\right], \tag{8.1}$$

where a summation is, of course, implied for any discrete eigenstates and an integration is taken for the continuum. [The wave functions in (8.1) are expressed in unbounded space.] If E is in the neighborhood of the continuous spectrum of ϕ, e.g.,

$$\mp\,\mathrm{Im}\lim_{\epsilon\to0^+}\sum_n\frac{|\psi_n(0;[\phi])|^2}{E-E_n[\phi]\pm i\epsilon}=\rho(E;[\phi])|\psi(0;E;[\phi])|^2\neq0\,, \tag{8.2}$$

hence (8.1) vanishes because of the over-all factor of ϵ. Barring any accidental degeneracies, for E in the region of the discrete spectrum the only terms contributing to (8.1) are those for which $k=n$, leading to the result

$$\rho_0(E;[\phi])=\sum_{\text{discrete states }n}|\psi_n(0;[\phi])|^4\,\delta(E-E_n[\phi])\,, \tag{8.3}$$

which clearly exhibits $p_0(E;\ [\phi])$ as a localization probability. It is convenient to extend the summation (8.3) to be over all states, thereby defining a quantity $q_0(E)$ which coincides with $p_0(E)$ in the discrete spectral region. Using (8.3) and the WKB approximation (6.4)–(6.7), Eq. (4.16) becomes

$$q_0(E)=[(2m)^3/(2\pi\hbar^2)^2]\sum\nolimits_n\langle|E_n[\phi]|\times T^{-2}(E_n[\phi];[\phi])\,\delta(E-E_n[\phi])\rangle_\phi\,, \tag{8.4}$$

where again the summation over n has been taken outside the ϕ averaging. Apart from over-all constants, (8.4) differs from (6.21) by the presence of the extra factor of $|E_n[\phi]|^{1/2}T^{-1}$. Therefore, using the generalized function form for the δ function in (8.4) as in (7.3) and evaluating the functional integral (8.4) by steepest descents leads to an equation for ϕ_1 which is identical to (7.6) except for the presence of a factor of 2 before $\delta\ln T/\delta\phi(R)$ and $E_n^{-1}\delta E_n/\delta\phi(R)$ and the substitution $\phi_0\to\phi_1$. Equation (7.7) and the argument following it can be used to remove the δ function from the ϕ averaging in (8.4) and have it evaluated at ϕ_1. This leads to

$$q_0(E)\propto\sum\nolimits_n\delta(E-E_n[\phi_1])\,\langle|E_n[\phi]|\,T^{-2}(E_n[\phi];[\phi])\rangle_\phi\,. \tag{8.5}$$

The SCF equation for ϕ_1 is obtained from (7.8) by multiplying the $\delta \ln T/\delta\phi(R)$ and the $\delta E_n/\delta\phi(R)$ in (7.8) by 2. Continuing as in Sec. VII, the equation for ϕ_1 is

$$\frac{a(E)}{E\rho(E)[E-\phi_1(R)]^{1/2}}\left(1+\frac{E}{2a(E)[E-\phi_1(E)]}\right)\Theta(r_0,R) = \tfrac{1}{2}C^{-3/2}R^2\phi_1(R)\,, \qquad (8.6)$$

where $a(E)$, $\rho(E)$, and C are as given in Sec. VII.

The form of ϕ_1 (and ϕ_0) in the classically inaccessible region can be determined by considering the contribution to $|\psi_n(0;[\phi])|^2$ arising from the finite electron density in the nonclassical region. This result can be used to prove that $\phi_1(R)\to 0$ as $R\to\infty$ as it must. For convenience, only one classical turning point is assumed to be present for the random fields $\phi(R)$ which contribute to $p_0(E)$ and admit of bound states. Using the WKB connection formulas, the unnormalized wave function $p(r)^{-1/2}\cos[\int_0^R p(r)\,dr/\hbar-\frac{1}{4}\pi]$ in the well connects with the wave function

$$\chi_{\text{n.c.}}(R)=[\phi(R)-E]^{-1/4}\exp\left(-\int_{r_0}^{R} dr\,\frac{\{2m[\phi(r)-E]\}^{1/2}}{\hbar}\right) \qquad (8.7)$$

(apart from an overall constant) in the nonclassical region. Introducing the Langer correction,[38] the magnitude of the normalized wave function at $R=0$ is just inversely proportional to the norm of this unnormalized function,

$$|\psi_n(0;[\phi])|^2 \propto |E_n[\phi]|^{1/2}/(T+N)\,, \qquad (8.8)$$

where

$$N\propto\int_0^\infty dR\,|\chi_{\text{n.c.}}(R)|^2\,. \qquad (8.9)$$

[The positive energy-independent proportionality factors in (8.8) and (8.9) are not required.] Because of the dependence of N on $E_n[\phi]$ and of the latter on $\phi(R)$ for R in the classically allowed region, N introduces a minor correction into the SCF equations for ϕ_1 in the classically accessible region, and this is ignored. However, N now enables ϕ_1 to be defined for $r_0<R$. Steepest descents leads to the following integral equation for ϕ_1 in the classically forbidden region:

$$\frac{\Theta(R,r_0)}{T(E_n[\phi_1];\,[\phi_1])\{\phi_1(R)-E_n[\phi_1]\}^{1/2}}\left[\frac{B(R)}{\phi_1(R)-E_n[\phi_1]}+\left(\frac{2m}{\hbar^2}\right)^{1/2}\int_R^\infty\frac{B(r)\,dr}{\{\phi_1(r)-E_n[\phi_1]\}^{1/2}}\right]=\gamma R^2\phi_1(R)\,, \qquad (8.10)$$

where

$$B(R)=\exp\left[-2\int_{r_0}^{R}\left(\frac{2m\{\phi_1(r)-E_n[\phi_1]\}}{\hbar^2}\right)^{1/2}dr\right] \qquad (8.11)$$

and γ is a constant independent of E. A solution to (8.10) and (8.11) clearly does not exist as $R\to r_0^+$ as is to be expected. For $R>r_0$, (8.10) implies that $\phi_1(R)\geq 0$. If $\phi_1(R)$ is finite as $R\to\infty$, the left-hand side of (8.10) vanishes as $R\to\infty$. Thus, the only possible solution gives $\phi_1(R)\to 0^+$ as $R\to\infty$, and $\phi_1(R)$ is of nonzero measure. For R large enough, ϕ_1 may be neglected in (8.11) and in the left-hand side of (8.10). This then implies that

$$\phi_1(R)\sim O[e^{-\kappa R}/\kappa^3\rho(E)R^2]\,,\quad R\to\infty \qquad (8.12)$$

where κ is defined in (6.15).

One possible interpretation of positive $\phi_1(R)$ in the nonclassical region—except in the immediate neighborhood of the turning point—is that this reflects the requirement of conservation of probability. In order to obtain localized states, negative potential fluctuations are required in some region of space. But (4.5) implies that, on average, $\phi(R)$ is everywhere zero. Therefore, if such negative fluctuations are found somewhere, it becomes highly likely that positive potential fluctuations must occur elsewhere in space. By specifying that an average electron is initially and finally at the origin, we make it more likely that a negative potential fluctuation is centered about this position—otherwise the average electron would not have "chosen" to be at that point in space in the first place.

Although the exact details of and the contributions from the classically forbidden region are difficult to extract from (8.10), they are not required. Equations (8.10)–(8.12) do imply the existence of a classical turning point $r_0(E)$ for $\phi_1(R;\,E)$ as required by the negative value of the SCF $\phi_1(R;\,E)$ in the classically allowed region and the probabilistic requirement that $\phi_1(R)\to 0$ faster than R^{-1} as $R\to\infty$. Because of the nonanalyticity of the WKB approximation [even (6.10) in the case] for the SCF, the potential ϕ_1 is uncertain in the region of the classical turning point for, say, a wavelength on either side. However, given ϕ_1 on either side of r_0 from (8.6) and (8.10), probabilistic arguments can be used to join the SCF in these two regions. First consider values of the random potential $\phi(r)$ in the integrand of (8.5) which are fairly smooth in the neighborhood for which ϕ_1 is presently uncertain, but which coincide with ϕ_1 in the region for which it has been determined. Here smoothness is taken to imply that $\phi(r)$ has no large positive or negative fluctuations about the potential $\bar{\phi}_1$ which is derived from ϕ_1 by continuing it through the uncertain region with a simple straight line. For such smooth $\phi(r)$, the difference $\phi(r)-\bar{\phi}_1(r)$ can be treated as a small perturbation on $\bar{\phi}_1$, since it would not qualitatively change the nature of, e.g., the energy dependence of the density of states and the magnitude of the wave function at the origin.

All such smooth potentials would also have similar measures, thereby contributing equally with $\overline{\phi}_1$. The second case is that set of potentials $\phi(r)$ for which $\phi(r) - \overline{\phi}_1$ is large and positive in the uncertain region. Although these potentials would minimize the penetration of the wave function into the classically forbidden region, this penetration is already small, since $\phi_1(r)$ becomes positive in the determined part of the nonclassical region. Furthermore, such large potential fluctuations would have very small measures, so their effects can be neglected. Similarly, those potentials for which $\phi(r) - \phi_1(r)$ becomes large and negative need not be considered because of their small measures. They would possibly have a qualitative effect upon the nature of the SCF: However, these potentials would also lead to a value of $p_0(E; [\phi])$ which is much less than $p_0(E; [\overline{\phi}_1])$ since the large negative potential fluctuation implies that the localized average electron of energy E spends a lot of time in the neighborhood of this fluctuation, and therefore less time in the vicinity of the origin. Thus, we conclude that the SCF ϕ_1 cannot differ much from $\overline{\phi}_1$, and we now consider that this must be the case.

The density of states $\rho(E)$ must still be evaluated in order to complete the determination of ϕ_1. By (7.30) and (6.8), the density of states is just

$$\rho(E; [\phi_1]) = (2m/\hbar^2)^{1/2} \int_0^{r_0} dR[E - \phi_1(R; E)]^{-1/2}$$
$$= (-2m/Eh^2)^{1/2} R_0 \int_0^{(r_0/R_0)} [f(x) - 1]^{1/2} dx\,. \tag{8.13}$$

Since r_0/R_0, and hence the integral in (8.13), is dimensionless and energy independent, (7.23) implies that (8.13) can be written as

$$\rho(E; [\phi_1]) \propto (b')^{3/4}(-E)^{-5/4}\,, \tag{8.14}$$

where b' $[(b')^{-3/2} \equiv \frac{1}{2}(b)^{-3/2}]$ is still energy dependent by (7.21) and (8.6). ρ' is defined in (7.16) as $\partial\rho/\partial E$ *when ϕ is E independent*. Hence, in the present case ρ' must imply $\{\partial\rho(E; [\phi])/\partial E\}_{\phi=\phi_1}$. If ϕ_1 were energy independent, b' would be a constant, so

$$\rho' = -5\rho/4E\,, \tag{8.15}$$

and hence $a(E) = \frac{7}{2}$ as stated above. Substituting b' into (8.14) gives

$$\rho(E) \propto [\rho(E)]^{-1/2}(-E)^{-7/4} \propto (-E)^{-7/6}\,. \tag{8.16}$$

The radial density of s-wave states (8.16) becomes infinite as $E \to 0^-$ since $E = 0^-$ is an accumulation point for the discrete spectrum from a potential which has the leading singularity $-b'R^{-4/3}$ at the origin. In the continuum ($E > 0$) the radial s-wave density of states (7.30) is proportional to the size of the radial well L which is introduced to provide the box normalization. As $L \to \infty$, this density of states is obviously infinite. The density of states must be continuous across $E = 0$, a fact which clearly follows from (7.30) since when $L < R_0$, i.e., as $E \to 0^-$, the box normalization also cuts off the discrete states. Hence for finite L there is really no difference between the highest-lying discrete states and the bottom of the continuum, and the singularity in $\rho(E)$ as $E \to 0^-$ is formally removed.

The result (8.16) implies that the localization radius R_0 varies as

$$R_0 \propto (-E)^{-2/3}\,, \tag{8.17}$$

and hence the localized states become more extended as we approach the transition energy $E = 0$ from below. Thus, those localized states near the mobility edge are profoundly affected by the presence of similar states which are centered elsewhere in the system. The present theory is, however, only a single-center theory—only spherically symmetric potentials enter—and therefore it cannot account for the effects of these other states. A proper SCF evaluation of the mobility, on the other hand, requires two centers, the initial and final positions of the average electron. Thus, these two center states are explicitly considered in the SCF treatment of the mobility—herein lies the mathematical difficulty—and this may lead to a shift of the mobility edge.

Evaluating the integrand of (8.5) at ϕ_1 and taking the continuum limit (7.28) leads to the result that

$$\begin{aligned} p_0(E) &\propto (-E)^{13/6}\,, \quad E < 0 \\ &\equiv 0\,, \qquad\qquad\; E > 0 \end{aligned} \tag{8.18}$$

with the mobility edge at $E = 0$. Intuitively $p_0(E)$ is expected to be inversely proportional to the localization range. The larger the size of a localized state, the lower the probability of the average electron being in the vicinity of the origin. The behavior $p_0(E) \to 0$ as $E \to 0^-$ is therefore indicative of the fact that the localization radius increases as $E \to 0^-$; the decrease in $p_0(E)$ due to the large value of R_0 dominates its increase because of an increasing density of states in this limit. The critical exponent behavior of (8.18) is indicative of, but not proof of, critical exponent behavior on the other side of the mobility edge, e.g., a mobility which increases as $(E)^\alpha$ for $\alpha > 0$, $E \geq 0$. If only the dominant part of the SCF $-b'R^{-4/3}$ is maintained, then for $E_1 > E > 0$, the states in this potential correspond to resonant states, ones which spend a long time in the vicinity of the origin. This is also suggestive of a continuous increase in the mobility for $E > 0$.

In contrast to derivations of the mobility edge which consider the probabilistic convergence properties of the renormalized perturbation expansion for the electron's self-energy, the present SCF method can provide a description of these localized and extended states. Furthermore, the method can, in principle, be generalized to treat the mobilities.

The results (8.16)–(8.18) follow from the use of ϕ_1; however, any single potential has zero weight, and it is necessary to consider the effects of fluctuations about ϕ_1. As shown in the next section, these fluctuations lead to energy-independent factors; consequently, the proportionality constants in (8.18), etc., have been omitted as these results also contain the effects of fluctuations. In Sec. X a discussion is given of the SCF theory of mobilities and the difficulties inherent in a two-center theory.

IX. FLUCTUATIONS

Within the semiclassical approximation it still remains to consider the contributions from the random fields $\phi(r)$ in the neighborhood of ϕ_1 in order to verify the results in the preceding section. The semiclassical approximation to (8.5) involves neglecting contributions from the nonclassical region; however, it is necessary to invoke the properties of ϕ_1 in the latter region in order that the SCF be taken to be continuous up to the classical turning point. The functional form for ϕ_1 is also assumed to be of the same form as in (7.22) and (7.24) with $b \to b'$. These assumptions correspond to the belief that the functional derivatives of $p_0(E;[\phi])$ with respect to $\phi(R)$ should remain analytic at the classical turning point, or at least lead to integrable (or square integrable) singularities.

Equation (8.18) just provides the values of

$$|E_n[\phi]|\, T^{-2}(E_n[\phi];[\phi])\,\delta(E-E_n[\phi])$$

in (8.5) at the saddle point ϕ_1. The measure of ϕ_1 is then given by

$$M[\phi_1]\delta\phi = \exp\left(-\frac{4\pi}{2\rho w}\int_0^\infty R^2\phi_1^2(R)\,dR\right)$$

$$= \exp\left(-\frac{4\pi}{2\rho w}\,R_0{}^3E^2\int_0^{(r_0/R_0)} x^2f^2(x)\,dx\right), \quad E \le 0 \tag{9.1}$$

since r_0/R_0 is dimensionless, and invoking (8.17) implies that (9.1) is a constant independent of energy. The integral is easily evaluated if only the leading part of ϕ_1 in (7.20) is maintained. In this case $r_0/R_0=1$ and $x^2f^2(x) \propto x^{-2/3}$. The corrections to (7.20) therefore are small.

As is customary in saddle-point integration, if the ϕ averaging in (8.5) is written as $\mathfrak{N}\int\delta\phi\, e^{F(E[\phi];[\phi])}$ and we define

$$\xi(r)=\phi(r)-\phi_1(r)\,, \quad \delta\phi(r)=\delta\xi(r)\,, \tag{9.2}$$

the ϕ averaging in (8.5) is written approximately as

$$\exp\{F(E[\phi_1];[\phi_1])\}\,\mathfrak{N}\int\delta\xi\,\exp\left(\frac{1}{2}\int dR\int dR'\,\frac{\delta^2F(E[\phi];[\phi])}{\delta\phi(R)\,\delta\phi(R')}\bigg|_{\phi=\phi_1}\xi(R)\,\xi(R')\right)[1+O(\xi^3)]\,, \tag{9.3}$$

where the terms of $O(\xi^3)$ and higher that arise from the functional Taylor series of F in powers of ξ are ignored but can be considered to yield a perturbative expansion in the usual fashion.[40] The factor $e^{F([\phi_1])}$ has already been considered, and we now show that the Gaussian functional integral in (9.3) is independent of the energy. Using the definition of partial functional differentiation in (7.13) and the shorthand ϕ and ϕ' for $\phi(R)$ and $\phi(R')$, respectively, it follows that

$$\frac{\delta^2F(E[\phi];[\phi])}{\delta\phi\,\delta\phi'}=\left[\frac{\Delta^2F}{\Delta\phi\,\Delta\phi'}+\frac{\delta E}{\delta\phi}\,\frac{\Delta}{\Delta\phi'}\left(\frac{\partial F}{\partial E}\right)+\frac{\delta E}{\delta\phi'}\,\frac{\Delta}{\Delta\phi}\left(\frac{\partial F}{\partial E}\right)+\frac{\delta E}{\delta\phi'}\,\frac{\delta E}{\delta\phi}\,\frac{\partial^2F}{\partial E^2}\right]_{E=E[\phi]}+\frac{\delta^2E[\phi]}{\delta\phi\,\delta\phi'}\,\frac{\partial F}{\partial E}\bigg|_{E=E[\phi]}\,, \tag{9.4}$$

where

$$\frac{\delta^2E[\phi]}{\delta\phi\,\delta\phi'}\equiv\frac{\Delta}{\Delta\phi'}\left(\frac{\delta E[\phi]}{\delta\phi}\right)_{E=E[\phi]}+\frac{\delta E[\phi]}{\delta\phi'}\left(\frac{\partial}{\partial E}\,\frac{\delta E[\phi]}{\delta\phi}\right)_{E=E[\phi]}\,, \tag{9.5}$$

and $\delta E[\phi]/\delta\phi$ is in (9.4) and (9.5) taken to be (7.11) with E instead of $E[\phi]$. Using (7.11), Eq. (9.5) is readily evaluated as

$$\frac{\delta^2E[\phi]}{\delta\phi\,\delta\phi'}=\left(\frac{(2m)^{1/2}\delta(R-R')}{2T(E-\phi)^{3/2}}-\frac{m}{T^2(E-\phi)^{1/2}(E-\phi')^{1/2}}\left[(E-\phi)^{-1}+(E-\phi')^{-1}+2\rho'/\rho\right]\right)_{E=E[\phi]}\,. \tag{9.6}$$

Similarly, the results

$$\frac{\delta^2\ln|E[\phi]|}{\delta\phi\,\delta\phi'}=\left(\frac{(2m)^{1/2}\delta(R-R')}{2ET(E-\phi)^{3/2}}-\frac{m}{ET^2(E-\phi)^{1/2}(E-\phi')^{1/2}}\right.$$

$$\left.\times\left[2E^{-1}+(E-\phi)^{-1}+(E-\phi')^{-1}+2\rho'/\rho\right]\right)_{E=E[\phi]}\Theta(r_0,R)\,\Theta(r_0,R') \tag{9.7}$$

and

$$\frac{\delta^2 \ln T(E[\phi];[\phi])}{\delta\phi\delta\phi'} = \left(\frac{(2m)^{1/2}\delta(R-R')}{2T(E-\phi)^{3/2}}\left[-\tfrac{3}{2}(E-\phi)^{-1}+\rho'/\rho\right]+\frac{m}{T^2(E-\phi)^{3/2}(E-\phi')^{3/2}}\right.$$
$$\times\left[-\tfrac{1}{2}+(E-\phi)(\rho'/\rho)(1-\rho'/\rho)+(E-\phi')(\rho'/\rho)(1-\rho'/\rho)+3(E-\phi)/2(E-\phi')\right.$$
$$\left.\left.+3(E-\phi')/2(E-\phi)+(E-\phi)(E-\phi')(2(\rho''/\rho)-4(\rho'/\rho)^2)\right]\right)_{E=E[\phi]}\Theta(r_0,R)\,\Theta(r_0,R') \tag{9.8}$$

can be obtained.

The Gaussian functional integral (9.3) has the value $\{\det K(RR';[\phi_1])\}^{-1/2}$, where det implies the Fredholm determinant and K is the kernel

$$K(RR';[\phi_1]) = -\frac{\rho w}{4\pi RR'}\,\frac{\delta^2 F(E[\phi];[\phi])}{\delta\phi(R)\delta\phi(R')}\bigg|_{\phi=\phi_1}. \tag{9.9}$$

The kernel K has a diagonal part, proportional to $\delta(R-R')$, which is dimensionless. In fact, if the second term in (8.6) in $(E-\phi_1)^{-3/2}$ is ignored, then this modified equation (8.6) is substituted into the diagonal part of (9.9), and finally when the leading term (7.20) of the SCF is used, this diagonal part is found to be $\frac{3}{2}\delta(R-R')\Theta(r_0,R)$. If we write

$$K=\tfrac{3}{2}\underline{1}+\tfrac{3}{2}K',$$
$$\det K = [\det(\tfrac{3}{2}\underline{1})][\det(\underline{1}+K')], \tag{9.10}$$

the Fredholm determinant of the first factor in (9.10) is infinite, being proportional to the dimension of the space. This divergence is in the standard form of the "unlinked cluster." It is an overall normalization which appears in all orders of perturbation theory, i.e., the expansion in (9.3) containing the terms of $O(\xi^3)$ and higher. However, in the expansion in powers of ξ^n, $n\geq 3$, there are also coefficients which are proportional to dirac δ functions. The terms in perturbation theory arising from these diagonal parts are then proportional to the trace of the dirac δ function (or powers thereof), i.e., to the dimensions of the function space. These diagonal terms in perturbation theory therefore directly correspond to the "unlinked clusters" which must cancel this infinite normalization in the familiar manner.

The nondiagonal part of $K(RR';[\phi_1])$ is symmetric and separable in R and R'. After the "unlinked clusters" have been factored out, the remainder of K can be written in the form

$$K''=\underline{1}+\sum_{\alpha,\beta=1}^{d} g_{\alpha\beta}A_\alpha(E,R/R_0)A_\beta(E,R/R_0)=\underline{1}+K', \tag{9.11}$$

where $g_{\alpha\beta}$ are constants independent of E and d is finite. By assumption, the functional derivatives with respect to ϕ are to be regularized at the classical turning point, so the integrals

$$\int_0^{r_0} A_\alpha(E,R/R_0)A_\beta(E,R/R_0)\,dR = S_{\alpha\beta} \tag{9.12}$$

exist. Employing the simplifications that led to (9.10), the functions A_α and A_β are obtained by taking RR' times the factors in (9.7) and (9.8). With this identification and using (8.15)–(8.17), when the change in variables $x=R/R_0$ is made in (9.12), the resulting integral is dimensionless, and hence the $S_{\alpha\beta}$ are independent of E. Since

$$\det K'' = \operatorname{tr}\ln(\underline{1}+K')=\sum_{i=1}^{d}\ln(1+\lambda_i), \tag{9.13}$$

where λ_i are the eigenvalues of the kernel K', i.e., the eigenvalues of the energy-independent matrix $\overleftrightarrow{g}\overleftrightarrow{S}$, the contribution from the fluctuations is energy independent as asserted.

X. TOWARDS A SCF THEORY OF MOBILITIES

From a discussion of $p_0(E)$, the probability that an average electron with energy E returns to its initial position after an infinite time, it is possible to deduce certain properties of the transport processes. However, in order to discuss these transport phenomena directly, it is necessary to consider average electrons which do not return to their original position. The simplest quantity which contains this information is the following generalization of (3.2):

$$p_{0R}(t)=\langle|c_{0R}(t|\{\vec{R}_j\})|^2\rangle$$
$$=\langle|\mathcal{G}(\vec{0}\vec{R};t|\{\vec{R}_j\})|^2\rangle. \tag{10.1}$$

Equation (10.1) is the probability that an average electron travel a distance R in time t, where c and $\mathcal{G}$ are defined in Sec. III. If the limit $R\to\infty$, $t\to R^\alpha$ is considered in (10.1), then the case of $\alpha=2$ would correspond to diffusive motion. Near the mobility edge a value of α differing from two may be expected. Introducing Fourier transforms of the probability amplitudes as in (3.3)–(3.6), Eq. (10.1) becomes

$$p_{0R}(t)=\lim_{\epsilon\to 0^+}(2\pi)^{-2}\int_{-\infty}^{\infty}dE\int_{-\infty}^{\infty}dE'\,e^{-i(E-E')t/\hbar}$$
$$\times\langle\mathcal{G}(\vec{0}\vec{R};E+i\epsilon|\{\vec{R}_j\})\mathcal{G}(\vec{R}\vec{0};E'-i\epsilon|\{\vec{R}_j\})\rangle. \tag{10.2}$$

It is clear that in the limit $t \to \infty$, $R \to t^{\alpha^{-1}}$, only values of $E \approx E'$ contribute to (10.2). Thus, introducing the sum and difference variables

$$\mathcal{E} = \tfrac{1}{2}(E + E') , \quad \omega = E - E' \tag{10.3}$$

transforms (10.2) into

$$p_{0R}(t) = \int_{-\infty}^{\infty} d\mathcal{E}\, p_{0R}(t; \mathcal{E}) , \tag{10.4}$$

where

$$\begin{aligned} p_{0R}(t; \mathcal{E}) = \lim_{\epsilon \to 0^+} (2\pi)^{-2} \int_{-\infty}^{\infty} d\omega e^{-i\omega t/\hbar} \\ \times \langle \mathcal{G}(\overrightarrow{0R}; \mathcal{E} + \tfrac{1}{2}\omega + i\epsilon \,|\, \{\vec{R}_j\}) \\ \times \mathcal{G}(\overrightarrow{R0}; \mathcal{E} - \tfrac{1}{2}\omega - i\epsilon \,|\, \{\vec{R}_j\}) \rangle \end{aligned} \tag{10.5}$$

and in the long-time large-R limit only small values of ω contribute to (10.5). $\mathcal{E}$ can then be taken as the energy of the average electron, and $p_{0R}(t; \mathcal{E})$ is related to the mobility for electrons of energy $\mathcal{E}$. The ϕ averaging of Sec. IV can be introduced into (10.5) as in (4.15) in place of the average over all the scatterer positions,

$$p_{0R}(t; \mathcal{E}) = \lim_{\epsilon \to 0^+} (2\pi)^{-2} \int_{-\infty}^{\infty} d\omega e^{-i\omega t/\hbar} p_{0R}(\mathcal{E}, \omega) , \tag{10.6}$$

with

$$\begin{aligned} p_{0R}(\mathcal{E}, \omega) \equiv \langle G(\overrightarrow{0R}; \mathcal{E} + \tfrac{1}{2}\omega + i\epsilon; [\phi]) \\ \times G(\overrightarrow{R0}; \mathcal{E} - \tfrac{1}{2}\omega - i\epsilon; [\phi]) \rangle_{\Phi} . \end{aligned} \tag{10.7}$$

We could consider the formal SCF obtained from (10.7) or (10.6) by evaluating the ϕ average by steepest descents. In the latter case, the SCF would be a sum of two terms of the form (5.4) with the replacement of W by the pseudopotential (7.1) and the indices $\overrightarrow{rr'} \to \overrightarrow{0R}$ and $\overrightarrow{R0}$, respectively. Since (5.4) is already too complicated when $\vec{r}$, $\vec{r}' \equiv 0$, the formal SCF from (10.7) cannot be treated. Alternatively, the formal SCF arising directly from (10.6) has a more complicated structure than (5.2) with $\overrightarrow{rr'} \to \overrightarrow{0R}$ and therefore leads to SCF equations which are too "complex." The important point to emphasize is that in both cases the SCF has cylindrical symmetry about the $\vec{0}$-$\vec{R}$ axis. Since the initial and final points are identical by time-reversal invariance, there is also a plane of symmetry bisecting the $\vec{0}$-$\vec{R}$ axis. The SCF's ϕ_2 from (10.6) and (10.7) therefore have $D_{\infty h}$ symmetry!

If the formal SCF's are obtained from (10.6) or (10.7) before the limit $\epsilon \to 0^+$ is taken, these SCF's must in general be complex. In order that only real SCF's occur, it is convenient to consider the spectral decompositions (6.11) of the Green's functions in (10.6) and (10.7) just as in Secs. VII and VIII. With some rearrangement (taking the limit $\epsilon \to 0^+$), these equations can be rewritten as

$$\begin{aligned} p_{0R}(\mathcal{E}, \omega) = \textstyle\sum_j \sum_k \langle \psi_j(\vec{0}; [\phi]) \psi_j^*(\vec{R}; [\phi]) \psi_k^*(\vec{0}; [\phi]) \\ \times \psi_k(\vec{R}; [\phi]) \delta(\mathcal{E} - \tfrac{1}{2}E_j[\phi] - \tfrac{1}{2}E_k[\phi]) \\ \times \delta(\omega - E_j[\phi] + E_k[\phi]) \rangle_{\Phi} , \end{aligned} \tag{10.8}$$

with

$$p_{0R}(t; \mathcal{E}) = (2\pi)^{-2} \int_{-\infty}^{\infty} d\omega e^{-i\omega t/\hbar} p_{0R}(\mathcal{E}, \omega) , \tag{10.9}$$

where ψ_j and ψ_k are the eigenfunctions corresponding to the energies $E_j[\phi]$ and $E_i[\phi]$, respectively, for the particular value of the random field $\phi(\vec{r})$ of $D_{\infty h}$ symmetry.

Considering the development in the preceding sections, it is natural to invoke the semiclassical approximations to the Green's functions in (10.6) and (10.7), $G^{\text{WKB}}(\overrightarrow{0R}; z; [\phi])$, or, equivalently, the states and energies $\{\psi_j(\vec{r}; [\phi])$ and $E_j[\phi]\}$ in (10.8) and (10.9) for arbitrary $D_{\infty h}$ symmetry fields $\phi(\vec{r})$. Unfortunately, however, the determination of such semiclassical Green's functions, etc., requires the general analytic solution for classical motion in a plane with an arbitrary potential with the two equivalent spatial origins $\vec{0}$ and $\vec{R}$. This is a restricted form of the general classical three-body problem. It is useful to recall that a general analytic solution is required because the SCF is unknown; it is to be determined from a steepest-descents evaluation of the ϕ averaging involving a functional differentiation. The latter operation requires an explicit representation of $G([\phi])$.

Given the present difficulty of obtaining $G([\phi])$ in this case, it is then permissible to consider crude approximations ϕ_2 to the SCF which enable some qualitative conclusions to be drawn. Before presenting the detailed mathematics, we discuss the physical implications. For large R a zeroth-order approximation to ϕ_2 can be guessed to be the sum of two attractive $|\vec{r}|^{-4/3}$ potentials $\phi_{\vec{0}}$ and $\phi_{\vec{R}}$ which are centered about the points $\vec{0}$ and $\vec{R}$, respectively. This result is, of course, correct in the limit $\vec{R} \to \vec{0}$. Thus, as is in fact demonstrated below,

$$\phi_2(\vec{r}) \approx \phi_{\vec{0}}(\vec{r}) + \phi_{\vec{R}}(\vec{r}) , \quad R \to \infty \tag{10.10}$$

where $\phi_{\vec{0}}$ and $\phi_{\vec{R}}$ have the same general structure as ϕ_1 except for some constants, the appearance of a different density of states, and the ω dependence. For $E < 0$ and cases in which classical motion is forbidden with the simple $|\vec{r}|^{-4/3}$ approximations in (10.10), the WKB wave functions in the nonclassical region can be used to obtain the SCF in this region. This leads to a SCF with a positive potential fluctuation in this nonclassical region, thereby making tunneling between the two wells even less likely. The qualitative picture is clear since the situation (10.10) resembles the case of the hydrogen molecular ion. The $-|\vec{r}|^{-4/3}$ potential is more singular at the origins ($\vec{0}$ and $\vec{R}$) than the Coulomb potential, and the former is of shorter range in space than the latter. Even for long times ($t \propto R^2$) an electron in a low-lying hydrogenic state will not hop to a very distant proton (i.e., for the case of clamped nuclei and $R \to \infty$). For the $-|\vec{r}|^{-4/3}$ potential, this hopping can only be more difficult for the low-lying levels than in the Coulomb problem. If an electron on a proton were, say, photoionized to a state with $E > 0$, it could hop to another proton which is fixed at a large distance R. Consequently, the SCF ϕ_2 will lead to a nonzero mobility for $E > 0$. The behavior of the mobility near $E \approx 0$ will depend intimately upon the presence or absence of positive potential fluctuations as $E \to 0$. If absent, the mobility edge might shift to a value of E which is less than zero and vice versa. In any event, the general qualitative conclusion from (10.10) is that the mobility vanishes for the low-lying states for $E < 0$ and is nonzero when E is sufficiently greater than zero. Hence a mobility edge occurs near $E \approx 0$ in a region of nonzero density of states. This inference of the presence of a mobility edge therefore is based upon Mott's criterion for a transition between localized and extended states. Section VIII also demonstrates that $E = 0$ represents such a transition when the criterion is represented in terms of the localization probability; however, as was noted in Sec. VIII, because of the long range of the states for $E \to 0^-$, potential fluctuations involving two wells might slightly alter the transition energy. Thus, the two formally equivalent operational definitions for the mobility edge are satisfied within the SCF approximation for the present work.

Most of the above conclusions leading to the structure of ϕ_2 in (10.10) and to the implications arising from this structure can be obtained quite generally directly from (10.8) and (10.9). Just as in the analysis of ϕ_0 and ϕ_1, the general features of ϕ_2 can be deduced directly from the measure associated with random fields $\phi(\vec{r})$ which have $D_{\infty h}$ symmetry about the focal points $\vec{0}$ and $\vec{R}$. Since this measure is

$$\mathfrak{N} M'[\phi]\delta\phi = \mathfrak{N} \exp[-(2\rho\omega)^{-1} \int d\vec{r}\phi^2(\vec{r})]\delta\phi , \quad (10.11)$$

the volume element $d\vec{r}$ for coordinate systems with $D_{\infty h}$ symmetry implies that $\phi(\vec{r})$ must approach 0 as either $|\vec{r}|$ or $|\vec{r}-\vec{R}| \to \infty$. Similarly, the only place where infinite potential fluctuations may occur are at the points $\vec{0}$ and $\vec{R}$. Since infinite positive potentials at $\vec{0}$ and $\vec{R}$ would lead to very small amplitudes of the wave functions at these points, the contributions from such fields $\phi(\vec{r})$ to (10.8) are very small. Again, the potentials $\phi(\vec{r})$ which approaches $-\infty$ as $\vec{r} \to \vec{0}$ and as $\vec{r} \to \vec{R}$ make the dominant contributions to (10.8). Hence the SCF $\phi_2(\vec{r})$ must have deep potential wells which are centered about $\vec{0}$ and $\vec{R}$.

Given that $\phi(\vec{r})$ with symmetric deep wells at $\vec{0}$ and $\vec{R}$ and $\phi(\vec{r}) \to 0$ as $|\vec{r}|$ or $|\vec{R}-\vec{r}| \to \infty$ provide the dominant contributions to (10.8), it then follows that for large $\vec{R}$, $\mathrm{Im}G(\vec{0}\vec{R};\, E;\, [\phi])$ vanishes for all such ϕ when E is in the vicinity of the low-lying states: For R large and low-lying states the wave functions are composed of two pieces which are centered on the wells and which have negligible overlap with each other. This implies that there are pairs of g and u states ψ_{gj} and ψ_{uj} in this double well (with energies E_{gj} and E_{uj}, respectively) which become degenerate when R is large and the states are sufficiently low lying. In this case, the wave functions at $\vec{R}$ and $\vec{0}$ correspond to

$$\psi_{gj}(\vec{0};\, [\phi]) = \psi_{gj}(\vec{R};\, [\phi]) \to \psi_{uj}(\vec{0};\, [\phi]) = -\psi_{uj}(\vec{R};\, [\phi]) , \quad (10.12a)$$

when

$$E_{gj}[\phi] \leftarrow E_{uj}[\phi] . \quad (10.12b)$$

For E in the neighborhood of a particular pair $j = a$ of degenerate states $E_{ga} = E_{ua}$, the imaginary part of the Green's function becomes

$$-\frac{1}{\pi} \mathrm{Im}G(\vec{0}\vec{R};\, E+i\epsilon;\, [\phi]) \to \psi_{ga}(\vec{0};\, [\phi])\psi^*_{ga}(\vec{R};\, [\phi])\, \delta(E - E_{ga}[\phi]) + \psi_{ua}(\vec{0};\, [\phi])\,\psi^*_{ua}(\vec{R};\, [\phi])\,\delta(E - E_{ua}[\phi]) \equiv 0 , \quad (10.13)$$

where the equality follows directly from (10.12). This vanishing of G for E low enough only ensues because $\vec{0}$ and $\vec{R}$ correspond to particularly related symmetry points of the random fields $\phi(\vec{r})$ which make the major contribution to (10.8) and which have the $D_{\infty h}$ symmetry restriction. Equation (10.13) implies that there cannot be any contribution to (10.8) and (10.9) when $E \pm \omega$ is low lying, i.e., *in the region of a finite density of states*. As only small ω can contribute to (10.9) in the limit $R \to \infty$, $t \to R^{\alpha}$, this provides a proof of the existence of the mobility edge. For these deep traps for R large where the degenerate states ψ_{ga} and ψ_{ua} have negligible overlap, the g and u states can be transformed into another pair of degenerate levels with the same energy which only have amplitude on one of the wells. Thus, these left- and right-well eigenstates are

$$\psi_{la} = (\psi_{ga} + \psi_{ua})/\sqrt{2} , \quad \psi_{ra} = (\psi_{ga} - \psi_{ua})/\sqrt{2} , \quad (10.12c)$$

where ψ_{la} is nonzero only in the neighborhood of the well centered at $\vec{0}$ and ψ_{ra} is nonvanishing only near the well at $\vec{R}$. The picture (10.12c) of the low-lying localized states is just the one used by Mott to show that the conductivity due to localized states vanishes as $\omega^2 \ln\omega$ when the frequency $\omega \to 0$.[3]

For the lowest-lying states a wave function in one well initially has zero amplitude on any distant wells at later times. Hence in the formal SCF (5.4) of Zittartz and Langer[7] $\vec{r}$ and $\vec{r}'$ can be taken to be close to each other for these deep states. The SCF then reduces to a potential with a single well as they assumed. Lukes has assumed that the result (10.10) can be used to consider electron conductivity in disordered systems as it represents the hopping of electrons between two Zittartz-Langer potential wells.[41] The explicit derivation of ϕ_2 below, albeit crude, provides a justification for this intuitive model. Equations (10.8) and (10.9) are again to be approximated by the use of WKB wave functions which are obtained as the residues of $G^{\mathrm{WKB}}(\vec{0}\vec{R};\, z;\, [\phi])$ at the singularities. The derivation below is designed to indicate that these residues can approximately be taken to have the structure associated with potential wells centered on $\vec{0}$ and $\vec{R}$ as in (10.10). The relationship between the path-integral representation of $G([\phi])$ in (4.9) and the semiclassical approximation which we now briefly review provides the impetus for this simple approximation.[34–37]

In the limit that $\hbar$ is small relative to typical values of Hamilton's principal function in the exponent of (4.9), neighboring paths $\vec{r}(\tau)$ will essentially have random phases with respect to each other. They will therefore all destructively interfere, unless these paths are in the vicinity of the path or paths which make the exponential in (4.9) stationary. These trajectories are therefore the solutions to

$$\delta \int_0^t d\tau \left\{ \tfrac{1}{2} m [\dot{\vec{r}}(\tau)]^2 - \phi[\vec{r}(\tau)] \right\} = 0 \,, \qquad (10.14)$$

where δ represents variations of the path $\vec{r}(\tau)$ subject to the end-point constraints $\vec{r}(0) = \vec{r}'$ and $\vec{r}(t) = \vec{r}$ and the fixed transit time t. By Hamilton's principle the solutions $\vec{r}_n(\tau)$ to (10.14) are the classical trajectories from $\vec{r}'$ to $\vec{r}$ in time t. In general, there are many such paths, and the semiclassical approximation to (4.9) must contain a summation of contributions from each of these. The paths in the neighborhood of the classical paths are included in the usual fashion by retaining terms up to quadratic in the difference $\vec{r}(\tau) - \vec{r}_n(\tau)$ when Hamilton's principal function is expanded in a Taylor series about the classical paths.

The semiclassical approximation to $G(E;\, [\phi])$ of (4.12) is then obtained by Fourier transformation. Consistent with the semiclassical limit, this Fourier time integration is evaluated by the method of stationary phase. (In cases where there is only tunneling, the point of stationary phase corresponds to a complex time.[37]) In this approximation the well-known result is[35]

$$G^{\mathrm{WKB}}(\vec{r}\vec{r}';\, E;\, [\phi]) = -(2\pi\hbar^2)^{-2} \sum_{\text{classical paths}} |N_A|^{1/2} e^{iA/\hbar - i\nu\pi/2} \,, \qquad (10.15)$$

where the classical action is

$$A(\vec{r}\vec{r}';\, E;\, [\phi]) = \int_{\vec{r}'}^{\vec{r}} \vec{p} \cdot d\vec{r} = \int_0^t d\tau \vec{p}(\tau) \cdot \dot{\vec{r}}(\tau) \,, \qquad (10.16)$$

the normalization is

$$N_A = \det \begin{vmatrix} \dfrac{\partial^2 A}{\partial \vec{r}\, \partial \vec{r}'} & \dfrac{\partial^2 A}{\partial \vec{r}\, \partial E} \\ \dfrac{\partial^2 A}{\partial E\, \partial \vec{r}'} & 0 \end{vmatrix} \,, \qquad (10.17)$$

and the quantity ν is the number of unit reductions of the rank of the determinant N_A^{-1} along the classical trajectory. (For one-dimensional motion ν is the number of traversals through the classical turning points.) In general, there are an infinite number of classical trajectories for a given $\vec{r}$, $\vec{r}'$, and E, and the contributions from these paths will destructively interfere unless the actions for all of these trajectories are somehow related; i.e., they all lie on some periodic (or multiply periodic) orbit. This then leads to the Bohr-Sommerfeld quantization condition for many-dimensional nonseparable potentials.[37] For one-dimensional radial motion, application of (10.15)–(10.17) leads to the results quoted in (6.8) [cf. (6.18) also].

In the case of (10.8) and (10.9), those periodic orbits passing through $\vec{0}$ and $\vec{R}$, for $|\vec{R}|$ large, are required. These planar orbits for the present case of $D_{\infty h}$ symmetry potentials with deep symmetrical wells about $\vec{0}$ and $\vec{R}$ can easily be deduced from the radial orbits which arise in the spherically symmetric case when $\vec{R} \to \vec{0}$. Consider first the lowest-lying states where classical motion from $\vec{0}$ to $\vec{R}$ may be forbidden. The tunneling orbits required must be those which lie on the $\vec{0}$-$\vec{R}$ axis, going from $\vec{0}$ to $\vec{R}$, $\vec{R}$ to $\vec{R}+\vec{a}$, $\vec{R}+\vec{a}$ back to $-\vec{a}$, and then back to $\vec{0}$, etc. Because of the deep wells surrounding $\vec{0}$ and $\vec{R}$ and the condition that the fields $\phi(\vec{r})$ contributing to (10.8) vanish as $|\vec{r} - \vec{R}|$ or $|\vec{r}| \to \infty$, this orbit is the one with minimum potential barrier in the classically forbidden region. Thus, our approximation is an adiabatic one in which we consider the motion as being along the one-dimensional coordinate representing the most favorable path. The semiclassical wave function is then the one-dimensional wave function for this path multiplied by a function of the coordinate orthogonal to the path. The assumption is that the latter function is rapidly decaying away from the most favorable path, so its effect upon the SCF can be ignored; only the motion along the most favorable path is used to obtain the SCF. During the classical motion in either of the deep wells, the contribution to the potential from the other well is negligible.

Hence, the motion corresponds to bounded radial motion in a spherically symmetric potential on the given well. During tunneling, in the region surrounding $\frac{1}{2}\vec{R}$, the dependence of the potential upon both $\vec{0}$ and $\vec{R}$ becomes of prime importance, and consequently, we are unable to deduce the precise shape of potential in the important "bar of the dumbbell." In summary, in the region near $\vec{0}$, the unnormalized wave function is of the form (apart from the Langer correction for radial wave functions which must eventually be included)

$$[p_{\vec{0}}(r)]^{-1/2}\cos[\int_0^r p_{\vec{0}}(r')\,dr'/\hbar-\tfrac{1}{4}\pi]\,, \qquad (10.18)$$

where

$$p_0(r)=\{2m[E-\phi_{\vec{0}}(r)]\}^{1/2}\,, \qquad (10.19)$$

and $\phi_{\vec{0}}(r)$ is the spherical part of the random field ϕ which is centered about $\vec{0}$. The function (10.18) connects with the exponentially decaying function

$$|p_0(r)|^{-1/2}\exp[-\int_{r_0}^r |p_0(r')|\,dt'/\hbar] \qquad (10.20)$$

for r just inside the nonclassical region beyond the turning point r_0, $\frac{1}{2}R\gg r_0>0$. The wave function (10.20) eventually joins up with the function which exponentially increases (as r increases) as we approach the turning point r_R, $R>r_R\gg\frac{1}{2}R$, i.e.,

$$|p_{\vec{R}}(r)|^{-1/2}\exp[-\int_r^{r_R} |p_{\vec{R}}(r')|\,dr'/\hbar]\,, \qquad (10.21)$$

where

$$p_{\vec{R}}(r)=\{2M[E-\phi_{\vec{R}}(r)]\}^{1/2}\,, \qquad (10.22)$$

and $\phi_{\vec{R}}$ is that spherical symmetric part of ϕ which is centered about $\vec{R}$. Lastly, (10.22) connects with

$$[p_{\vec{R}}(r)]^{-1/2}\cos[\int_r^{r_R} p_R(r')dr'/\hbar-\tfrac{1}{4}\pi] \qquad (10.23)$$

inside the well around $\vec{R}$.

The evaluation of the SCF now proceeds just as in Secs. VII and VIII. The steepest-descents evaluation of (10.8) is performed with a particular j and k and with ω small. The wave function $\psi_j(\vec{A};[\phi])$, $\vec{A}=\vec{0}$, $\vec{R}$ (with the Langer correction), is proportional to

$$|E_j[\phi]|^{1/4}(T_{\vec{0}}+N_{\vec{0}}+T_{\vec{R}}+N_{\vec{R}})^{-1/2}\,, \qquad (10.24)$$

where $T_{\vec{A}}$ is the period for the radial classical motion in the well about $\vec{A}$ [cf. (7.14)], $N_{\vec{A}}$ is the contribution from the nonclassical region [cf. (8.7) and (8.8)] near the well on $\vec{A}$, and the small contribution from the region about $\frac{1}{2}R$ is ignored. The energies $E_j[\phi]$ can be taken as approximately those for a single well—the presence of the second well could be treated by perturbation theory. After using the ϵ form for the two dirac δ functions in (10.8), these δ functions are shown to be slowly varying in the region of the saddle point ϕ_2 just as in the case of (7.6)–(7.9) and (8.4)–(8.5). This slow variation arises because (10.8) is only needed for ϵ and ω small, and hence

$$|E_j[\phi_2]|^{-1}\approx|E_k[\phi_2]|^{-1}$$
$$\gg\frac{\mathrm{P}}{\mathcal{E}-\frac{1}{2}(E_j[\phi_2]+E_k[\phi_2])}\,,\quad\frac{\mathrm{P}}{\omega-E_j[\phi_2]+E_k[\phi_2]}\,. \qquad (10.25)$$

Thus the δ functions in (10.8) can again be removed from the ϕ averaging and are evaluated at ϕ_2. The remaining saddle-point determination proceeds identically as in Secs. VII and VIII leading to $\phi_{\vec{0}}$ and $\phi_{\vec{R}}$ being $-|\vec{r}|^{-4/3}$ wells centered at $\vec{0}$ and $\vec{R}$, respectively, with positive potential fluctuations in the nonclassical region. (Because of the negligible overlap between low-lying functions on either well, we can safely take $\phi_{\vec{0}}$ and $\phi_{\vec{R}}\to 0$ at $\frac{1}{2}\vec{R}$ as the first approximation.) Although the above derivation only considers the wave function along the $\vec{0}$-$\vec{R}$ axis, clearly the form of the wave function is known throughout all of space, thereby leading to a more complete derivation of the ϕ_2 quoted above.

As $\mathcal{E}$ increases and the parts of the wave functions centered on the wells at $\vec{0}$ and $\vec{R}$ begin to overlap for those dominant contributing random fields $\phi(\vec{r})$, the above arguments still lead to $-|\vec{r}|^{-4/3}$ wells about $\vec{0}$ and $\vec{R}$, with greater uncertainty about the region around $\frac{1}{2}\vec{R}$. When the overlap begins to grow large, $\phi_{\vec{0}}$ and $\phi_{\vec{R}}$ are still primarily $-|\vec{r}|^{-4/3}$ wells, but they are increasingly perturbed by the presence of the other well. This perturbation arises mainly from the dependence of the energies $E_j[\phi]$ on both wells in the overlap region; the basic structure of (10.24) is retained except that $N_{\vec{0}}$ and $N_{\vec{R}}$ cannot be separated but must be combined into a single $N_{\vec{0}\vec{R}}$.

The next range of energies to be considered are those for which classical motion from $\vec{0}$ to $\vec{R}$ is no longer forbidden. In this case there are a number of types of classical periodic orbits which contribute to the semiclassical Green's function (10.15)–(10.17). For instance, let the points $\vec{R}_0$ and $\vec{R}_0'$ be those which are common to the plane bisecting the $\vec{Q}-\vec{R}$ axis and either the turning point surface or the wall which is included to provide box normalization. There is then a periodic orbit where the particle travels from $\vec{0}$ to $\vec{R}_0$, then $\vec{R}_0$ to $\vec{R}$, $\vec{R}$ to $\vec{R}_0'$, and finally from $\vec{R}_0'$ back to $\vec{R}$. In this case the orbit does not intersect the $\vec{0}-\vec{R}$ axis at points other than $\vec{0}$ and $\vec{R}$. Clearly there are also periodic orbits which intersect this axis at other points an arbitrary number of times, the simplest being of the form of a figure eight with the orbit intersecting itself at $\frac{1}{2}\vec{R}$ (by symmetry).

In the simplest case, when $\vec{R}$ and $\vec{R}_0$ are large, the motion from $\vec{0}$ to $\vec{R}_0$ can be approximated as purely radial motion in the spherically symmetric well $\phi_{\vec{0}}(r)$, etc., for motion near $\vec{R}$. In order to determine the dependence of the over-all normalization (10.17) on the number of full traversals of the periodic orbit, it would be necessary to consider the stability of the orbit,[35] a task complicated by the general nature of $\phi(\vec{r})$. Our adiabatic hypothesis in part corresponds to ignoring the dependence of this normalization on the number of full traversals. With this assumption, the phases from all the classical paths (say, for the case that the orbits do not intersect the $\vec{0}-\vec{R}$ axis other than at $\vec{0}$ and $\vec{R}$) can be summed to yield

$$G^{\mathrm{WKB}}(\vec{0}\vec{R};\; z;\; [\phi]) \approx -(2\pi\hbar)^{-1} \left| N_A(\vec{0}\vec{R};\; z;\; [\phi]) \right|^{1/2} \times e^{(i\theta/2)}(1-e^{i\theta})^{-1} \;, \qquad (10.26)$$

where

$$\hbar\,\theta \simeq 2\int_0^{\bar{R}_0} dr\{2m[z-\phi_{\vec{0}}(r)]\}^{1/2} + 2\int_{\bar{R}_0}^{R} dr\{2m[z-\phi_{\vec{R}}(r)]\}^{1/2} - \pi h \,. \qquad (10.27)$$

The poles of (10.15) lead to the quantization condition $\hbar\,\theta = 2\pi n$, $n = 1, 2, \ldots$, for standing waves in the box-normalized states or some of the high-lying bound states [cf. (6.4)–(6.6)]. Introducing the Langer correction for the radial motion, the spectral representation is then written as

$$G^{\mathrm{WKB}}(\vec{0}\vec{R};\; z;\; [\phi]) \simeq \sum_j \frac{|E_j[\phi]|^{1/2} M_j(\vec{0}\vec{R};\; E_j[\phi];\; [\phi])}{(z-E_j[\phi])\{T_{\vec{0}}(E_j[\phi];\; [\phi]) + T_{\vec{R}}(E_j[\phi];\; [\phi])\}} \,, \qquad (10.28)$$

where, for instance,

$$T_{\vec{R}}(z) = \int_{R_0}^{R} dr\{(2/m)[z-\phi_{\vec{R}}(r)]\}^{-1/2} \qquad (10.29)$$

is that part of the period which is spent in the well at $\vec{R}$. The term M_j contains the dependence of G on motions perpendicular to the most favorable path, and this dependence is ignored in the saddle-point evaluation of ϕ averaging. This steepest-descents calculation proceeds just as in the analyses of ϕ_0 and ϕ_1 leading to a $\phi_2(\vec{r})$ with the structure given in (10.10) and $-|\vec{r}|^{-4/3}$ wells centered at $\vec{0}$ and $\vec{R}$.

A general solution to the present problem would, of course, be of interest, but given the inherent mathematical complexities, the crude approach taken here is sufficient to exhibit the general structure (10.10). In fact, given this result, it will be instructive to consider simple model potentials which exhibit the general structure of ϕ_2, but which are even simpler to handle mathematically. One such model involves the "dumbbell potential" which is made up of three parallelepiped sections, where allowance is made for the differences in potential between the bar and the two ends. Similarly, the sizes of the three wells are kept arbitrary and are then determined "variationally" as in the case of Edward's simple van der Waals–type model. This variation in size, therefore, includes the possibility that the dumbbell degenerates down to a simple parallelepiped with the symmetry points $\vec{0}$ and $\vec{R}$.

XI. CONCLUSIONS

The model of an electron in the presence of dense weak random scatterers, or equivalently an electron in a Gaussian random potential, is used in an attempt to elucidate the general features of the electronic structure of disordered systems. The model leads to a mathematical description of the ensemble-averaged one-electron properties which is analogous to that for the general many-body problem. Thus, a solution is sought within the framework of a self-consistent-field (SCF) formulation. Because the existence of localized states in the translationally invariant ensemble-averaged system represents a breaking of symmetry, it is important to indicate how the use of a SCF approximation naturally introduces this symmetry breaking. The resulting symmetry of the SCF is also an important aspect of the approach.

In order that only real SCF's need be considered, separate SCF's are to be determined for the real and imaginary parts of averaged properties. This is an essential simplification over the occurrence of complex SCF's when this separation is not performed.

The Green's functions for electron motion in the Gaussian random potential are approximated using semiclassical techniques. The transition between localized and extended states is found to occur at $E = 0$, the average energy. The probability density that an electron return to its initial position $\vec{0}$ after an infinite time, $p_0(E)$, varies as $(-E)^{13/6}$ below the mobility edge and is zero above it. The SCF obtained for $p_0(E)$ is a spherically symmetric $-|\vec{R}|^{-4/3}$ energy-dependent potential well. The localization range, the classical turning point from the SCF, is found to vary as $(-E)^{-2/3}$. Outside of the classically allowed region, the SCF becomes positive and then decays as $e^{-\kappa R}/R^2$ as $R \to \infty$, thereby reinforcing the association of the turning point with the size of the localized states. Another slightly different measure comes from equating the localization volume with the ratio of $n_0(E)/p_0(E)$. This leads to a localization radius which varies as $(-E)^{-5/9}$.

Note added in proof. R. M. White and P. W. Anderson [Phil. Mag. 25, 737 (1972)] have shown that the large size of the localized states near the mobility edge contributes to the enhancement of the diamagnetic susceptibility of amorphous semiconductors (e.g., As_2S_3 and As_2Se_3) relative to the corresponding crystals.

It is important to note that the SCF's determined for $n_0(E)$, the density of states at the original (and final) position, and $p_0(E)$ are identical except for some inconsequential factors of 2. Since the former is related to the average Green's function, while the latter is obtained from the average of the product of two Green's functions $\langle \mathcal{G}\mathcal{G}\rangle$, there remains the possibility that the position of the mobility edge can generally be inferred from the average Green's function alone, whereas a rigorous determination requires a consideration of $\langle \mathcal{G}\mathcal{G}\rangle$.

In order to directly calculate the electron mobility in the disordered system, the simplest quantity to consider is $p_{0R}(E, t)$, the ensemble-averaged probability that an average electron with energy E at $\vec{0}$ will be at $\vec{R}$ at time t, in the long-time large-distance limit of diffusive or nearly diffusive motion. The SCF for this property has $D_{\infty h}$ symmetry, the same symmetry as the nuclear field in the hydrogen molecular ion, thereby complicating the determination of the semiclassical Green's function for motion in such an arbitrary nonseparable potential. However, it is generally demonstrated that the SCF must have deep symmetrical wells which are centered at $\vec{0}$ and $\vec{R}$, and these wells are shown to have the same $-|\vec{r}|^{-4/3}$ energy-dependent behavior as is found for the SCF's for $n_0(E)$ and $p_0(E)$. This $-|\vec{r}|^{-4/3}$ dependence arises because the average electron, when in the neighborhood of one of the wells, has its motion determined by the nature of the singularity of the potential at that well. Because of the mathematical complexities inherent in potentials of $D_{\infty h}$ symmetry, it has not been possible to determine generally the nature of the SCF in the important region between the wells—near $\frac{1}{2}\vec{R}$. However, for the lowest-lying levels the general features of the SCF in this midregion are deduced, and the results are used to show that the conductivity due to electrons in these low-lying states vanishes. The resultant SCF for $p_{0R}(E, t)$ provides a justification for the model used by Mott to show that the conductivity due to localized states vanishes as $\omega^2 \ln\omega$ as the frequency $\omega \to 0$. It likewise yields the *ad hoc* model of Lukes which describes hopping between two Halperin-Lax-Zittartz-Langer-type deep wells. Similarly, it provides another justification for Halperin and Lax's and Zittartz and Langer's use of spherically symmetric SCF's and their neglect of distant wells in discussing the lowest-lying levels.

In the case of $n_0(E)$ and $p_0(E)$ the contributions from the fluctuations about the SCF that preserve the symmetry of the SCF are maintained. Those potential fluctuations with other symmetries could be included by perturbation theory using the techniques of Zittartz and Langer. In considering $p_{0R}(E, t)$, it is probably more instructive to perform model calculations with simpler random potentials, say of a form which represents a natural generalization of Edward's van der Waals model, than to explicitly consider the fluctuations about the SCF.

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Bulk Moduli of Simple Metals Calculated from the Method of Homogeneous Deformations and the Method of Long Waves

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It is customary in the model-potential theory of simple metals to solve the Schrödinger equation for the conduction electrons by perturbation theory and to retain only terms to second order in the lattice structure factor. This method of solution leads to a simple expression for the total energy of a metal. Two values of the bulk modulus of the metal may be deduced from this expression: one (B_D) by direct differentation with respect to volume and the other ($B_{\rm LW}$) by an application of the method of long waves. These two approximations to the bulk modulus are not equal in a second-order theory. However, equality may be obtained, for local electron-ion potentials, if certain terms of third and fourth order are retained in the perturbation solution of the Schrödinger equation. The magnitude of these terms has been estimated for several potentials and metals and has often been found to be large. Results are also extremely sensitive to the potential used. In this paper, it is argued that the variation among existing results implies that the full nonlocality and energy dependence of the electron-ion potential must be retained if reliable estimates of ($B_D - B_{\rm LW}$) are to be made. Consistent and complete expressions for the total energy of a metal in terms of an optimized form of the Heine-Abarenkov model potential are presented and it is shown that these expressions give an adequate account of the cohesive energies and lattice parameters of several simple metals. From the expression for total energy, formulas for B_D and $B_{\rm LW}$ are obtained which are qualitatively different from those of a local approximation. The nonlocal and energy-dependent contributions are found to be numerically important in calculations of B_D and $B_{\rm LW}$ for three simple metals. The expressions obtained imply small differences between B_D and $B_{\rm LW}$ for these metals, when one of the parameters of the theory is suitably adjusted. This parameter, which represents the spatial distribution of the depletion charge, is not obtainable within the framework of conventional model-potential theory. Thus the calculations suggest that further work is necessary before a complete statement about the influence of higher-order perturbation terms on ($B_D - B_{\rm LW}$) can be made.

I. INTRODUCTION

The majority of detailed calculations of properties of simple metals have involved the use of a single-particle model Schrödinger equation to describe the conduction-electron energies. In this equation, the true conduction-electron–ion potential is often replaced by an effective or model potential.[1] This replacement is justified, since the effective potential is chosen to maintain, modulo π, the correct scattering phase shifts for conduction electrons. In order to guarantee that this latter condition is fulfilled, it is found that the effective potential must be a function of both the angular momentum and energy of the scattered electrons.

Since the effective potential (including electron-screening effects) is weak, the model Schrödinger