The general behavior of the current is consistent with a model of tunneling of carriers through the reversed biased barrier. Such a barrier becomes broadened, but sharply peaked. Again, it is required that the barriers be of different height in order to explain the difference in behavior with difference in sign of voltage.

It is to be noted in comparing Figs. 6 and 7 that for values of dc bias for which the equilibrium value of $\epsilon$ coincides with the theoretical value in Fig. 7, the equilibrium value is reached instantaneously as shown in Fig. 6. Where experimental points in Fig. 7 fall below theoretical values, there is an observable delay between application of electric field and final value of capacitance taken from Fig. 6. This corresponds to the fact that time is required for space-charge layers to build up. Initially (in time) after application of the electric field, the normal dielectric constant is observed. As the space-charge layer broadens, the observed capacitance (or apparent $\epsilon$) decreases.

## VI. CONCLUSION

Unraveling the assorted anomalous effects that have been reported in $BaTiO_3$ which have been attributed to some form of surface layer has not led to any consistent picture of the layer except in the most qualitative terms. The results reported here are representative of measurements made on a number of crystals in which evidence of space-charge layers whose thickness is voltage dependent may be seen. The detailed quantitative interpretation of results is hampered by complicated electric field distributions and our general ignorance of $BaTiO_3$ surfaces. On the other hand, the observations indicate that further work in which impurity concentrations and dielectric constant are varied (the latter by varying temperature) as well as thickness of samples would be worthwhile in trying to understand details of surface layers and fields in insulators and $BaTiO_3$ in particular.

It is felt that measurements of this kind will shed light on the general problem of mapping of space-charge regions in insulators. It is clear that experiments that actually probe such regions are difficult to imagine on the general insulating material. The special property that makes a ferroelectric amenable to such probing is the sensitivity it exhibits to reasonably attainable fields in its Kerr effect and dielectric constant.

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# Effect of the Lattice on Dielectric Properties of an Electron Gas*

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A system of $N$ electrons in the presence of a rigid periodic background of positive charge is considered. Following Martin and Schwinger, an inverse dielectric operator, $\mathcal{K}'$, is introduced. An approximate equation which takes into account the long-range nature of the Coulomb field is derived for $\mathcal{K}'$. A representation is used where $\mathcal{K}'$ is a matrix with rows and columns labeled by vectors of the reciprocal lattice. Poles and zeros in the dielectric operator are found to be manifestations of Bragg's law. Assuming these to be the major effect of the lattice, the equation for $\mathcal{K}'$ is solved. The result is examined in the weak-binding limit and seen here, except at the Bragg reflections, to agree with that of Nozières and Pines. Finally the ground-state energy of the system is exhibited.

## INTRODUCTION

A GOOD deal of attention has been devoted lately to the properties of a gas of interacting electrons in the presence of a uniform background of positive charge. Much of the interest in this system stems from the hope that it will, for some applications, be a good model for the electrons in a solid. Now in a solid, of course, the positive charge is not uniformly distributed but rather concentrated on ions which vibrate about equilibrium positions that form a lattice structure containing various kinds of defects. The existence of the lattice as well as the defects in it and the vibrations about it may be expected to have some effect on the dielectric properties of the electron gas. It is the purpose of this paper to investigate the effect of the lattice, ignoring defects and vibrations, in order to see where the free electron gas results are valid and where and how they must be modified because of the presence of the lattice. To this end the inverse dielectric operator of Martin and Schwinger will be considered here and techniques suited to the weak but long-ranged nature of the Coulomb field will be used to derive an approximate equation for it. This equation will be solved and the effect of the lattice on this operator and hence on, say, the ground-state energy of the system, will be seen.

Consider a system of volume $\Omega$ containing $N$ electrons

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imbedded in a rigid periodic background of positively charged ions which we shall describe by the potential $V_I(\mathbf{r})$. The spatial structure of the positive lattice may be described by means of a set of $N$ lattice vectors, typified by $\mathbf{R}$, which go from one (arbitrarily chosen) ion to each of the others. In terms of these vectors the periodicity is expressed by

$$V_I(\mathbf{r})=V_I(\mathbf{r}+\mathbf{R}). \tag{1}$$

An electron at $(\mathbf{r},t)$ has a direct interaction with one at $(\mathbf{r}',t')$ described by

$$v(x-x')=v(\mathbf{r}-\mathbf{r}')\delta(t-t')=\frac{e^2}{|\mathbf{r}-\mathbf{r}'|}\delta(t-t'). \tag{2}$$

We then describe the system by a Hamiltonian

$$H=\int d\mathbf{r}\,\psi^\dagger(\mathbf{r},t)[(-\hbar^2\nabla^2/2m)+V_I(\mathbf{r})]\psi(\mathbf{r},t)$$

$$+\tfrac{1}{2}\int d\mathbf{r}d\mathbf{r}'\psi^\dagger(\mathbf{r},t)\psi^\dagger(\mathbf{r}',t)v(\mathbf{r}-\mathbf{r}')\psi(\mathbf{r}',t)\psi(\mathbf{r},t), \tag{3}$$

where the operators $\psi(\mathbf{r},t)$, $\psi\dagger(\mathbf{r},t)$ obey the anticommutation relations

$$\{\psi(\mathbf{r},t),\psi^\dagger(\mathbf{r}',t)\}=\delta(\mathbf{r}-\mathbf{r}'),$$
$$\{\psi(\mathbf{r},t),\psi(\mathbf{r}',t)\}=0=\{\psi^\dagger(\mathbf{r},t),\psi^\dagger(\mathbf{r}',t)\}. \tag{4}$$

We want to determine the effect of the detailed electron-electron interaction on the energy of a degenerate electron gas at zero temperature. We calculate this energy change as a perturbation on the energy of a system of $N$ electrons subject to the same average Hartree potential and occupying the lowest $N$ single-particle levels. The highest filled level is called the Fermi level. The eigenfunctions and eigenvalues of the Hartree problem are assumed to be known and to satisfy

$$[-(\hbar^2\nabla^2/2m)+V_I(\mathbf{r})+V_H(\mathbf{r})]\psi_n(\mathbf{k},\mathbf{r})=E_n(\mathbf{k})\psi_n(\mathbf{k},\mathbf{r}), \tag{5}$$

where $m$ is the mass of the electron. The Hartree potential is given by

$$V_H(\mathbf{r})=\int v(\mathbf{r}-\mathbf{r}')\rho(\mathbf{r}')d\mathbf{r}', \tag{6}$$

where $\rho$ is the density of electrons,

$$\rho(\mathbf{r})=\frac{1}{N}\sum_{n<m}\int_0^{\mathbf{P}}\frac{d\mathbf{k}}{(2\pi)^3}\psi_n^*(\mathbf{k},\mathbf{r})\psi_n(\mathbf{k},\mathbf{r}). \tag{7}$$

and the notation on the integral is intended to convey that we sum over only those levels below the Fermi level (at band $m$, momentum $\mathbf{P}$), i.e., only over occupied levels.

Using the techniques for the many-electron system developed by Martin and Schwinger,[1] we should like to calculate the effects of the electron-electron interaction on the energy, that is, we want the exchange and correlation energies. This problem has been considered in detail for the free electron gas[2] i.e., a uniform background of positive charge. It will be our purpose here to see how the presence of the periodic potential, $V_I(\mathbf{r})$, affects the usual result.

It is worth noting that while the presence of $V_I(\mathbf{r})$ in general tends to complicate things, it may in some cases simplify the interpretation. Thus consider the $N$ electrons to consist of $N-1$ electrons filling the atomic core and valence levels of an insulator or semiconductor and one electron with momentum $\mathbf{k}$ in the conduction band which is separated from the valence band by an energy gap of width $E_g$.[3] In this case there will be real energies for excited states ($\mathbf{k}\neq 0$) provided the excitation energy is less than $E_g$. In the free electron gas, for any excitation energy, $E_e$, one can always construct states with the same momentum but smaller excitation energy by distributing the energy and momentum over more than the one electron. Thus any single-particle excitation will have a finite decay time, or, crudely, a complex energy. With the energy gap, however, for $E_e<E_g$, one may unambigously consider the excitation as a one-particle excitation as there are no multiparticle states to which it can decay.

## THE APPROXIMATE EQUATION

In an electron gas, where the interactions are weak but long ranged, divergences occur when calculations are performed by standard perturbation theory. It is well known, however, that these divergences, due to the range of the Coulomb field, are cancelled by polarization effects[4]; that is, a charge placed in the medium has its field altered by the medium which tends to shield the charge. Equivalently, if an external potential, $U(x)$, is applied to the medium, an effective potential, $V'(x)$, consisting of the external potential together with the induced change in potential produced by the medium, will be experienced in the medium.

Let us therefore consider the operator $\mathcal{K}'(x,x')$

[1] P. C. Martin and J. Schwinger, Phys. Rev. **115**, 1342 (1959)
[2] E.g., J. Lindhard, Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd. **28**, No. 8 (1954); D. Pines, *Solid-State Physics*, edited by F. Seitz and D. Turnbull (Academic Press, Inc., New York, 1955), Vol. 1; J. Hubbard, Proc. Roy. Soc. (London) **A243**, 336 (1958); P. Nozières and D. Pines, Phys. Rev. **109**, 762 (1958).
[3] It will be noted that this case is not exactly the degenerate gas since there will be unoccupied levels in the conduction band below the level with momentum $\mathbf{k}$. However, the theory of this paper may still be used provided that these levels are included in the class of unoccupied levels in the sum over levels, and that the level with momentum $\mathbf{k}$ is considered as occupied. Thus, in the sum over levels there will be an integral over the valence band plus the contribution from the lone occupied conduction band level, whatever it might be.
[4] M. Gell-Mann and K. A. Brueckner, Phys. Rev. **106**, 364 (1957).

which relates $U(x')$ and $V'(x)$:

$$V'(x)=\int \mathcal{K}'(x,x')U(x')dx'. \tag{8}$$

To recognize $\mathcal{K}'$, assume that the potential $U$ is set up by a charge distribution $\rho$. Then the Fourier transform in space and time of $U$ is given by

$$U(\mathbf{k},\omega)=(4\pi/\mathbf{k}^2)\rho(\mathbf{k},\omega). \tag{9}$$

If we, for the moment, specialize to the case of spatial (as well as temporal) translational invariance, we may write the Fourier transform of (8) as

$$V'(\mathbf{k},\omega)=\mathcal{K}'(\mathbf{k},\omega)(4\pi/\mathbf{k}^2)\rho(\mathbf{k},\omega). \tag{10}$$

Now, classically the potential, $\phi$, at large distances from a static-charge distribution, $\rho$, in a dielectric medium is given by

$$\phi(\mathbf{k})=(4\pi/\epsilon\mathbf{k}^2)\rho(\mathbf{k}), \tag{11}$$

where $\epsilon$ is the dielectric constant. Equation (11) is just the Fourier transform of Poisson's equation in a dielectric. We may generalize (11) to include small distances and temporally varying charge distributions by letting $\epsilon$ depend on space and time, so that its Fourier transform depends on momentum and frequency.[5] Then we have

$$V'(\mathbf{k},\omega)=[4\pi/\epsilon(\mathbf{k},\omega)\mathbf{k}^2]\rho(\mathbf{k}). \tag{12}$$

Comparison of (10) and (12) shows $\mathcal{K}'$ to be the inverse of $\epsilon$. Even without translational invariance, if we consider both $\mathcal{K}'$ and $\epsilon$ as *operators*,[6] we may write

$$\mathcal{K}'=\epsilon^{-1}. \tag{13}$$

Thus $\mathcal{K}'$ tells us the dielectric properties of the medium. It is more useful than $\epsilon$ in that it also allows the calculation of the inelastic scattering of fast charged particles by thin solid foils[7] and of the ground-state energy of the medium.[8] Further, it may be used to develop single-particle equations to improve the results of the Hartree equation in band-structure calculations.[9]

Martin and Schwinger[1] have shown that $\mathcal{K}'$ satisfies

$$\mathcal{K}'(x,x')=\delta(x-x')-(i/\hbar)\int dx''dx'''\, v(x-x'')\times\left[\frac{\delta}{\delta V'(x''')}\bar{G}(x'',\mathbf{r}''t''+0)\right]\mathcal{K}'(x''',x'), \tag{14}$$

where $\bar{G}(x,x')$ is the Green's function which describes the propagation of an electron (or hole) through the medium from $x'$ to $x$ and satisfies

$$\left[i\frac{\partial}{\partial t}+\frac{\hbar^2\nabla^2}{2m}-V_I(\mathbf{r})-V'(x)-i\int dx''dx'''\times v(x-x'')\mathcal{K}'(x''',x'')\delta/\delta V'(x''')\right]\bar{G}(x,x')=\delta(x-x'). \tag{15}$$

The Hartree approximation consists of neglecting the last term in (15), from which it easily follows that

$$\delta\bar{G}_H(x,x')/\delta V'(x'')=\bar{G}_H(x,x'')\bar{G}_H(x'',x'). \tag{16}$$

If we then insert (16) into (14) as a first approximation, we arrive at

$$\mathcal{K}'(x,x')=\delta(x-x')-(i/\hbar)\int dx''dx'''\, v(x-x'')\times\bar{G}_H(x'',x''')\bar{G}_H(x''',x'')\mathcal{K}'(x''',x'). \tag{17}$$

The Hartree Green's function is given by[10]

$$iG_H(\mathbf{r}t,\mathbf{r}'t')=\frac{1}{N}\sum_{n>m}\int_{\mathrm{P}}^{\infty}\frac{d\mathbf{k}}{(2\pi)^3}\psi_n^*(\mathbf{k},\mathbf{r})\psi_n(\mathbf{k},\mathbf{r}')\times e^{-(i/\hbar)E_n(\mathbf{k})(t-t')},\quad t>t' \tag{18}$$

$$=-\frac{1}{N}\sum_{n<m}\int_{0}^{\mathrm{P}}\frac{d\mathbf{k}}{(2\pi)^3}\psi_n^*(\mathbf{k},\mathbf{r})\psi_n(\mathbf{k},\mathbf{r}')\times e^{-(i/\hbar)E_n(\mathbf{k})(t-t')},\quad t<t'.$$

## SOLUTION OF THE EQUATION

Let us introduce some alternative forms of the Hartree wave functions $\psi_n(\mathbf{k},\mathbf{r})$. As both $V_I(\mathbf{r})$ and $V_H(\mathbf{r})$ have the periodicity of the lattice, we may write the $\psi_n$ in Bloch form:

$$\psi_n(\mathbf{k},\mathbf{r})=e^{i\mathbf{k}\cdot\mathbf{r}}u_n(\mathbf{k},\mathbf{r}), \tag{19}$$

where the $u_n$ are periodic

$$u_n(\mathbf{k},\mathbf{r}+\mathbf{R})=u_n(\mathbf{k},\mathbf{r}). \tag{20}$$

We may therefore expand the $u_n$ in a Fourier series

$$u_n(\mathbf{k},\mathbf{r})=\sum_{\mathbf{K}}\chi_n(\mathbf{k},\mathbf{K})e^{-i\mathbf{K}\cdot\mathbf{r}}, \tag{21}$$

where the reciprocal lattice vectors $\mathbf{K}$ are defined by

$$e^{i\mathbf{K}\cdot\mathbf{R}}=1. \tag{22}$$

Some properties of the chosen wave functions and

[5] J. Lindhard, reference 2; P. Nozières and D. Pines, reference 2; J. J. Quinn and R. A. Ferrell, Phys. Rev. **112**, 812 (1959).
[6] U. Fano, Phys. Rev. **103**, 1202 (1956).
[7] P. Nozières and D. Pines, Phys. Rev. **113**, 1254 (1959).
[8] J. Hubbard, reference 2.
[9] G. W. Pratt, Jr. (to be published).
[10] P. C. Martin and J. Schwinger, reference 1; J. Hubbard, reference 2; J. J. Quinn and R. A. Ferrell, reference 5; A. Klein and R. Prange, Phys. Rev. **112**, 994 (1958).

energies are

$$\sum_n \chi_n^*(\mathbf{k},\mathbf{K})\chi_n(\mathbf{k},\mathbf{K}')=\delta_{\mathbf{K},\mathbf{K}'}, \quad (23)$$

$$\sum_{\mathbf{K}} \chi_n^*(\mathbf{k},\mathbf{K})\chi_{n'}(\mathbf{k},\mathbf{K})=\delta_{n,n'}, \quad (24)$$

$$\chi_n(\mathbf{k}-\mathbf{K},\mathbf{K}')=\chi_n(\mathbf{k},\mathbf{K}'+\mathbf{K}), \quad (25)$$

$$\chi_n^*(\mathbf{k},\mathbf{K})=\chi_n(-\mathbf{k},-\mathbf{K}), \quad (26)$$

and

$$E_n(\mathbf{k})=E_n(-\mathbf{k})=E_n(\mathbf{k}+\mathbf{K}). \quad (27)$$

We may expand $\mathcal{K}'$ as

$$\mathcal{K}'(\mathbf{r}t,\mathbf{r}'t')=\sum_{\mathbf{k}}\int \frac{d\mathbf{k}}{(2\pi)^3}\frac{d\omega}{2\pi}e^{i\mathbf{K}\cdot\mathbf{r}}e^{-i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}e^{-i\omega(t-t')} \times\mathcal{K}'(\mathbf{k},\mathbf{K};\omega). \quad (28)$$

Then inserting (28) and (18) in (17) and performing the integrations in analogy with the free electron case,[2] we obtain

$$\mathcal{K}'(\mathbf{k},\mathbf{K};\omega)+\sum_{\mathbf{K}'}\alpha(\mathbf{k}-\mathbf{K}',\mathbf{K}-\mathbf{K}';\omega) \times\mathcal{K}'(\mathbf{k},\mathbf{K}';\omega)=\delta_{\mathbf{K},0}, \quad (29)$$

where

$$\alpha(\mathbf{k}-\mathbf{K}',\mathbf{K}-\mathbf{K}';\omega) =\frac{4}{N}\sum_n\sum_{n'<m}\int_0^{\mathrm{P}}\frac{d\mathbf{k}'}{(2\pi)^3} \times\frac{[E_n(\mathbf{k}-\mathbf{k}')-E_{n'}(\mathbf{k}')]}{[E_n(\mathbf{k}-\mathbf{k}')-E_{n'}(\mathbf{k}')-i\eta]^2-\hbar^2\omega^2} \times v(\mathbf{k}-\mathbf{K})\rho_{\mathbf{k}',\mathbf{k}'-\mathbf{k}}^{n'n}(\mathbf{K})\rho_{\mathbf{k}',\mathbf{k}'-\mathbf{k}}^{n'n*}(\mathbf{K}'). \quad (30)$$

where $\eta\to 0+$,

$$v(\mathbf{k}-\mathbf{K})=4\pi e^2/|\mathbf{k}-\mathbf{K}|^2, \quad (31)$$

and

$$\rho_{\mathbf{k},\mathbf{k}'}^{nn'}(\mathbf{K})=\sum_{\mathbf{K}'}\chi_n^*(\mathbf{k},\mathbf{K}+\mathbf{K}')\chi_{n'}(\mathbf{k}',\mathbf{K}'). \quad (32)$$

If we expand $\epsilon$ in a manner analogous to (28), we may write (13) as

$$\sum_{\mathbf{K}'}\epsilon(\mathbf{k}-\mathbf{K}',\mathbf{K}-\mathbf{K}';\omega)\mathcal{K}'(\mathbf{k},\mathbf{K}';\omega)=\delta_{\mathbf{K},0}. \quad (33)$$

Comparison with (29) then shows

$$\epsilon(\mathbf{k},\mathbf{K};\omega)=\delta_{\mathbf{K},0}+\alpha(\mathbf{k},\mathbf{K};\omega). \quad (34)$$

From (5) and the definitions at the beginning of this section one may easily derive an equation for $\rho_{\mathbf{k},\mathbf{k}'}^{nn'}(\mathbf{K})$:

$$\{(\hbar^2/2m)[(\mathbf{k}'+\mathbf{K})^2-\mathbf{k}^2] -[E_{n'}(\mathbf{k}')-E_n(\mathbf{k})]\}\rho_{\mathbf{k},\mathbf{k}'}^{nn'}(\mathbf{K}) =i(\hbar^2/m)(\mathbf{k}-\mathbf{k}'-\mathbf{K})\cdot\sum_{\mathbf{K}'}\mathbf{K}'\chi_n^*(\mathbf{k},\mathbf{K}') \times\chi_{n'}(\mathbf{k}'+\mathbf{K},\mathbf{K}'). \quad (35)$$

Hence, for $\mathbf{k}-\mathbf{k}'-\mathbf{K}\to 0$ it is easily seen that

$$\rho_{\mathbf{k},\mathbf{k}'}^{nn'}(\mathbf{K})\to\delta_{n,n'}[1+(\mathbf{k}-\mathbf{k}'-\mathbf{K})\cdot f(\mathbf{k})]+(1-\delta_{n,n'}) \times\frac{(i\hbar^2/m)(\mathbf{k}-\mathbf{k}'-\mathbf{K})\cdot\sum_{\mathbf{K}'}\mathbf{K}'\chi_n^*(\mathbf{k},\mathbf{K}')\chi_{n'}(\mathbf{k},\mathbf{K}')}{E_n(\mathbf{k})-E_{n'}(\mathbf{k})}, \quad (36)$$

where $f(\mathbf{k})$ is a function of $\mathbf{k}$, the $\chi_n$'s and $E_n$'s. From (36), (32), (30), (27), and (24) it follows that for $\mathbf{k}\to\mathbf{K}$

$$\alpha(\mathbf{k}-\mathbf{K}',\mathbf{K}-\mathbf{K}';\omega) \to-\frac{(\mathbf{k}-\mathbf{K})}{|\mathbf{k}-\mathbf{K}|^2}\cdot\frac{16\pi e^2}{N}\sum_n\sum_{n'}\int_0^{\mathrm{P}}\frac{d\mathbf{k}'}{(2\pi)^3} \times(1/\omega^2)(i\hbar^2/m)\sum_{\mathbf{K}''}\mathbf{K}''\chi_{n'}^*(\mathbf{k}',\mathbf{K}'')\chi_n(\mathbf{k}',\mathbf{K}'') \times(1-\delta_{n,n'})\sum_{\mathbf{K}'''}\chi_{n'}^*(\mathbf{k}'-\mathbf{K}',\mathbf{K}''') \times\chi_n(\mathbf{k}'-\mathbf{K},\mathbf{K}''')+[\text{terms finite for } \mathbf{k}=\mathbf{K}]. \quad (37)$$

Since the summation over $\mathbf{K}'''$ in (37) yields $\delta_{n,n'}$ for $\mathbf{K}'=\mathbf{K}$, we see that $\alpha(\mathbf{k}-\mathbf{K}',\mathbf{K}-\mathbf{K}';\omega)$, and hence $\epsilon(\mathbf{k}-\mathbf{K}',\mathbf{K}-\mathbf{K}';\omega)$, has a simple pole for $\mathbf{k}=\mathbf{K}\neq\mathbf{K}'$. For $\mathbf{k}\to\mathbf{K}'$ everything is of the same form except for the factor of $|\mathbf{k}-\mathbf{K}|^2$ in the denominator arising from $v(\mathbf{k}-\mathbf{K})$. Hence we see that $\epsilon(\mathbf{k}-\mathbf{K}',\mathbf{K}-\mathbf{K}';\omega)$ has a simple zero for $\mathbf{k}=\mathbf{K}'\neq\mathbf{K}$.

To understand these poles and zeros let us consider an electromagnetic wave (e.g., an x-ray beam) in a vacuum impinging on the surface of a dielectric medium. The reflection coefficient, $R$, (the ratio of reflected to incident intensities) is given as[11]

$$R=[(\epsilon^{\frac{1}{2}}-1)/(\epsilon^{\frac{1}{2}}+1)]^2. \quad (38)$$

Thus, for $\epsilon=0$ and $\epsilon=\infty$ we have $R=1$, i.e., the reflected intensity equals the incident intensity; there is total reflection at the zeros and poles of $\epsilon$. Evidently we may understand these zeros and poles to be simply manifestations of Bragg's law.

Explicitly exhibiting the zeros and poles, we may write

$$\alpha(\mathbf{k}-\mathbf{K}',\mathbf{K}-\mathbf{K}';\omega) =\frac{|\mathbf{k}-\mathbf{K}'|}{|\mathbf{k}-\mathbf{K}|}\beta(\mathbf{k}-\mathbf{K}',\mathbf{K}-\mathbf{K}';\omega), \quad (39)$$

where $\beta(\mathbf{k}-\mathbf{K}',\mathbf{K}-\mathbf{K}';\omega)$ is finite and non zero for $\mathbf{k}=\mathbf{K}'$ and $\mathbf{k}=\mathbf{K}$. We may reasonably expect that these poles and zeros constitute the major effect of the lattice and that to a good approximation we may neglect the $\mathbf{K}'$ dependence of $\beta$ in (39). Then (29)

[11] E.g., J. A. Stratton, *Electromagnetic Theory* (McGraw-Hill Book Company, Inc., New York, 1941).

becomes

$$\mathcal{K}'(\mathbf{k},\mathbf{K};\omega)+\frac{\beta(\mathbf{k},\mathbf{K};\omega)}{|\mathbf{k}-\mathbf{K}|}\sum_{\mathbf{K}'}|\mathbf{k}-\mathbf{K}'|\mathcal{K}'(\mathbf{k},\mathbf{K}';\omega)=\delta_{\mathbf{K},0}, \quad (40)$$

which has the solution

$$\mathcal{K}'(\mathbf{k},\mathbf{K};\omega)=\delta_{\mathbf{K},0}\left[\frac{1+\sum_{\mathbf{K}'\neq 0}\beta(\mathbf{k},\mathbf{K}';\omega)}{1+\sum_{\mathbf{K}'}\beta(\mathbf{k},\mathbf{K}';\omega)}\right]-(1-\delta_{\mathbf{K},0})\frac{|\mathbf{k}|}{|\mathbf{k}-\mathbf{K}|}\frac{\beta(\mathbf{k},\mathbf{K};\omega)}{1+\sum_{\mathbf{K}'}\beta(\mathbf{k},\mathbf{K}';\omega)}, \quad (41)$$

as may be verified by direct substitution.

Let us discuss this result in the weak-binding limit. Here the electrons are almost a free electron gas and we may expect the contributions from $\mathbf{K}'\neq 0$ in the summations to be small (since for free electrons these contributions are zero, only the $\mathbf{K}=0$ term contributing). Then we may write

$$\mathcal{K}'(\mathbf{k},\mathbf{K};\omega)\approx\delta_{\mathbf{K},0}\frac{1}{1+\beta(\mathbf{k},0;\omega)}-(1-\delta_{\mathbf{K},0})\frac{|\mathbf{k}|}{|\mathbf{k}-\mathbf{K}|}\frac{\beta(\mathbf{k},\mathbf{K};\omega)}{1+\beta(\mathbf{k},0;\omega)}. \quad (42)$$

The first term (42) is just of the form of the free electron gas result[2] [note: $\beta(\mathbf{k},0;\omega)=\alpha(\mathbf{k},0;\omega)$], while the second term is small with respect to the first except at the Bragg reflection. For $|\mathbf{k}|\ll|\mathbf{K}|$ the second term is negligible, a result conjectured by Nozières and Pines.[7] Thus in the weak-binding approximation the form of $\mathcal{K}'$ is essentially that of the free electron gas result except at the Bragg reflection. In general, even away from Bragg reflections, the form of $\mathcal{K}'$ is modified somewhat by the lattice.

It should be noted that in obtaining (41) the only details of the form of $\epsilon$ that have been used are the nature and positions of the poles and zeros. Since we have seen these to be simply manifestations of the Bragg reflections, they must be a generally valid property of $\epsilon$, not at all restricted to the use of (16). Thus the result (41) should be valid no matter what approximation is taken for $\delta\bar{G}/\delta V'$ in (14).

## THE ENERGY

Hubbard[2] has related the ground-state energy of the system to $\mathcal{K}'$[12]:

$$E=\sum_{n<m}\int_0^{\mathrm{P}}\frac{d\mathbf{k}}{(2\pi)^3}E_n(\mathbf{k})-\tfrac{1}{2}N\int\frac{d\mathbf{k}}{(2\pi)^3}\frac{4\pi e^2}{\mathbf{k}^2}-\tfrac{1}{2}\int\rho(\mathbf{r})v(\mathbf{r}-\mathbf{r}')\rho(\mathbf{r}')d\mathbf{r}d\mathbf{r}'+\mathcal{E}, \quad (43)$$

where

$$\mathcal{E}=\frac{i\hbar}{2}\int_0^{e^2}\frac{de^2}{e^2}\int dx\delta(t)\lim_{x'\to x}[\mathcal{K}'(x,x')-\delta(x-x')]. \quad (44)$$

Using (28) we have

$$\mathcal{E}=\frac{i\hbar}{2}\Omega\int_0^{e^2}\frac{de^2}{e^2}\int\frac{d\mathbf{k}}{(2\pi)^3}\frac{d\omega}{2\pi}[\mathcal{K}'(\mathbf{k},0;\omega)-1], \quad (45)$$

which, by (41), becomes

$$\mathcal{E}=-\frac{i\hbar}{2}\Omega\int_0^{e^2}\frac{de^2}{e^2}\int\frac{d\mathbf{k}}{(2\pi)^3}\frac{d\omega}{2\pi}\frac{\beta(\mathbf{k},0;\omega)}{1+\sum_{\mathbf{K}}\beta(\mathbf{k},\mathbf{K};\omega)}. \quad (46)$$

Noting that $\beta\sim e^2$, we may perform the $e^2$ integration and obtain finally

$$\frac{\mathcal{E}}{\Omega}=-\frac{i\hbar}{2}\int\frac{d\mathbf{k}}{(2\pi)^3}\frac{d\omega}{2\pi}\frac{\beta(\mathbf{k},0;\omega)}{\sum_{\mathbf{K}}\beta(\mathbf{k},\mathbf{K};\omega)}\times\ln[1+\sum_{\mathbf{K}}\beta(\mathbf{k},\mathbf{K};\omega)], \quad (47)$$

a rather simple generalization of the free electron gas result.

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[12] The transition to Hubbard's notation is simply made noting:

$$F(x,x')=\mathcal{K}'(x,x')-\delta(x-x'),$$

$$\mathcal{U}(x,x')=\int\mathcal{K}'(x,x'')v(x''-x')dx''.$$