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Iterative procedure for calculating Green's functions for systems of finite extent

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We present a method for efficiently calculating the one-particle Green's function (OPGF) for the interaction of a particle with a static potential using an iterative procedure that avoids the necessity for inversion of large matrices. The OPGF for a hierarchy of successively larger systems converging to the full system under study are thereby also obtained. We demonstrate the usefulness of the method, applying it to determine the bound-state spectrum and density of states of one particle interacting with mesoscopic size and extended two-dimensional systems. Applications to a variety of physical systems are briefly discussed.

I. INTRODUCTION

The importance of the one-particle Green's function (OPGF) for potential scattering is well known. Its central role in condensed-matter physics has been emphasized in the book of Economu.[1] Interpretation of experimental spectra is in many cases intimately tied to the density of states $N(E)$ which can be directly computed from the Green's function.[1-3] Expressions for calculating absorption spectra,[3] Raman spectra,[4,5] and many other physical quantities can be directly written in terms of the OPGF. In fact, any physical quantity that can be expressed in terms of second-order perturbation theory can be written as a matrix element of the OPGF.[5]

In this paper we present an efficient algorithm for the calculation of OPGF of finite and quasiextended systems. As intermediate results we obtain the OPGF for a hierarchy of successively larger systems converging to the full system under study. We apply our method to study the bound-state spectrum and the density of states of a two-dimensional disk and briefly discuss its application to other physical systems of interest. We also suggest how to use this algorithm for the evaluation of the Green's function of a many-particle system.

The precise form of the OPGF depends crucially on the boundary condition of the problem under study. The choice of boundary condition is dictated by the physical quantity to be studied. To illustrate this let us first consider a one-particle system in a one-dimensional potential $V(x)$ (energy E, mass m, and wave number $k=\sqrt{2mE}/\hbar$), and suppose that we want to evaluate the density of states. The density of states of a one-dimensional system governed by the Hamiltonian $H=H_0+V(x)$ can be evaluated in terms of the OPGF $G(x,x';E)$ with outgoing wave boundary conditions as $|x|\to\infty$. The well-known expression for $N(E)$ in terms of $G(E)$ is given by $N(E)=(2\pi)^{-1}\mathrm{Im}\,\mathrm{Tr}G(E)$.[1,2] The physical interpretation behind the requirement of outgoing wave boundary conditions is that the outgoing waves carry information regarding the spectrum of the system. This is connected to the intimate connection between the S matrix and the density of states, as expressed by Levinson's theorem,[6] and by the Dashen, Ma, and Bernstein relationship[7] between the trace of the Green's function of a system and its S matrix.

We therefore consider the Green's function $G(x,x';E)$ with outgoing wave boundary conditions. As is well known, the free OPGF $G_0(x,x';E)$ with outgoing wave conditions has the configuration-space representation $G_0(x,x';E)=e^{ik|x-x'|}/2ik$, and the full Green's function $G(x,x';E)$ can be obtained in terms of $G_0(x,x';E)$ by a solution of the Lipmann-Schwinger equation. Clearly, numerical solution of this equation, when $G(x,x';E)$ is needed for long systems (e.g., a disordered metallic wire), requires inversion of large matrices. The iterative procedure suggested below is meant to avoid this problem.

If only the density of states is needed, the Dashen-Ma-Bernstein method for calculating density of states is more efficient than the Green's-function approach since it only involves knowledge of the wave functions in the asymptotic region of coordinate space. In fact, we have shown that, for one-dimensional systems, all one needs in order to calculate the density of states is the phase of the transmission amplitude.[8] However, evaluating the S matrix is often not much simpler than the evaluation of the full Green's function, while the Green's function contains much more information about the system.

In Sec. II we explain our method as applied to the Green's function with outgoing boundary conditions in two dimensions. Starting from the coupled system of Lipmann-Schwinger integral equations for the Green's function partial-wave components, we then introduce an iterative method which avoids the necessity of inversion of very large matrices. Numerical results for the bound-state spectrum and density of states of a two-dimensional extended system with periodic potential are presented and discussed in Sec. III. Finally, in Sec. IV we briefly discuss potential applications to various one-particle systems as well as an extension to the N-particle system.

II. GREEN'S FUNCTION FOR ONE-PARTICLE POTENTIAL SCATTERING IN TWO DIMENSIONS

We begin by considering the quantum mechanics of one particle in a two-dimensional system which, for convenience, has geometrical symmetry. For definiteness, consider a circular or rectangular sample having the potential $V(x,y)$ which is different from zero within a domain D. We neglect electron-electron interactions and assume zero temperature so that electron-phonon interactions are also absent. Thus, we consider a single-particle scattering problem in two dimensions where the scattering potential (which may have been obtained from an energy-dependent optical potential[9]) can be extended over many atomic units.

The boundary conditions to be imposed on the wave function are of crucial importance. We formulate the analog of the outgoing wave boundary conditions discussed in connection with the one-dimensional problem for the two-dimensional case. Here the requirement of outgoing circular waves is adopted. The use of polar coordinates is superior to that of Cartesian coordinates for treating outgoing circular wave boundary conditions, even if $V(x,y)$ has Cartesian symmetry. Thus, if m is the effective mass of the particle and E is its energy, we define $k=\sqrt{2mE}/\hbar$, $v(r,\theta)=(2m/\hbar^2)V(r\cos\theta,r\sin\theta)$ and denote by $\mathbf{k}$ the wave vector corresponding to the initial direction (which we take as the positive x direction) and $\mathbf{r}=(r,\theta)$. The free Green's function

$$G_0(\mathbf{r},\mathbf{r}';k)=\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{2\pi\sqrt{k|\mathbf{r}-\mathbf{r}'|}} \tag{2.1}$$

satisfies the equation

$$(\Delta+k^2)G_0(\mathbf{r},\mathbf{r}';k)=\delta^2(\mathbf{r}-\mathbf{r}') . \tag{2.2}$$

The full Green's function can be defined in terms of the Lipmann-Schwinger integral equation

$$G(\mathbf{r},\mathbf{r}';k)=G_0(\mathbf{r},\mathbf{r}';k) + \int_D G_0(\mathbf{r},\mathbf{r}'';k)v(\mathbf{r}'')G(\mathbf{r}'',\mathbf{r}';k)d\mathbf{r}'' . \tag{2.3}$$

In order to solve Eq. (2.3), we perform the angular momentum expansion of the free and full one-particle Green's functions in terms of the angular functions $e^{in\theta}$ $(n=0,\pm1,\pm2,\ldots,)$

$$G_0(\mathbf{r},\mathbf{r}';k)=\sum_n J_n(kr_<)H_n^{(1)}(kr_>)e^{in(\theta-\theta')} , \tag{2.4}$$

$$G(\mathbf{r},\mathbf{r}';k)=\frac{1}{\sqrt{rr'}}\sum_{m,n} G_{mn}(r,r';k)e^{i(m\theta-n\theta')} . \tag{2.5}$$

Here $J_n(kr)$ and $H_n^{(1)}(kr)$ are the regular Bessel function and the Hankel function of the first kind, respectively, and $r_<=\min(r,r')$, $r_>=\max(r,r')$. It is convenient to define the radial coefficient in the expansion of the free one-particle Green's function as

$$g_n(r,r';k)=\sqrt{rr'}J_n(kr_<)H_n^{(1)}(kr_>) , \tag{2.6}$$

which satisfies the differential equation

$$\left[\frac{\partial^2}{\partial r^2}-\frac{n^2-1/4}{r^2}+k^2\right]g_n(r,r';k)=\delta(r-r') . \tag{2.7}$$

The radial coefficients $G_{mn}(r,r';k)$ in the expansion (2.5) are the solutions of the coupled set of integral equations

$$G_{mn}(r,r';k)=\delta_{mn}g_n(r,r';k) + \sum_p \int_D g_m(r,r'';k)v_{mp}(r'') \times G_{pn}(r'',r';k)dr'' \tag{2.8}$$

where

$$v_{mp}(r)=\int_0^{2\pi} e^{i(m-p)\theta}v(r\cos\theta,r\sin\theta)d\theta . \tag{2.9}$$

In terms of the radial coefficients $G_{mn}(r,r';k)$ the density of states now reads as

$$N(k)=-\frac{1}{\pi D}\mathrm{Im}\sum_n\left[\int_D G_{nn}(r,r;k)dr\right] . \tag{2.10}$$

Equation (2.8) includes an infinite number of coupled equations. However, from classical considerations, angular momentum is related to the product kb where b is the impact parameter. We therefore expect that the actual number of partial waves that must be retained in numerical calculations can be limited to a cutoff number, $L=kR$, R being somewhat larger than the radius of the system. This is born out in our numerical example discussed in Sec. III.

We now show how equations such as Eq. (2.8) can be treated numerically even when the domain of integration in coordinate space is very large. If the integral in Eq. (2.8) is replaced by a sum over M mesh points, the matrix that must be inverted is of dimension $MN\times MN$ where N is the number of partial waves in the sum over P. We expect both N and M to be at least a few tens. Therefore, determination of G from Eq. (2.8) requires the inversion of the complex matrix $1-\mathbf{gV}$ of large dimension. Due to the special (Lipmann-Schwinger) structure of the integral equation for the Green's function, Eq. (2.8) can be solved iteratively in, say, K iterations where in each iteration one inverts a matrix whose dimension is MN/K. Let us write Eq. (2.8) as an operator equation in matrix form (dropping for the moment the k dependence),

$$\mathbf{G}=\mathbf{g}+\mathbf{gvG} . \tag{2.11}$$

We divide the range of integration $[0,R]$ into K segments at points $0=r_0<r_1<r_2\cdots<r_{K-1}<r_K=R$ and write the interaction matrix $\mathbf{v}$ as the sum,

$$\mathbf{v}=\sum_{k=1}^{K}\mathbf{v}_k;\quad \mathbf{v}_k=\begin{cases}\mathbf{v} \text{ if } r_{k-1}<r<r_k\\ 0 \text{ otherwise} .\end{cases} \tag{2.12}$$

With the notation $\mathbf{G}_0=\mathbf{g}$ let us inspect the following iterative scheme:

$$\mathbf{G}_k=\mathbf{G}_{k-1}+\mathbf{G}_{k-1}\mathbf{v}_k\mathbf{G}_k \quad (k=1,2,\ldots,K) . \tag{2.13}$$

Since Eq. (2.11) is a resolvent equation, it is evident from Eq. (2.3) that $\mathbf{G}_\mathbf{k}$ is the Green's function corresponding to the interaction truncated at $r=r_k$, and hence $\mathbf{G}_K=\mathbf{G}$. Our method is an *Aufbau* method wherein *the Green's functions for all size samples up to the full system size are obtained simultaneously.* To see how the iterative scheme (2.13) avoids inversion of large matrices, we rewrite it as an integral equation recalling that the integration domain is limited to $r\in[r_{k-1},r_k]$ in which $\mathbf{v}_k(r)$ does not vanish. Taking $\mathbf{r}'$ as a parameter, we first consider $\mathbf{G}_k(r,r')$ only for $r_{k-1}<r<r_k$,

$$\mathbf{G}_k(r,r')=\mathbf{G}_{k-1}(r,r')+\int_{r_{k-1}}^{r_k}\mathbf{G}_{k-1}(r,r'')v_k(r'')\mathbf{G}_k(r'',r')dr'' ,\quad r_{k-1}<r<r_k . \tag{2.14}$$

Since the domain of integration is K times smaller than the original domain $[0,R]$ for which M mesh points are necessary, the integral in Eq. (2.14) can be replaced by a sum over M/K mesh points, and hence, the dimension of the matrix that must be inverted is NM/K. Once Eq. (2.14) is solved, its solution can be substituted back into the same equation in order to evaluate $\mathbf{G}_k(r,r')$ this time for all $r\in[0,R]$. This second step does not require matrix inversion, but only quadrature integration. Thus, we circumvent the problem of large matrix inversion (although we are unable to avoid the storage problem since $\mathbf{G}_k$ for all $r,r'\in[0,R]$ is needed). Most of the computer time is consumed in the quadrature integration, not matrix inversion. In any case, this somewhat elementary procedure tremendously expedites computation of the Green's function. We now consider a specific example.

III. DENSITY OF STATES OF A TWO-DIMENSIONAL SYSTEM

As an illustrative example for the above algorithm we calculate the OPGF and evaluate the density of states of a particle in a two-dimensional extended system. Physically we may think of conduction electrons in a metal (at zero temperature) interacting with the frozen atoms with electron-electron interaction neglected. Consider a two-dimensional system of large but finite extent characterized by potential $V(x,y)$ which is periodic in Cartesian coordinates x,y within the sample domain, $0<r<R_0$. Outside the sample boundaries, $V(x,y)=V_1$, where V_1 is the potential barrier of height equal to the Fermi energy plus work function. The work function potential barrier is taken to be V_1 within domain $R_0<r<R$ and is cutoff at radius R, where the cutoff radius R is chosen to simulate the experimental resolution of the measurements of the bound-state energy. Cutoff of the barrier allows application of scattering methods to determine bound-state properties. Thus, the conduction electrons move in the potential

$$V(x,y)=V(r,\theta)=\begin{cases}V_0[\cos(k_xx)\cos(k_yy)+1]=V_0[\cos(k_xr\cos\theta)\cos(k_yr\sin\theta)+1], & R<R_0\\ V_1, & R_0<r<R\\ 0, & r>R.\end{cases} \tag{3.1}$$

We take $V_1>V_0$, and both V_0 and V_1 positive. There are no stable bound states for this potential, however, in complete analogy with the double barrier potential in one dimension (see the discussion in the Introduction) we expect peaks in the density of states of the potential (3.1) to approximate the true bound states of the potential

$$V(x,y)=V(r,\theta)=\begin{cases}V_0[\cos(k_xx)\cos(k_yy)+1]=V_0[\cos(k_xr\cos\theta)\cos(k_yr\sin\theta)+1], & r<R_0\\ V_1, & r>R_0.\end{cases} \tag{3.2}$$

Our aim is, therefore, to evaluate the OPGF related to the potential of Eq. (3.1) using the algorithm developed in Sec. II.

The approximate number of coupled equations (2.8) can now be estimated using the classical relation between momentum k, impact parameter b, and angular momentum L, $kb=L$. Since we study the dependence of the Green's function on energy, the value of k is in the range of typical values of k_F in metals, i.e., a several Å^{-1}. The maximum value of the impact parameter is the radius R of the system. Thus, the number of coupled integral equations N is given approximately by the relation $N=2kR+1$. In the special case of potential Eq. (3.1), we reduce the number of equations by assuming $k_x=k_y$ so that the x and y directions are identical and the system has a 90° rotational symmetry. In this case the matrix elements v_{mp} [Eq. (2.9)], vanish unless $|mp|=4$, so that the number of equations is reduced by a factor of 4.

In order to test our program we evaluated the density of states for a circular disk with $V_0=0$ and with a very high circular barrier V_1. The resonance energies for $V_1=\infty$ are the zeros of the Bessel functions $J_n(kR_0)$, and the calculated density of states with $V_1=8$ eV, $R_0=23$ Å, and $R=25$ Å, has peaks at these energies. In Fig. 1, the energy range contains no resonances.

We now consider a circular disk of radius $R=25$ Å, $V_0=3$ eV, $V_1=8$ eV, $R_0=23$ Å, $k_x=k_y=1.25$ Å^{-1} and we calculate the density of states as a function of energy E in the range $2.4<E<V_0$ (below $E=2.4$ eV there is a monotonic rise of the density of states without any notable structure). We find that the cutoff angular momentum L can be fixed at 24, and

$$-\mathrm{Im}\int_D G_{nn}(r,r;k)dr \ll -\mathrm{Im}\int_D G_{00}(r,r;k)dr \quad (\text{for } n\geq 24) . \tag{3.3}$$

In Table I we give the values of the two expressions $-\text{Im}[\int_D G_{nn}(r,r;k)dr]$ and $-\text{Im}[\int_D g_n(r,rk)dr]$ for $n=0$, 4, 8, 12, 16, 20, 24, and 24, for $E=2.412$ eV. From the table we conclude that fixing L at 24 leads to an error of a few percent. We also found that the contribution of two sets of channels with no coupling between them (e.g., the set of channels -24, -20, -16, -12, -8,. . . and the set of channels -23, -19, -15, -11, -7,. . .) is almost identical if L is large enough. Hence we evaluate the contribution of a single set and multiply it by 4, which leads to a substantial savings in computer time.

The spectrum of the one particle in the above potential is shown in Fig. 1. The sharp peaks correspond to stable bound states, and their finite width is a consequence of the finiteness of the circular barrier, which allows tunneling outside the potential range. The broader peaks correspond to resonances. It is important to point out here that we have in fact calculated the OPGF in all configuration space and, therefore, it can be used for the calculation of other observables in addition to the density of states. Ideally, we would like to study much larger systems, since electrons within a disc of radius 25 Å cannot be considered as Bloch electrons. Only in the limit of very large radius we may expect the Bloch momentum to have its physical significance and argue that the precise form of the boundaries is not important. Unfortunately, with our present computing facilities we cannot reach this limit. In order to test the effect of the system size we consider a circular system of radius $R=50$ Å, with all other parameters (except, of course, the number of partial waves) as before. The density of states of this larger system is plotted as function of energy in Fig. 2. The one-particle spectrum of the larger system is richer and contains both narrow and broad resonances. In both cases the bound states do not lie at the bottom of the potential well but appear at higher energies. A study of much larger systems would require use of supercomputers.

TABLE I. Imaginary part of race of partial-wave n (first column) Green's functions for the system with interaction (second column) and the free one (third column). The system consists of a single particle moving in the potential field given in Eq. (4.1) with the parameters $v_0=3.0$ eV, $v_1=8.0$ eV, $k_x=k_y=1.250$ Å^{-1}, $R=25.0$ Å, and $R_0=23.0$ Å. The effective mass of the particle is taken as that of a free electron.

	$-\text{Im}\left[\int_D G_{nn}(r,r;k)dr\right]$	$-\text{Im}\left[\int_D g_n(r,r;k)dr\right]$
$n=0$	$0.7617E+00$	$0.2526E+01$
$n=4$	$0.6286E+00$	$0.2506E+01$
$n=8$	$0.4524E+00$	$0.2239E+01$
$n=12$	$0.2999E+00$	$0.2088E+01$
$n=16$	$0.1630E+00$	$0.1660E+01$
$n=20$	$0.4231E-01$	$0.2184E+00$
$n=24$	$0.2349E-02$	$0.1786E-02$

It is useful to point out here that the choice of a circular shape is a matter of convenience. If the shape of the system is more complex, the symmetry disappears and the integration in Eq. (2.9) becomes more difficult to carry out, but after the partial-wave matrix elements of the interaction are computed at all relevant radii, the iterative procedure is unchanged.

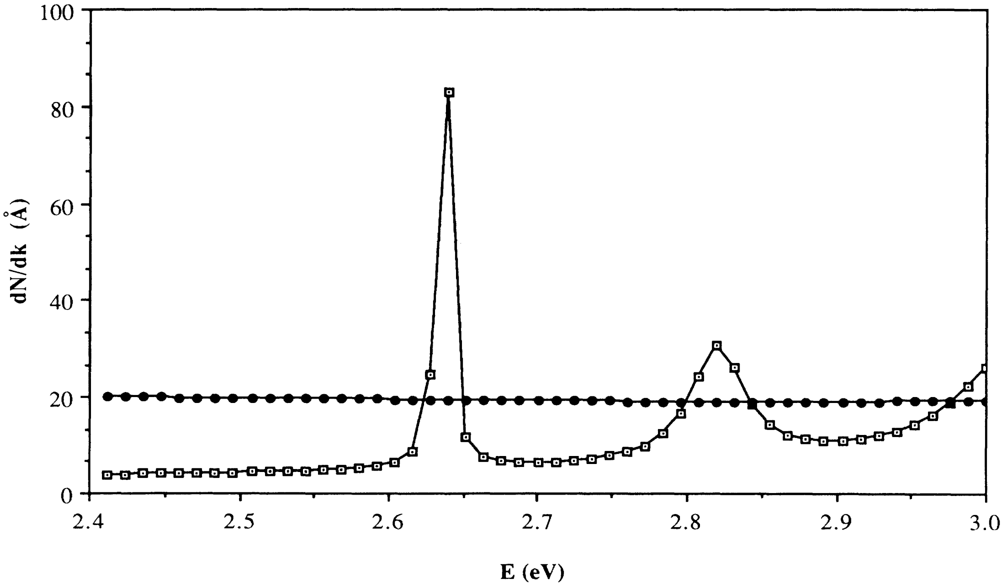

FIG. 1. Density of states per unit wave number of the system with full interaction (squares) and with the corregated part of the potential (circles). The system consists of a single particle moving in the potential field given in Eq. (4.1) with parameters $V_0=3$ eV, $V_1=8$ eV, $k_x=k_y=1.250$ Å^{-1}, $R=25$ Å, and $R_0=23$ Å. The effective mass of the particle is taken as that of a free electron.

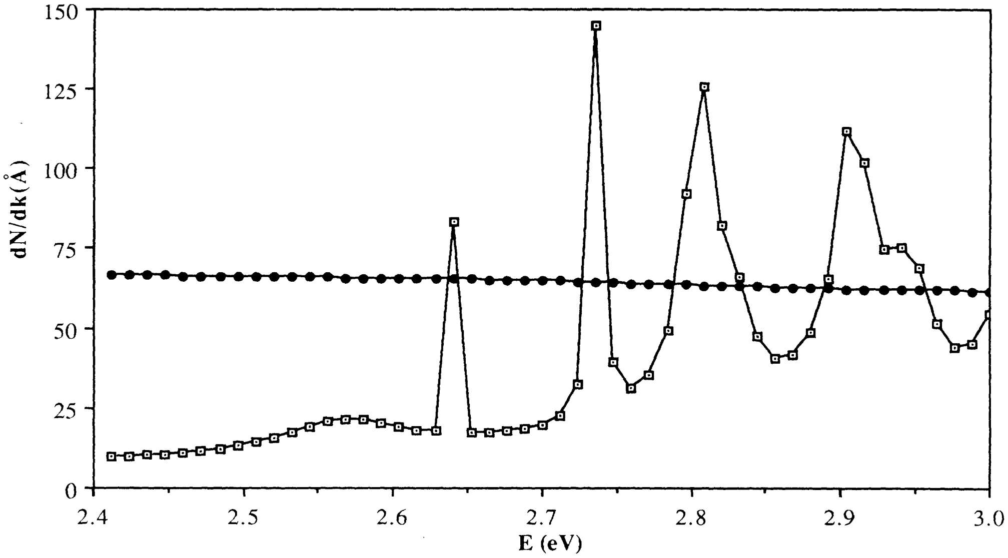

FIG. 2. Same as Fig. 1 but with $R = 50$ Å and $R_0 = 48$ Å.

IV. APPLICATION TO SEVERAL PHYSICAL SYSTEMS OF INTEREST

In this section we briefly point out a few other directions in which the ideas presented above can be used to evaluate Green's functions of interest in condensed matter physics. The list below is by no means complete.

A. Green's function of a three-dimensional system

In complete analogy with the one- and two-dimensional systems we may think of a three-dimensional system characterized by a potential $V(x,y,z)$ which is periodic in Cartesian coordinates up to a certain distance from the surface boundaries.

The angular momentum quantum numbers are the orbital angular momentum l and its projection m on some fixed axis. The radial matrix elements of the potential $V(x,y,z)=V(r,\theta,\phi)=V(r,\Omega)$ [analog of Eq. (2.9)] are then

$$V_{l'm',lm}(r)=\int Y^*_{lm}(\Omega)V(r,\Omega)Y_{lm}(\Omega)d\Omega \ . \tag{4.1}$$

The number of coupled equations are, approximately,

$$N=\sum_{l=0}^{L}(2l+1)=\frac{L^2+3L}{2} \ . \tag{4.2}$$

The value of the cutoff angular momentum L is approximately kR where R is the radius of the system. It is evident that if we want R to be a few tens of angstroms and k a few inverse angstroms, we will have to use supercomputers to solve Eq. (2.14). Nevertheless, the algorithm sketched above should be most efficient in evaluation of Green's function for one particle in an extended three-dimensional system.

B. Green's function for quasi-one-dimensional systems

Systems in which particles propagate freely only in one direction (say along the x axis) while in the other directions the wave function has standing wave boundary conditions, are termed quasi-one-dimensional systems. Such systems play a central role in the study of electrical conductance. To calculate the dc conductance, it is sufficient to know the transmission and reflection matrix amplitudes and then use the well-known relations between conductance and transmission and reflection.[10] However, when the ac conductance is required, we need the full Green's function to evaluate it using the Kubo formula.[1]

To this end we construct the free Green's function which vanishes on the boundaries of the system and has outgoing wave boundary conditions when $|x|$ is outside the interaction region. Let $\mathbf{y}$ denote the transverse coordinates in which the motion is bounded to a finite region. The standing-wave wave function $\phi_m(\mathbf{y})$ belongs to the energy eigenvalue ε_m and the wave number k_m of the propagating wave in the x direction is given by

$$k_m^2=k^2-\varepsilon_m \ , \tag{4.3}$$

where k^2 is the total energy. The free Green's function is then given by

$$G_0(x\mathbf{y},x'\mathbf{y}')=\sum_m \frac{\exp(ik_m|x-x'|)}{2ik_m}\phi_m(\mathbf{y})[\phi_m(\mathbf{y}')]^* \ . \tag{4.4}$$

The full Green's function $G(x\mathbf{y},x'\mathbf{y}')$ which takes into account the interaction $v(x,\mathbf{y})$ of the electron with the sample is given by the standard Lipmann-Schwinger equation. Using the orthogonality of the standing-wave wave functions we turn the Lipmann-Schwinger equation into a set of coupled equations for the coefficients $G_{mn}(x,x')$ in the expansion

$$G(x\mathbf{y},x'\mathbf{y}')=\sum_{mn}G_{mn}(x,x')\phi_m(\mathbf{y})[\phi_m(\mathbf{y}')]^* \ , \qquad (4.5)$$

in terms of the matrix elements of the potential

$$v_{mp}(x)=\int d\mathbf{y}\phi_m(\mathbf{y})v(x,\mathbf{y})[\phi_p(\mathbf{y})]^* \qquad (4.6)$$

which reads as

$$G_{mn}(x,x')=\frac{\exp(ik_m|x-x'|)}{2ik_m}\delta_{mn} + \int dx''\frac{\exp(ik_m|x-x''|)}{2ik_m} \times\sum_p v_{mp}(x'')G_{pn}(x'',x') \ . \qquad (4.7)$$

The sum over the discrete indices should run to infinity. However, a cutoff at some value N large enough to include all the physical channels for which k_m^2 is positive, in addition to a few evanescent channels should be sufficient. The dimension of G in Eq. (4.7) will then be $NM\times NM$ where M is the number of integration points. The recommended technique here is therefore to divide the domain of x over which the interaction $v(x,\mathbf{y})$ is nonzero into small intervals and to use the iteration technique developed in Sec. II. Evaluation of Im(TrG) gives the density of states having these boundary conditions. This density of states is sensitive to the number of physical channels for which k_m^2 is positive. Each time the energy passes through a zero of k_m^2 a new channel opens and the density of states is discontinuous at such points. A trivial example is the density of states for free motion, which is proportional to the sum $\sum_{n=1}^{N_{\text{phys}}}1/k_n$ where N_{phys} is the number of physical channels.

C. The quantum Hall effect

One of the central quantities related to the integral quantum Hall effect is the density of states of an electron in a two-dimensional disordered sample in the presence of a strong perpendicular magnetic field. In the absence of the disorder potential, the density of states is simply given by the sum $N(E)=\sum_n\delta(E-E_n)$, where the sum rums over the Landau energies $E_n=(n+\frac{1}{2})\hbar\omega$, $n=0,1,\ldots$, and ω is the cyclotron frequency. The disordered (impurity) potential is often taken as an infinite sum of localized potentials

$$v(x,y)=\sum_{m=1}^{\infty}v_m(x,y) \ , \qquad (4.8)$$

where each function v_m is localized around the point (x_m,y_m), the position of impurity number m. The modifications of the density of states upon introducing the interaction (4.8) are not yet fully understood.

Studies of the quantum Hall effect (including the density of states) have been limited to a single Landau level, but there is a growing belief that despite the substantial energy separation between adjacent Landau levels, the coupling between Landau levels is important. Some attempts to include a finite number of Landau levels in the calculations of the density of states has been reported but to our knowledge, no attempt has been made to include all the Landau levels at the onset.

Since the sum of localized interactions in Eq. (4.8) is infinite, an exact solution is, of course, out of the question. Instead, an iterative procedure which takes into account successively more terms with an attempt to identify the limit of an infinite number of terms is suggested below. We introduce the magnetic field B through the magnetic length $L=\sqrt{\hbar c/eB}$ and consider the Hamiltonian H_0 of an electron in a two-dimensional plane with a perpendicular magnetic field in the Landau gauge $A_x=By$. As shown by Comtet,[11] the Green's function $G_0=(k^2-H_0)^{-1}$ can be evaluated analytically in configuration space. Therefore we can consider the following iterative procedure, $G_{m+1}=G_m+G_m v_{m+1}G_{m+1}$ for $m=0,1,2,\ldots$, and use the fact that each impurity potential is localized at the point (x_m,y_m) and employ the technique developed in Sec. II to evaluate $g_{m+1}(xy,x'y';k^2)$ at any x' and y' but for x and y only in the vicinity of (x_{m+1},y_{m+1}). This procedure obviates the necessity for inversion of large matrices and at the same time provides a natural iteration scheme since each Green's function G_m is the exact Green's function for the case in which there are only m terms in the expression for the disordered potential (4.8).

D. Green's function of an N-particle system

Finally, we suggest how the method developed here can be employed to evaluate Green's functions of N-particle systems. We base our suggestion on the hyperspherical expansion approach to the many-body problem, which has been used intensively in atomic and nuclear physics. The Laplacian operator is written in terms of one radial coordinate ρ (the hyper-radius) and a grand angular momentum operator $L^2(\Omega)$ where Ω is a set of $3N-1$ angles which, together with the hyper-radius, are sufficient for a complete kinematical specification of the N-particle system.[12,13] The angular eigenfunctions $Y_{[L]}(\Omega)$ of $L^2(\Omega)$ (the hyperspherical harmonics) are known, and hence, the partial-wave components $V_{[L][L']}(\rho)$ of the total interaction $V(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)=V(\rho,\Omega)$ can be computed. The interaction $V(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)$ may include three- and many-body interactions in addition to the sum over two-body interactions. The procedure is completely analogous to the one explained in Sec. IV A for the case of one particle in a three-dimensional extended system.

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