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On the escape of a particle from a potential well

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Abstract. An expression is obtained for the time-dependent wavefunction of a spinless non-relativistic particle escaping from a spherically symmetrical potential well having an outer barrier through which the particle can penetrate. The initial state of the particle, at time $t=0$, is taken to be a normalised wavepacket, located in the well, but otherwise arbitrary. The time-dependent Schrödinger equation of the system is solved by means of a Laplace transform, and the form of the wavefunction at a distance from the well is used to determine the conditions under which the process would appear to a suitable particle detector as an emission with one or more exponential decay rates.

1. Introduction

The quantum-mechanical problem of the escape of a spinless non-relativistic particle from a potential well having an outer barrier through which the particle can penetrate is of continuing interest, both for its own sake and in the general context of the theoretical treatment of 'metastable' states and associated phenomena, such as alpha-emission, auto-ionisation, scattering resonances, and certain solid-state processes. For recent contributions in this field from various points of view, and references to earlier work, see e.g. Schulman *et al* (1978), Sharma and Ogunsulire (1978) and Drukarev *et al* (1979).

To understand this continuing interest, it should be remembered that the treatment of the problem originally given in connection with the theory of alpha-emission (Gamow 1928, Gamow and Critchfield 1949) requires the use of so-called 'quasi-stationary' states. These are solutions of the time-dependent Schrödinger equation of the system, $H\psi = i\hbar\partial\psi/\partial t$, say, which have the same form as stationary states, i.e. $\psi(\boldsymbol{r}, t) = \phi_E(\boldsymbol{r}) \exp(-iEt/\hbar)$, with $H\phi_E = E\phi_E$, but which, unlike stationary states, satisfy the boundary condition of representing purely outgoing waves at infinity.

It was shown that one or more discrete solutions of this type exist if the outer barrier is high enough, and that in such solutions E necessarily has a negative imaginary part. Because of this $|\psi|^2$ at any point decreases exponentially with time, thus compensating for the net outflow of particles at infinity. The probability flux vector also decreases exponentially with time, and, by a suitable choice of potential well and barrier, the essential features of alpha-emission could be accounted for (Gamow and Critchfield 1949).

However, this treatment is open to objection in two ways.

(1) The momentum of the particle at a distance from the well also has a negative imaginary part, as a result of which the amplitude of the wavefunction at any time t

increases exponentially without limit with increasing distance from the well. Hence there is no time, $t = 0$ say, at which the particle can be said to be definitely in the well; on the contrary, it is at all times most likely to be at infinity.

(2) In general, the use in quantum mechanics of wavefunctions satisfying boundary conditions which are such that operators representing dynamical variables, e.g. energy, have complex eigenvalues and so are not Hermitian leads to serious logical and mathematical inconsistencies, in spite of attempts by a number of authors to justify their use. For a detailed discussion of this and allied topics the reader is referred to Sharma and Ogunsulire (1978).

Recent attempts to treat the problem in a way which avoids these objections are of two kinds.

(a) Schulman *et al* (1978), and other authors referred to therein, consider first the so-called 'finite-volume' problem, in which the potential consists of two wells, A and B say, separated by a barrier. If penetration through the barrier is neglected, the stationary states of the system below the barrier consist of the bound states of the particle in well A, and those of the particle in well B. Transitions from a state in which the particle is in well A, say, to states in which it is in well B can occur by barrier penetration. The limiting case in which the outer boundary of well B is removed to infinity should then provide a solution of the present problem. However, the treatment used by these authors leads to certain as yet unresolved difficulties, for details of which the reader is referred to the paper by Schulman *et al* (1978).

(b) Since the system is not in a stationary state, Drukarev *et al* (1979) do not look for a solution in the form of a modified or perturbed stationary state. Instead they solve the time-dependent Schrödinger equation of the system with an initial wavefunction, at time $t = 0$, of the form of a normalised wavepacket, located in the well, but otherwise arbitrary. It is a property of the equation that the solution is then normalised at all times. They express the solution as an expansion in terms of the usual continuum of positive energy eigenstates of the system, as used, for example, in the treatment of elastic scattering. Finally, they obtain an expression for the overlap integral of the wavefunction of the particle at time $t > 0$ with the wavefunction at time $t = 0$. The square modulus of this quantity gives the probability that the particle would be found at time t to be still in its initial state in the well. They show that this probability decreases almost entirely exponentially, with one or more decay constants, depending on the potential.

Although the work of these authors is not open to the objections discussed above, it does not constitute a complete treatment of the problem, since they do not consider explicitly what would be observed by a suitable particle detector placed at a distance from the well, nor is this obvious from their form of solution.

It is the purpose of the calculation given in § 2 *et seq* of the present paper to remedy this omission. Starting from the same premises, i.e. taking the initial state of the system at time $t = 0$ to be a normalised wavepacket located in the well but otherwise arbitrary, the time-dependent Schrödinger equation of the system is solved for $t > 0$ by means of a Laplace transform with respect to t. The resulting solution is in a convenient form for the present purpose, since it leads (§ 3) to simple expressions for the component parts of the wavefunction at a distance from the well. The results are summarised and discussed in § 4.

It will be assumed that the potential $V(r)$ (see figure 1) is real, spherically symmetrical and finite everywhere, that $V(r) \to 0$ faster than r^{-1} as $r \to \infty$, and that the particle is in an s-state. It is shown in § 5 how to generalise the results to potentials

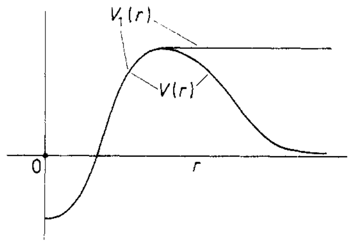

Figure 1. The potential $V(r)$, consisting of a potential well with an outer barrier, and the comparison potential $V_1(r)$, which is the same as $V(r)$ from $r=0$ to the top of the barrier, and from there on remains constant.

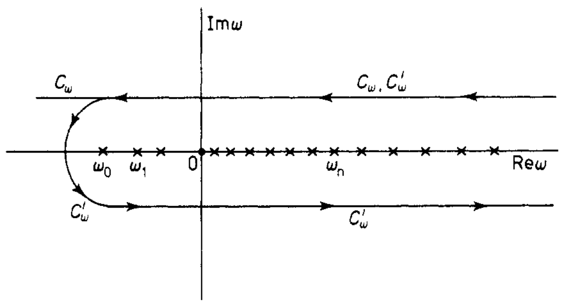

Figure 2. The energy eigenvalues ω_n of the system for finite R, given by the poles in the complex ω-plane of the function $\Phi(r, \omega)$ defined by equation (2.6). The contours C_ω and C'_ω are those used in the evaluation of the integral (2.4) for the wavefunction of the particle.

having a 'Coulomb tail', i.e. such that $V(r) \sim Cr^{-1}$ as $r \to \infty$, and to higher states of orbital angular momentum of the particle.

2. The solution of the Schrödinger time-dependent equation of the system

If we write the time-dependent wavefunction of the particle in an s-state as $\Psi(\boldsymbol{r}, t) = r^{-1}\psi(r, t)$, then Ψ satisfies the Schrödinger time-dependent equation of the system, and hence, using units in which $\hbar = 2m = 1$, ψ satisfies the 'radial' equation:

$$H_r\psi \equiv -\partial^2\psi/\partial r^2 + V(r)\psi = \mathrm{i}\partial\psi/\partial t. \tag{2.1}$$

We shall solve this equation with the boundary conditions $\psi = 0$ at $r = 0$ and at $r = R$. Here $R \gg r_0$, where $r_0 \sim$ the radius of the well; later we let $R \to \infty$. For the initial value of ψ at $t = 0$ we write $\psi(r, 0) = \psi_0(r)$. For $\Psi(\boldsymbol{r}, t)$ to represent a single particle, we require it to be normalised to unity at all times $t \geqslant 0$, and this will be so provided that, at time $t = 0$,

$$\int |\Psi(\boldsymbol{r}, 0)|^2 \,\mathrm{d}\boldsymbol{r} = 4\pi \int_0^{r_0} |\psi_0(r)|^2 \,\mathrm{d}r = 1 \tag{2.2}$$

in which the first integral is in principle over all space, and the initial wavepacket represented by $\psi_0(r)$ is assumed to have negligibly small amplitude for $r > r_0$.

We now use a Laplace transform with respect to t, slightly modified for later convenience. Thus, if one defines

$$\Phi(r, \omega) = -\mathrm{i} \int_0^\infty \psi(r, t) \exp(\mathrm{i}\omega t) \,\mathrm{d}t, \qquad \mathrm{Im}\,\omega > 0 \tag{2.3}$$

then

$$\psi(r, t) = (2\pi\mathrm{i})^{-1} \int_{C_\omega} \Phi(r, \omega) \exp(-\mathrm{i}\omega t) \,\mathrm{d}\omega, \qquad t > 0 \tag{2.4}$$

where the contour C_ω is as shown in figure 2.

By multiplying each term of equation (2.1) by $\exp(\mathrm{i}\omega t)$ and integrating with respect to t from 0 to ∞, we obtain, for $\operatorname{Im}\omega > 0$,

$$\mathrm{d}^2\Phi(r, \omega)/\mathrm{d}r^2 + [\omega - V(r)]\Phi(r, \omega) = \psi_0(r). \tag{2.5}$$

It can be verified by direct substitution that the expression

$$\Phi(r, \omega) = W(\omega)^{-1}\left(\chi(r, \omega)\int_0^r \phi(r', \omega)\psi_0(r')\,\mathrm{d}r' + \phi(r, \omega)\int_r^R \chi(r', \omega)\psi_0(r')\,\mathrm{d}r'\right) \tag{2.6}$$

is the solution of equation (2.5) with the required boundary conditions $\Phi(0, \omega) = \Phi(R, \omega) = 0$ for all ω, provided that $\phi(r, \omega)$ and $\chi(r, \omega)$ are solutions of $H_r\phi = \omega\phi$ and $H_r\chi = \omega\chi$ such that $\phi = 0$ at $r = 0$ and $\chi = 0$ at $r = R$, and that $W(\omega)$ is the Wronskian of ϕ and χ, namely

$$W = \phi\,\mathrm{d}\chi/\mathrm{d}r - \chi\,\mathrm{d}\phi/\mathrm{d}r. \tag{2.7}$$

It can easily be verified that $\mathrm{d}W/\mathrm{d}r = 0$ for all r, and hence that W is independent of r. Note that the form of the expression (2.6) is such that no particular normalisation of ϕ or of χ is needed.

Equations (2.4) and (2.6) thus give the required solution for $t > 0$ and finite R. It can be shown that ϕ and χ and their derivatives are analytic functions of ω for all finite ω, and that the only singularities of $\Phi(r, \omega)$ are simple poles which occur where $W(\omega) = 0$. For details, see Titchmarsh (1958 Part I, ch I), whose approach to the theory of eigenfunction expansions provided the inspiration for the treatment given in this section.

Now if $W(\omega_n) = 0$, $(n = 0, 1, 2, \ldots)$, say, then, by (2.7), $\chi(r, \omega_n) = a_n\phi(r, \omega_n)$, where a_n is a constant. It follows that $\phi(r, \omega_n) = 0$ at $r = R$ as well as at $r = 0$, i.e. that $\phi(r, \omega_n)$ is an eigenfunction of H_r, for finite R, with eigenvalue ω_n. Conversely, if ω_n is an eigenvalue, then $\chi(r, \omega_n) \propto \phi(r, \omega_n)$, and hence, by (2.7), $W(\omega_n) = 0$. Since H_r is Hermitian with respect to the assumed boundary conditions, all ω_n are real; they are in fact, in the units used here, the energy eigenvalues of the system for finite R (figure 2).

Note that the contour C_ω can be completed below to give C'_ω (figure 2), and the theory of residues then gives

$$\psi(r, t) = \sum_n [a_n/W'(\omega_n)]\left(\int_0^R \phi(r', \omega_n)\psi_0(r')\,\mathrm{d}r'\right)\phi(r, \omega_n)\exp(-\mathrm{i}\omega_n t) \tag{2.8}$$

which is the expansion of the solution in eigenfunctions of H_r for finite R. Note that the ϕ's are real for real ω.

We now consider what happens as $R \to \infty$. For any potential which $\to 0$ as $r \to \infty$, the 'positive energy' $(\omega > 0)$ eigenvalues of the system close up to form a continuum in $0 < \omega < \infty$, and only the remaining eigenvalues, if any, with negative ω, i.e. the bound states of the system, now give contributions to the wavefunction of the form (2.8) (see figure 3).

It is convenient from now on to use $k = \omega^{1/2}$ instead of ω, choosing the root to be such that $\operatorname{Im} k > 0$ for all ω on C'_ω. The corresponding contour C_k in the complex k-plane is shown in figure 4.

Assuming, as previously stated, that $\psi_0(r)$ is negligible for r greater than some value r_0, then, for $r > r_0$, the solution given by equations (2.4) and (2.6) reduces, apart from

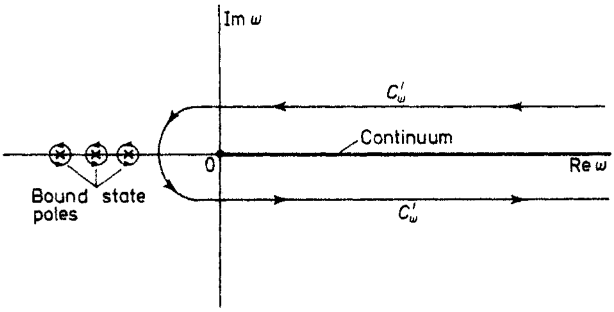

Figure 3. The limiting case $R \to \infty$ of figure 2.

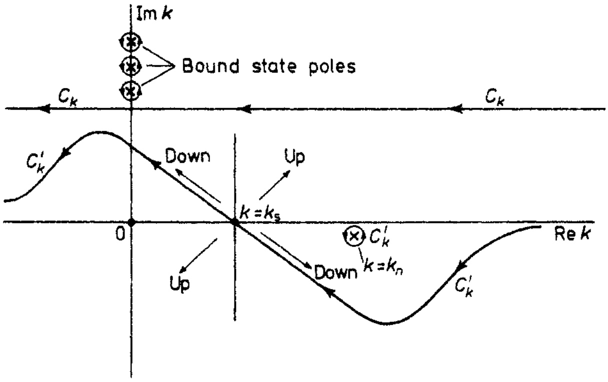

Figure 4. Properties in the complex k-plane of the integrand of expression (3.3) for the wavefunction of the particle at a distance from the well. The saddle-point at $k = k_s = r/2t$, and a pole at $k = k_n$ just below the real axis, are shown. The arrows marked UP (or DOWN) indicate the directions in which the modulus of the integrand increases (or decreases) most rapidly away from the saddle point. The contours C_k and C'_k are those used in the evaluation of (3.3).

bound state contributions of the form (2.8) which will be omitted from now on, to

$$\psi(r, t) = (2\pi \mathrm{i})^{-1} \int_{C_k} [F(k)/W(k)]\chi_k(r) \exp(-\mathrm{i}k^2 t) 2k \, \mathrm{d}k \tag{2.9}$$

where $F(k)$ is the 'ϕ-transform' of the initial state, i.e.

$$F(k) = \int_0^{r_0} \phi_k(r)\psi_0(r) \, \mathrm{d}r \tag{2.10}$$

and all functions of ω have been rewritten as functions of k. Thus $\phi_k(r)$ and $\chi_k(r)$ are solutions of $H_r\phi_k = k^2\phi_k$, $H_r\chi_k = k^2\chi_k$, such that $\phi_k = 0$ at $r = 0$ as before, and now, in the limit $R \to \infty$, $\chi_k \to 0$ as $r \to \infty$, at least for all k on C_k, i.e. for Im $k > 0$.

3. The wavefunction at a distance from the potential well

Since, by hypothesis, $V(r) \to 0$ faster than r^{-1} as $r \to \infty$, we can, for large enough r, use the asymptotic form

$$\phi_k(r) \sim A(k)\exp(\mathrm{i}kr) + B(k)\exp(-\mathrm{i}kr) \tag{3.1}$$

where $A(k)$ and $B(k)$ depend on the potential; also we can take

$$\chi_k(r) \sim \exp(\mathrm{i}kr) \tag{3.2}$$

since χ is required to be the solution of $H_r\chi = k^2\chi$ which $\to 0$ as $r \to \infty$ if $\operatorname{Im} k > 0$, and no particular normalisation is required. Then, since $W(k)$ is independent of r, and so can be evaluated anywhere, we have, by (2.7), (3.1) and (3.2), $W(k) = 2\mathrm{i}kB(k)$, and hence, for large enough r:

$$\psi(r, t) \sim -(2\pi)^{-1}\int_{C_k} [F(k)/B(k)]\exp[\mathrm{i}(kr - k^2 t)]\,\mathrm{d}k. \tag{3.3}$$

Note that we can write

$$\exp[\mathrm{i}(kr - k^2 t)] = \exp[-\mathrm{i}t(k - r/2t)^2]\exp(\mathrm{i}r^2/4t) \tag{3.4}$$

which shows that the integrand has a saddle point at $k = r/2t = k_s$, say (figure 4).

So far the calculation would have been valid whether $V(r)$ had an outer barrier or not. Now it is known that a potential with an outer barrier has a zero of $B(k)$ just below the real axis of k near any real value k_b of k which is such that $E_b = k_b^2$ is the energy of a bound state of the comparison potential $V_1(r)$ shown in figure 1, provided E_b is above the zero of energy, i.e. $V(\infty)$, used here. The broader the barrier, the nearer the zero of $B(k)$ is to k_b. For details, see e.g. Drukarev *et al* (1979), who give a precise method for locating such zeros, and references to earlier work.

Let there be such zeros of $B(k)$ at $k = k_n = k_{nR} - \mathrm{i}\gamma_n$, $(n = 1, 2, \ldots)$, say, with $0 < \gamma_n \ll k_{nR}$. The contour C_k in (3.3) can then be deformed continuously into C'_k (figure 4), leaving behind small loops round any pole of the integrand, i.e. any zero of $B(k)$, that the contour passes through in the process. We can now write

$$\psi(r, t) \sim \psi_S(r, t) + \sum_n \psi^{(n)}(r, t) \tag{3.5}$$

where, by integrating across the saddle point, the method of steepest descents gives, for large enough t,

$$\psi_S(r, t) = \tfrac{1}{2}(\pi t)^{-1/2}[F(k_s)/B(k_s)]\,exp(ir^2/4t - \mathrm{i}\pi/4); \tag{3.6}$$

also, for each pole:

(a) for $k_s = r/2t < k_{nR}$, i.e. $r < 2k_{nR}t$,

$$\begin{aligned}\psi^{(n)}(r, t) &= -\mathrm{i}[F(k_n)/B'(k_n)]\exp[\mathrm{i}(k_n r - k_n^2 t)] \\ &= -\mathrm{i}[F(k_n)/B'(k_n)]\exp[\gamma_n(r - 2k_{nR}t)]\exp[\mathrm{i}(k_{nR}r - k_{nR}^2 t)];\end{aligned} \tag{3.7}$$

(b) for $k_s = r/2t < k_{nR}$, i.e. $r > 2k_{nR}t$,

$$\psi^{(n)}(r, t) = 0 \tag{3.8}$$

since in the latter case the contour does not pass through the pole in the process of deformation. Thus, for each pole, the corresponding component $\psi^{(n)}$ of the wavefunction has a 'cut-off' at $r = 2k_{nR}t$, which moves outwards with velocity $2k_{nR}$, followed by an oscillation of wavenumber k_{nR} whose envelope is a decaying exponential also moving with velocity $2k_{nR}$ (figure 5, full curves). Note that in the units used here, $2k_{nR}$ is the classical velocity of a particle of momentum k_{nR} and energy $(k_{nR})^2$.

A more precise evaluation of the expression (3.3), to be given elsewhere, shows that the envelope of the wavefunction in fact displays small oscillatory departures near the cut-off from the approximate result given here (figure 5, broken curves). These do not, however, affect the conclusions drawn in the next section.

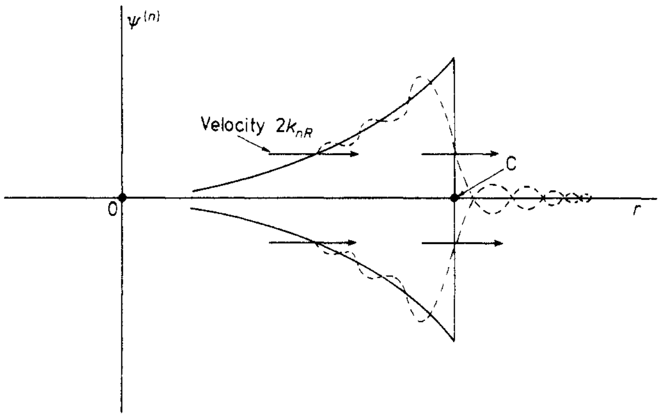

Figure 5. The envelope, moving with velocity $2k_{nR}$, of the oscillation of wavenumber k_{nR} which consititutes the component $\psi^{(n)}$ of the wavefunction of the particle at a distance from the well. Full curves: the approximate result obtained here; broken curves: the result of a more precise calculation to be given elsewhere. C: 'cut-off' at $r = 2k_{nR}t$.

4. Summary of results and discussion

We have seen that provided the comparison potential $V_1(r)$ (figure 1) has at least one bound state with energy above the zero of energy $V(\infty)$ used here, then the radial wavefunction $\psi(r, t)$ of a particle known to be in the potential well $V(r)$ at time $t = 0$ will, for each such bound state of $V_1(r)$, have a component $\psi^{(n)}(r, t)(n = 1, 2, \ldots)$ given by equations (3.7) and (3.8) (see figure 5).

At any point r, after the passage of the 'cut-off' (figure 5), $\psi^{(n)}$ consists of an oscillation of wavenumber k_{nR} with an amplitude which varies with t as $\exp(-2\gamma_n k_{nR} t)$. Provided the particle detector used to observe the process has sufficient momentum resolution, it will respond separately to the momenta k_{nR} of the particle in the different components $\psi^{(n)}$ of the wavefunction. The process will then, for each such component, appear as the emission of a particle of momentum k_{nR} and energy $(k_{nR})^2$, with, as can be seen from equation (3.7), a peak probability flux per unit solid angle of $2k_{nR}|F(k_n)/B'(k_n)|^2$; this flux then decays exponentially with decay constant $4\gamma_n k_{nR}$. Integration of the flux over all time and angles gives the total probability $2\pi(\gamma_n)^{-1}|F(k_n)/B'(k_n)|^2$ that the particle would be found to have been emitted in the 'state' $\psi^{(n)}$.

Note that for the above to be the case the particle need not have been in any particular initial state in the well; a necessary and sufficient condition is that the 'ϕ-transform' $F(k)$ of the initial state, defined by equation (2.10), should not vanish at $k = k_n$.

It is satisfactory to observe that the decay constants $4\gamma_n k_{nR}$ agree, in the units used here, with those found by Drukarev *et al* (1979) for the decay of the probability that the particle would be found to be still in its initial state in the well.

We have tacitly assumed that the particle detector used does not respond appreciably to the 'non-exponential decay' component ψ_s of the wavefunction given by equation (3.6). This seems reasonable since at any given point r, ψ_s represents the passage of a wave of continuously changing wavenumber and frequency. However, it is intended to study further the physical significance of this term, which would be the only surviving one if the potential had no barrier, and its importance in connection with particular potential wells, initial states, and detecting processes. The results will be submitted for publication in this journal.

5. Generalisations

If the particle is assumed to be in a state with angular momentum quantum number $l > 0$, its time-dependent wavefunction can be written as $\Psi(r, t) = r^{-1}\psi(r, t) Y_l(\theta, \phi)$, where Y_l is a spherical harmonic of order l, normalised to 4π on the surface of a unit sphere. It can then be verified that the calculation given above remains valid provided (1) that $V(r)$ is replaced throughout by $V^{(l)}(r) = V(r) + l(l+1)r^{-2}$, and the corresponding comparison potential $V_1^{(l)}(r)$ is defined to be equal to $V^{(l)}(r)$ from $r = 0$ to the top of the barrier of $V^{(l)}(r)$, and to be constant from thereon, and (2) that a factor $|Y_l(\theta\phi)|^2$ is inserted in the expression for the peak probability flux per unit solid angle given in § 4.

If the potential has a 'Coulomb tail', i.e. if $V(r) \sim Cr^{-1}$ as $r \to \infty$, where C is a constant, then the asymptotic forms (3.1) and (3.2) are modified by the addition of the well known Coulomb phase term. In the units used here, $\exp(\pm ikr)$ must be replaced by $\exp[\pm i(kr - C \ln 2kr/2k)]$. However the added term becomes negligible compared with kr for large enough r, and it can be verified that the results previously obtained are still valid.

Acknowledgments

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