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PROBABILISTIC METHODS IN SOME PROBLEMS OF SCATTERING THEORY

M. KAC*

Introduction. We give three applications of probability to scattering theory. The first question we consider is that of the "scattering length." We obtain a probabilistic expression for scattering length and use this expression to prove that in the case of an impenetrable obstacle ("hard" potential) the scattering length Γ is the same as the electrostatic capacity.

Next, we briefly touch upon a problem which is inherently probabilistic — namely, scattering in a medium with random boundary. We find that if a large number of small hard spheres ("dust particles") are distributed at random in the medium, the effect is to shift all the eigenvalues by a constant.

Our final topic is the so-called "inverse problem" of scattering theory: given the scattering operator, to compute the potential. For certain spherically symmetric potentials, this problem was solved in a famous paper of Gel'fand and Levitan. Here we show that their result can be included in the circle of potential-theoretic problems which can be solved by means of Brownian motion and Wiener integrals.

We quickly sketch some of the physical background.

We are concerned with the Schrodinger equation of non-relativistic quantum mechanics. In its stationary or time-independent form, this equation is

$$[(1/2)\nabla^2 + (k^2 - q(\vec{R}))]\psi = 0. \tag{1}$$

The "wave function" ψ depends on both the position vector $\vec{R} \in R^3$ and the wave number k. The real parameter k^2 is proportional to the energy. The function $q(\vec{R})$ is called the "potential." It represents the interaction of the quantum-mechanical "particle" with some force field. The "scattering problem" is, roughly speaking, to determine the effect of this interaction asymptotically for large $\vec{R}$. More precisely, we seek a solution of (1) which at $|\vec{R}| = \infty$ is of the asymptotic form $e^{i\sqrt{2}kz} + f_k(\vec{e})e^{i\sqrt{2}k\|\vec{R}\|}/\|\vec{R}\|$ where $\vec{e}$ is the unit vector in the direction of $\vec{R}$. The first term, $e^{i\sqrt{2}kz}$, is an incident wave in the direction of the z-axis; the second term $f_k(\vec{e})e^{i\sqrt{2}k\|\vec{R}\|}/\|\vec{R}\|$, is the "scattered wave."

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The central problem of scattering theory is to find the function $f_k(\vec{e})$, which is known as the scattering amplitude. The modulus square of the scattering amplitude, integrated over unit vectors $\vec{e}$, is the scattering cross-section,

$$\sigma^2 \equiv \int_0^{2\pi} d\theta \int_0^{\pi} |f(\theta, \phi)|^2 \sin\phi \, d\phi.$$

Now it is easy to show formally, by the use of a very classical transformation (I am not certain who first did it, although I believe credit is given to Schwinger) that to solve equation (1), with the given boundary condition, is equivalent to solving the following integral equation:

$$\psi(\vec{r}) = e^{i\sqrt{2k}z} - \frac{1}{2\pi} \int \frac{e^{i\sqrt{2k}\|(\vec{R}-\vec{r})\|}}{\|\vec{R}-\vec{r}\|} q(\vec{R})\psi(\vec{R}) \, d\vec{R}, \tag{2}$$

where the integration is taken over all of three-space. This is of course just a standard Green's function representation, and it is extremely easy to verify directly that it satisfies the equation. The only thing that we have to do, which is done in all the textbooks on this subject, is to show that the solution of the integral equation (2) has the appropriate asymptotic form for large values of r. I briefly outline a little geometrical argument that demonstrates how one can show this.

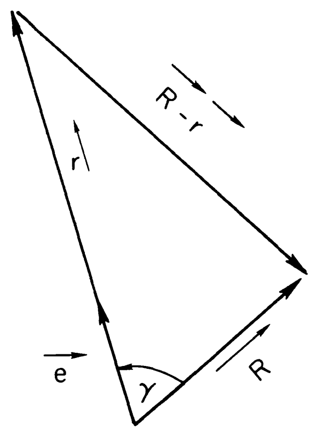

Fig. 1

Referring to figure 1 we see by the law of cosines that

$$|\vec{R} - \vec{r}| = \{|R|^2 + |r|^2 - 2|R|\,|r| \cos\gamma\}^{1/2}$$

which for $(R/r)^2 \ll 1$ (for example if q has finite range) satisfies

$$|\vec{R} - \vec{r}| \sim r\left(1 - \frac{R}{r}\cos\gamma\right) = r - R\cos\gamma = r - \vec{R}\cdot\vec{e}.$$

If we plug this into the integral equation (2) and neglect the term $\vec{R}\cdot\vec{e}$ in the denominator of the integrand, we obtain the asymptotic expression

$$(3)\quad \psi(r) \sim e^{i\sqrt{2}kz} + \frac{e^{i\sqrt{2}k\|r\|}}{\|r\|}\left[-\frac{1}{2\pi}\int e^{\,i\sqrt{2}k\vec{R}\cdot\vec{e}}\; q(\vec{R})\psi(\vec{R})\, dR\right],$$

which is in the correct asymptotic form. In fact, this last expression gives us an elegant but largely useless formula for the scattering amplitude in terms of the solution to the wave equation. There are however two limiting cases which can be handled.

The first case is that of high energy, or large k. (Since everything is dimensionless, it is a little complicated to say in relation to what it is large!). This case ought to be easy, since then the effect of the potential in the differential equation is that of a perturbation. When you carry out the details, you get what is known as the Born approximation. This approximation is also used when $q(\vec{r})$ is a "hard" potential, (i.e., it is infinite within a finite region). In that case of course it takes a certain amount of optimism, which physicists are endowed with in large quantities, to believe that it is okay, and fortunately, it is. I am reminded that many years ago, Professor Bocher, then at Harvard, said to one of his students, who then was one of my colleagues at Cornell, that the tragedy with physics is not that by wrong reasoning it arrives at wrong conclusions, but that by wrong reasoning it arrives at right conclusions.

Now the other limit, $k \to 0$, the low energy case, has some very nice connections with the theory of Wiener integrals. If we attack the problem formally, displaying the same amount of optimism as in the high energy case, the leading term on the right-hand side of (2) becomes 1 and so does the exponential within the integrand. If we call the resulting initial approximation ψ_0, then this function satisfies the simpler integral equation

$$(4)\qquad \psi_0(\vec{r}) = 1 - \frac{1}{2\pi}\int \frac{q(\vec{R})}{|\vec{R} - \vec{r}|}\psi_0(\vec{R})\, d\vec{R}$$

which should look familiar to people who work in probability theory. The asymptotic estimate (3) becomes

$$\psi_0(\vec{r}) \sim 1 + \frac{1}{r}\left[-\frac{1}{2\pi}\int q(\vec{R})\psi_0(\vec{R})\,dR\right].$$

In order for the quantity ψ_0 to be dimensionless it is necessary that the quantity in brackets in the formula above have the dimension of length, and without the minus sign it is called the scattering length, designated by the symbol Γ. The scattering cross section, which has dimensions of area, will be the square of the above scattering length.

There are many mathematical questions that I have not discussed in the preceding analysis, and I am not even sure whether they have all been considered, although they probably have been. They are not causing any great difficulty; for instance, the passage to the limit under the integral sign in some of our steps is clearly an operation which fills mathematicians with horror, but if you put enough assumptions on the potential, clearly everything is going to be all right. I am not going to be concerned with that, since my story will largely start from the above expression for the scattering length Γ.

The interesting thing is that the quantity Γ has an extremely simple interpretation in terms of Wiener integrals, which I think can already be suspected if you ask yourself what happens in the physically very interesting case of "hard" repulsive potential. (As I remarked earlier, a "hard" potential is one that is infinite in some region.) So, you have a "hard" object with an incident wave of very low energy, and the question is how this "hard" object scatters the wave. It is known, although the proofs do leave a certain amount to be desired, that the scattering length is exactly the capacity of the region over which the "hard" potential is distributed. Since capacity has been the bread and butter of people working in probabilistic potential theory for God knows how long, it is not at all strange that the scattering length, which is a generalization of capacity, also has a probabilistic interpretation.

A Wiener Integral for the Scattering Length. Let me now leave this physical background. Except for a few passages of which I shall warn you, all of what follows is in a completely rigorous state — a situation which I find rather strange for myself. I will assume

(a) $q(\vec{R}) \geqq 0$

(b) $\int q(\vec{R})\,d\vec{R} < \infty$, where $\int \cdots d\vec{R}$ with no region indicated will always mean an integration over all of 3-space.

We are going to consider the following expression, which is perhaps somewhat unmotivated, although most of you who have studied a certain amount of probabilistic potential theory, especially the way I do it, must have seen such formulas ad infinitum:

$$G_s(\vec{r}) = s \int_0^\infty e^{-st} E\{e^{-\int_0^t q(\vec{r}+\vec{r}(\tau))\, d\tau}\}\, dt. \tag{5}$$

Here $\vec{r}(\tau)$ stands for Brownian motion, and E is integration with respect to Wiener measure. Note that in the above expression there is no restriction on the Brownian motion. Except for a factor s this expression is just the Laplace transform of the expected value of the exponential written above, and you have seen such functionals floating around all over the place in this conference. As a background reference for the theory of the above functions, I refer you to "Quelques Aspects Probabilistique de la Theorie du Potential," University of Montreal Lectures Notes, 1970. Although in those notes I only did it for a two dimensional problem, one can parallel that derivation to show that the above function satisfies the equation

$$G_s(\vec{r}) = 1 - \frac{1}{2\pi} \int \frac{e^{-\sqrt{2s}\|\vec{R}-\vec{r}\|}}{\|\vec{R} - \vec{r}\|} q(\vec{R}) G_s(\vec{R})\, d\vec{R}, \quad (s > 0). \tag{6}$$

There are literally hundreds of derivations of this formula, take whichever you want to. The simplest one is to expand the expected value in formula (5) in a power series in the exponent, and use the theory of Wiener integrals to derive the integral equation. For those who are not familiar with the theory, let me point out that it is important that in the above integral equation, the kernel

$$\frac{1}{2\pi} \frac{e^{-\sqrt{2s}\|\vec{r}-\vec{R}\|}}{\|\vec{r} - \vec{R}\|}$$

arises as the Laplace transform of the fundamental transition density of the 3-dimensional Brownian motion, i.e.,

$$\frac{1}{2\pi} \frac{e^{-\sqrt{2s}\|\vec{r}-\vec{R}\|}}{\|\vec{r} - \vec{R}\|} = \int_0^\infty e^{-st} P(\vec{r} \mid R; t)\, dt$$

where

$$P(\vec{r} \mid \vec{R}; t) = \frac{1}{(2\pi t)^{3/2}} e^{-\|\vec{r}-\vec{R}\|^2/2t} .$$

(The two-dimensional case is much more complicated. One gets Bessel functions in the kernel, which produces rather interesting phenomena.)

Now, it does not take great perspicacity to note that the integral equation (6) for the function G_s is very similar to the original integral equation (2) for the wave function ψ. The differences are that instead of the imaginary term $e^{i\sqrt{2}kz}$, we have the number 1, and instead of the complex kernel, we have the real-valued kernel written above. To a physicist this is not a very important point, but to a mathematician it is. The integral equation for the function ψ is rather difficult, because although it is symmetric, what is needed for a complex integral equation of this form is a Hermitian kernel, which it is not. Consequently, the theory of Fredholm equations for ψ encounters a whole slew of difficulties which are completely absent for the integral equation for G_s when s is positive. The integral equation for G_s is very well behaved and has a nice kernel which can easily be symmetrized; in fact, a little later I shall symmetrize it for you. This last type of equation has several advantages. One speaks of Schwinger variational principles, although in fact such principles are usually formal statements about the stationary points of certain functionals, and I would not really call them variational principles. However, if one has a variational principle to go with a nice well behaved Hermitian kernel in an integral equation, that *is* a variational principle that can be used for estimating and so on.

Now clearly I would like to pass to the limit $s \to 0$ in equation (6) for this would yield a solution of (4). But before I pass to the limit, it might be convenient to form the function $1 - G_s(\vec{r})$ and integrate with respect to $\vec{r}$ over the whole space. One then obtains the formula

$$\int [1 - G_s(\vec{r})]\, d\vec{r} = \frac{1}{s} \int q(\vec{R})G_s(\vec{R})\, d\vec{R}. \tag{7}$$

To obtain this formula we interchange the order of integration and use the fact that the integrand for the integration in $\vec{r}$ was the Laplace transform of a probability density, and when you integrate the probability density you get 1; finally we use the fact that the Laplace transform of the function 1 is $1/s$. Another approach to evaluating the first integral is simply to carry it out using a simple polar coordinate argument. We would like very much to let $s \to 0$ in formula (6). The difficult approach to the problem would be to let the imaginary variable $ik \to 0$ in equation (2). The easy way is to let the variable $s \to 0$ along the real axis in (6). We remark that the left-hand side of the equation (7) is by definition (after an interchange of the order of integration) equal to the quantity

$$s \int_0^\infty e^{-st} \int d\vec{r}[1 - \mathrm{E}\{e^{-\int_0^t q(\vec{r}+\vec{r}(\tau))\, d\tau}\}]\, dt.$$

We would like to determine the behavior of the interior integration in the above formula for large t. As is well known, this is equivalent to determining the behavior of its Laplace transform for $s \to 0$. Since the above expression is, modulo the factor s, exactly the Laplace transform of the interior integral, we can equate the above expression to the right hand side of the formula (7) and divide by s to obtain the following quantity whose behavior for s is of interest: $(1/s^2) \int q(\vec{R})G_s(\vec{R})\, d\vec{R}$. All we need to do is show that the function $G_s(\vec{R})$ goes to a limit, and this is extremely easy to do. In fact, the original formula (5) for G_s shows us that in the limit as s goes to 0 we have

$$\lim_{s\to 0} G_s(\vec{R}) = \mathrm{E}\{e^{-\int_0^\infty q(\vec{R}+\vec{R}(\tau))\, d\tau}\} = G_0(\vec{R})$$

and this limit surely exists as a finite quantity. You may think that it is 0. Actually it is not. For every path, the function $\int_0^t q(\vec{R} + \vec{R}(\tau))\, d\tau$ is increasing as $t \to \infty$ (recall that q is a non-negative function). So the exponential within the expected value symbol approaches a limit boundedly and decreasingly. Since expectation is merely an integration, one can use the theorem on bounded convergence, from which it follows that the limit is finite and in fact is $G_0(\vec{R})$. By doing a little bit more, you can see that the function $G_0(\vec{R})$ is exactly equal to the function $\psi_0(\vec{R})$, since they satisfy exactly the same integral equation (4). (The equation for G_0 is obtained by setting $s = 0$ in equation (6).) Therefore, we have the asymptotic relation

$$\frac{1}{s^2} \int q(\vec{R})G_s(\vec{R})\, d\vec{R} \sim \frac{1}{s^2}\int q(\vec{R})\psi_0(\vec{R})\, d\vec{R}, \quad s \to 0,$$

and this last expression is just $2\pi\Gamma/s^2$. Consequently we arrive at the conclusion

$$\int d\vec{r}\,[1 - \mathrm{E}\{e^{-\int_0^t q(\vec{r}+\vec{r}(\tau))\, d\tau}\}] \sim 2\pi\Gamma t, \quad t \to \infty,$$

where we have of course made use of a Tauberian theorem. This last formula then represents a *probabilistic* interpretation of Γ. If we divide the above asymptotic formula by $2\pi t$ and let $t \to \infty$ then we have a limiting expression for the scattering length Γ that does not involve any imaginary quantities. One can of course prove a great many theorems based on the above formula, depending on a specific assumption on q.

Now let me connect this with something that is known. Consider the above integral equation for G_s when $s = 0$, i.e.,

$$G_0(\vec{r}) = 1 - \frac{1}{2\pi}\int \frac{1}{|\vec{R} - \vec{r}|} q(\vec{R})G_0(\vec{R})\, d\vec{R}.$$

Suppose that

$$q(\vec{r}) = \begin{cases} 1, & \vec{r} \in \Omega, \\ 0, & \vec{r} \notin \Omega, \end{cases}$$

and in order to avoid getting into any kind of trouble with regular and irregular points, let me assume that Ω is as nice a region as you can have. Then the quantity $\int_0^t q(\vec{R} + \vec{R}(\tau))\,d\tau$ represents that amount of time within the time interval $[0, t]$ which is spent in the region Ω. Then $G_0(\vec{r})$ is simply the expectation of exp(−"time spent in Ω"), and it is a well known result that this quantity satisfies the above integral equation for G_0. Next let us assume that

$$q(\vec{r}) = \begin{cases} +\infty, & \vec{r} \in \Omega, \\ 0, & \vec{r} \in \Omega. \end{cases}$$

The equation for G_0 must be reinterpreted, but it is quite easy to see what happens. The quantity $\int_0^t q(\vec{R} + \vec{R}(\tau))\,d\tau$ will give a contribution to the negative exponential only if the time spent in the region is 0. Consequently, the expected value of the exponential is the probability that 0 time is spent in the region Ω, and

$$(8) \qquad 1 - E\{e^{-\int_0^t q(r + r(\tau))\,d\tau}\} \equiv Q_\Omega(\vec{r}; t)$$

is the probability that in the time interval $[0, t]$ you will spend some positive time in the region. Spitzer [1] has already shown (in fact, he showed considerably more) that $\int Q_\Omega(\vec{r}; t)\,d\vec{r} \sim 2\pi\, C(\Omega)t$, $t \to +\infty$, where the quantity $C(\Omega)$ is the capacity of the region Ω. Spitzer, in fact, actually obtained the next term as well in the asymptotic expansion for $t \to \infty$. A Belgian mathematician by the name of Louchard [2] has taken the Laplace transform and has determined a whole succession of consecutive terms in the asymptotic expansion. But we need only the first term to confirm (heuristically) that capacity equals scattering length for a "hard" potential. A rigorous proof requires a little more effort.

Returning to the integral equation

$$(4) \qquad \psi_0(\vec{r}) = 1 - \frac{1}{2\pi} \int \frac{q(\vec{R})}{\|\vec{R} - \vec{r}\|} \psi_0(\vec{R})\,d\vec{R}$$

we rewrite it in the symmetrized form

$$\sqrt{q(\vec{r})}\psi_0(\vec{r}) = \sqrt{q(\vec{r})} - \frac{1}{2\pi} \int \frac{\sqrt{q(\vec{r})}\,\sqrt{q(\vec{R})}}{\|\vec{R} - \vec{r}\|} \psi_0(\vec{R})\sqrt{q(\vec{r})}\,d\vec{r}.$$

Denoting by $\phi_n(\vec{R})$ and λ_n the normalized eigenfunctions and eigenvalues of the kernel

$$K_0(\vec{r}, \vec{R}) = \frac{1}{2\pi} \frac{\sqrt{\tilde{q}(\vec{r})}\,\sqrt{\tilde{q}(\vec{R})}}{\|\vec{R} - \vec{r}\|},$$

(it is a Hilbert-Schmidt kernel, since $q(\vec{r}) \in L^1(R^3)$ or $\sqrt{q(\vec{r})} \in L^2(R^3)$) we obtain without any difficulty that

$$\sqrt{q(\vec{r})}\psi_0(\vec{r}) \sim \sum_{n=1}^{\infty} \frac{(\sqrt{q}, \phi_n)}{1+\lambda_n} \phi_n(\vec{r})$$

and therefore

$$\Gamma = \frac{1}{2\pi} \int q(\vec{r})\psi_0(\vec{r})\, d\vec{r} = \frac{1}{2\pi} \sum_{n=1}^{\infty} \frac{(\sqrt{q}, \phi_n)^2}{1+\lambda_n}.$$

Here the symbol $(\sqrt{q}, \phi_n)$ means the integral over the whole space of $\phi_n\sqrt{q}$. Once you have it in this form it is very easy, and I leave it as an exercise, to obtain a bona fide variation characterization of Γ,

$$\Gamma = \operatorname*{lub}_{f\in L^2(R)} \frac{(f, \sqrt{q})^2}{(f,f) + (K_0 f, f)}.$$

(For a development of some of the ideas related to this I refer you again to the University of Montreal Notes mentioned earlier, which were written in flowing English by Professor Stroock, and translated into flowing French by Professor Van Moerbeke. Professor Stroock has quoted me the statement of James Thurber, that he always liked to see his work translated into French, because it lost something in the original.)

Let me go a little more into the capacity business, because the connection is rather interesting. Suppose instead of the potential q I use the potential uq, where u is a positive constant which later I shall let approach infinity. Then nothing changes in the integral equation (4) except that there will be a factor u in front of the integral sign. This means that the eigenfunctions will not be changed, while the eigenvalues will be multiplied by a factor of u. Of course, the scattering length will be changed, and we will have the new scattering length

$$\Gamma_u = \frac{1}{2\pi} \sum_{n=1}^{\infty} \frac{(\sqrt{q}, \phi_n)^2}{1/u + \lambda_n}.$$

Everything being positive we get

$$\lim_{u\uparrow\infty} \Gamma_u = \frac{1}{2\pi} \sum_{n=1}^{\infty} \frac{(\sqrt{q}, \phi_n)^2}{\lambda_n},$$

but we do not know whether the right-hand side is finite.

Suppose that

$$q(\vec{r}) = 0 \quad \text{outside a closed region } \Omega,$$

$$q(\vec{r}) > 0 \quad \text{in the } \textit{interior } \Omega_0 \text{ of } \Omega,$$

and consider

$$H_u(\vec{r}) = \mathrm{E}\{e^{-u\int_0^\infty q(\vec{r}+\vec{r}(\tau))\,d\tau}\}.$$

$H_u(\vec{r})$ can be shown to satisfy the integral equation

$$H_u(\vec{r}) = 1 - \frac{u}{2\pi}\int_\Omega \frac{q(\vec{r})}{\|\vec{R}-\vec{r}\|} H_u(\vec{R})\,d\vec{R}$$

and it is clear that $\lim_{u\uparrow\infty} H_u(\vec{r}) = \text{Prob.}\{\vec{r} + \vec{r}(t)$ spends 0 time in $\Omega\}$.

From previous work (see, for example, Quelques Aspects Probabilistic de la Theorie du Potential, University of Montreal Notes, Summer, 1968) $\lim_{u\uparrow\infty}(1 - H_u(\vec{r}))$ = capacitory potential of Ω and therefore for every Borel set B, $\lim_{u\uparrow\infty} \int_B uq(\vec{R})H_u(\vec{R})\,d\vec{R} = \int_B \mathrm{fr}\,(d\vec{R})$ where fr is the equilibrium charge distribution.

It follows that if the support of q is Ω

$$\lim_{u\uparrow\infty} \Gamma_u = \frac{1}{2\pi}\sum_{n=1}^{\infty}\frac{(\sqrt{q},\phi_n)^2}{\lambda_n} = C(\Omega) = \text{capacity of } \Omega.$$

If you carefully read my University of Montreal Notes, in fact even if you read them not so carefully, you will discover that if you have a region Ω satisfying certain mild conditions and if q were identically 1 in this region Ω and 0 outside, then the above integral equation simplifies considerably and the eigenvalues are just those of the kernel $1/\|\vec{R}-\vec{r}\|$ in the region Ω, i.e., of the unrestricted Green's function, which is exactly the formula for the capacity which I derived in my University of Montreal Notes. The above requires $q \equiv 1$ in the region Ω and the eigenfunctions and the eigenvalues to be interpreted appropriately. I claimed, and everyone apparently believed me, that $\lim_{u\to\infty}\Gamma_u$ would give you the capacity, since it does not matter how the potential $uq \to \infty$. If this is the case, then the quantity

$$\left(\frac{1}{2\pi}\right)\sum_{n=1}^{\infty}\frac{(\sqrt{q},\phi_n)^2}{\lambda_n}$$

should represent the capacity of the support of the function q, regardless of the particular function q being considered, i.e., we should not need the special requirement that $q \equiv 1$ on its region of support. As we vary q the eigenfunctions and eigenvalues change, but the above remarkable combination remains constant. This is an extremely interesting result, and is an example of the type of windfall one can obtain. It is an extremely difficult thing to prove analytically, since the eigenfunctions and eigenvalues depend in the most complicated way on q, and yet the summation written above always gives you the capacity. An interesting question is what the shape of q does to regular and irregular points. One can also distinguish whether the points are regular according to the behavior of such limits as u goes to infinity in various expansions. In the interior and exterior nothing is going to change. But if the function q is going to become strongly 0 at an irregular point, then what used to be irregular for the ordinary potential theory will no longer be so.

Let me say a few words about what happens if q is not positive. The most straightforward case is when $q(r) \leqq 0$. In this case there is only a sign change all the way through in q so things are rather straightforward, formally. I do not know what happens in the case that q changes sign, although later I will state a conjecture. In the case $q(\vec{r}) \leqq 0$, I introduce $\tilde{q}(\vec{r}) = -q(\vec{r})$ and the integral equation (4) for ψ_0 differs only in that the minus sign in front of the integral is changed to a plus. Then everything goes through except that the formula for Γ changes to the following:

$$\Gamma = \frac{1}{2\pi} \sum_{n=1}^{\infty} (\sqrt{\tilde{q}}, \phi_n)^2/(1 - \lambda_n).$$

The eigenfunctions and eigenvalues remain the same. However, in order to ensure that the theory be applicable you must be certain that the maximum eigenvalue of the integral equation be less than 1. If it is $\geqq 1$, you clearly get nonsense from the above expression, since the left-hand side would be positive while the right-hand side would be negative or infinite. And of course this gives you a clue as to what is happening. The condition $\lambda_1 < 1$ is a necessary and sufficient condition not to have bound states. Now this statement is in terms of the eigenvalues of an integral equation with kernel $K_0(\vec{r}, \vec{R})$. Therefore, in order that the original problem not have bound states, it is necessary and sufficient that the maximum eigenvalue of the kernel be smaller than 1. Probabilistically this is equivalent to saying

$$E\{e^{\int_0^\infty q(r+r(\tau))\,d\tau}\} < +\infty .$$

At first it might seem that it is never possible that this expectation should be finite, but now we know in fact that if the largest eigenvalue is < 1, it will be finite. One can actually show, and for the characteristic function of a set I showed it way back in 1949, that the distribution of the integral within the above expectation has an exponential tail, i.e.,

$$\text{(9)} \qquad \text{Prob.} \left\{ \int_0^\infty q(r + r(\tau))\, d\tau > \alpha \right\} \sim e^{-\alpha/\lambda_1} \text{ as } \alpha \to \infty .$$

From this estimate one can also see that the integral in the above expectation will in fact be finite.

It is a matter of some historical interest and perhaps some amusement, how one gets involved in problems that affect one's life. It was the problem described by (9) that got me into this area, and like many things in my career, it has to do with Erdös. Erdös came to Ithaca and said: "Do you know, Kakutani and I were asking what is the probability that the time spent by a Brownian motion in a region is very large." Erdös had been able to estimate that it goes as an exponential, and he told me that he suspected it was exactly an exponential and would like to know what the constant is. Now, of course, this is one of the infinitely many problems that one hears and passes on. But somehow it drew my attention, so I began to get interested in this problem of proving that when q is a characteristic function of a region the distribution has an exponential tail. After about a week of hard work I had the answer, and then I noticed that all I was really doing was a certain amount of probabilistic potential theory.

If q changes sign I still suspect that the condition (9) is still necessary and sufficient for the non-existence of bound states. But I can no longer analyze the integral equation, nor can I write down a variational principle simply because when q changes sign, I can no longer symmetrize in any obvious way.

The "Wiener Sausage". Before I go on to the other things, let me make a connection between some of the preceding results and the so-called "Wiener sausage." I give you a few examples of how some very different looking things all connect together, which is one of the few reasons why mathematics is fun. Of course, some of you may not agree with me, but then you would be wrong. Allow me to make a digression on the "Wiener sausage."

What is the "Wiener sausage?" It is simply a tube, of radius, say, δ whose centerline is a Brownian path. We let $r(\tau)$, $0 \leqq \tau \leqq t$, be the Brownian path, and $W_\delta(t)$ be the Wiener sausage. To do things completely rigorously, let me divide the interval $(0, t)$ into 2^n parts. Let $\tau_k = kt/2^n$, $\vec{r}_k = \vec{r}(kt/2^n)$, $k = 0, 1, \cdots, 2^n$. The path is just a plain ordinary continuous path in three dimensions. We define $S_\delta(\vec{r}_k)$ to be the sphere of radius δ centered at $\vec{r}_k$. We have in a sense discretized the sausage. Now we form the union of these spheres, the "approximate Wiener sausage", $\bigcup_{k=1}^{2^n} S_\delta(\vec{r}_k)$. As $n \to \infty$, this sequence of unions is ascending, because the radius is fixed and we always use our previous centers. So the limit of the sequence of sets, as $n \to \infty$, exists and is clearly the Wiener sausage, $W_\delta(t)$. In fact, because of the monotonicity the following is true:

$$\lim_{n\to\infty} \bigcup_{k=1}^{2^n} |S_\delta(\vec{r}_k)| = |W_\delta(t)|.$$

(Here I use $|S|$ to mean the Lebesgue measure of S.) Let $\chi_k(\vec{r})$ be the indicator function (characteristic function) of $S_\delta(\vec{r}_k)$. Then I claim that $1 - \prod_{k=1}^{2^n} (1 - \chi_k(\vec{r}))$ is the indicator function of the approximate Wiener sausage. Integrating this quantity, we obtain the quantity $|\bigcup_{k=1}^{2^n} S_\delta(\vec{r}_k))|$. There has been no probability so far; we have just done some elementary analysis and fooled around with some simple sets. Now the probability comes in. If we integrate the above expressions, we obtain the equality

$$\left| \bigcup_{k=1}^{2^n} S_\delta(r_k) \right| = \int d\vec{r} \left\{ 1 - \prod_{k=1}^{2^n} (1 - \chi_k(r)) \right\}.$$

If we take the limit as $n \to \infty$ and then take the average with respect to Wiener measure, the left-hand side converges to $E\{|W_\delta(t)|\}$. For the right-hand side we can easily interchange limit and integral, and it is quite easy to give a probabilistic interpretation of the averaged integrand before taking the limit in n. The product within the integrand is the probability that the Brownian motion starting at 0 is not within the sphere of radius δ about $\vec{r}$ at any of the times τ_k, $k = 1, \cdots, 2^n$. Because of the complete spatial homogeneity of Brownian motion, we can rephrase this as asserting that the Brownian motion starting at $\vec{r}$ is not within a sphere about the origin of radius δ at any of the times τ_k. Therefore, we have the following equality

$$E\{|W_\delta(t)|\} = \int d\vec{r}\,[1 - \text{Prob.}\{\vec{r} + \vec{r}(\tau) \notin S_\delta(0), 0 \leqq \tau \leqq t\}.$$

Now 1 minus the probability that we are not in something is exactly the probability that we are in something, and therefore the integrand in the above equation is exactly my quantity $Q_{S_\delta(0)}(\vec{r}; t)$ (Eq. (8)). Using our previous asymptotic expansion for this quantity, we obtain the asymptotic result $\lim_{t\to\infty} |W_\delta(t)|/t = 2\pi\delta$. Similarly one can calculate $E\{|W_\delta(t)|^2\}$, and one obtains

$$\begin{aligned} E\{|W_\delta(t)|^2\} = \iint d\vec{r}\, d\vec{\rho}\, [1 &- \text{Prob.}\{|\vec{r}(\tau) - \vec{r}| > \delta,\ 0 \leqq \tau \leqq t\} \\ &- \text{Prob.}\{|\vec{r}(\tau) - \vec{\rho}| > \delta,\ 0 \leqq \tau \leqq t\} \\ &- \text{Prob.}\{|\vec{r}(\tau) - \vec{r}| > \delta, \text{ and} \\ &\quad |\vec{r}(\tau) - \vec{\rho}| > \delta,\ 0 \leqq \tau \leqq t\}], \end{aligned}$$

and by a more complicated argument, one can show that

$$E\{|W_\delta(t)|^2\} \sim (2\pi\delta t)^2, \quad t \to \infty.$$

It follows that

$$\lim_{t\to\infty} \frac{|W_\delta(t)|}{t} = 2\pi\delta \tag{10}$$

in probability, and equivalently,

$$\lim_{\delta\to 0} \frac{|W_\delta(t)|}{\delta} = 2\pi t \tag{11}$$

in probability.

In fact, a somewhat stronger theorem has been proved by Erdös, Kakutani, and Dvoretzky.

Formula (11) will be needed below, when we consider the problem of scattering in a random medium. I now pose the following conjecture, which should not be difficult to prove.

We write down the expression

$$\int d\vec{r}\,[1 - e^{\int_0^t q(\vec{r}+\vec{r}(\tau))\,d\tau}].$$

Notice that this expression really does not contain any probability, since for any given path we merely carry out the indicated integrals. It is also easy to show that this integral is finite for each t. This expression is precisely the analogue of the Wiener sausage. The conjecture is that this expression is asymptotic to $2\pi\Gamma t$ as $t \to \infty$, in probability.

I should remark that a great many of the results stated above dealing with the relationship between scattering length and the Wiener sausage represent joint work with Professor J. Luttinger. The original problem was to investigate Bose condensation in a container with random impurities. By investigating this problem, I was led to analysis using the Wiener integral. It was Professor Luttinger who remarked to me that if one replaces "hard" spheres by potentials, then one must replace capacity by scattering length, and this was the key observation and led to the above results. It should also be mentioned that in certain of the applied problems related to what I have talked about today there is an extra condition that the path should end at the origin at time t. Fortunately, all of the above results do go through in amended form, using conditional Wiener measure.

Scattering in a Random Medium. Our next topic is an interesting area to work in because there are a number of interesting and difficult unsolved problems. The problem I am going to consider is in a sense academic, but it is a simplified version of a problem that has some oomph to it. I will deal with a region Ω in three dimensions, and I should remark that I do not quite know what happens in two dimensions. You have a region Ω in three dimensions and distributed within it, to be precise with centers uniformly randomly distributed, you place M spheres S_k, $k = 1, \cdots, M$ of radius δ. Having placed them, I will call this configuration C. (Of course, there are many configurations, depending on where the centers have fallen.) I now consider the following problem:

$$(\tfrac{1}{2}\nabla^2 + \lambda)\phi = 0,\ \ \phi = 0 \text{ on } \partial\Omega,\ \ \phi = 0 \text{ on } \partial S_k, k = 1, \cdots, M.$$

This is in fact a problem of solving the Schrodinger equation in a region Ω in which we have placed little "hard" spheres randomly. The question is what happens to the eigenvalues $\lambda_n^{(C)}$ as $M \to \infty$, $\delta \to 0$. The symbol $\lambda_n^{(0)}$ will designate the eigenvalues for the unperturbed problem with $M = 0$, which is equivalent to removing the second boundary condition on the problem stated above for the function ϕ. Here the probabilistic treatment is extremely useful, because from the analytic point of view the problem looks impossible, unless you do it by the perturbation method, which few of us are willing to buy. The problem is easy to do probabilistically, and depends on a well known probabilistic argument which many of us have exploited in different contexts, related to the partition function or the Slater sum of the eigenvalues. This formula holds for any region:

$$\sum_{n=1}^{\infty} e^{-\lambda_n^{(C)}t} = \frac{1}{(\sqrt{2\pi t})^3}\int_\Omega d\vec{r}\, \text{Prob.}\{\vec{r} + \vec{r}(\tau) \in \Omega, \quad \text{for } 0 \leqq \tau \leqq t,$$

$$\text{and } \vec{r} + \vec{r}(\tau) \notin S_k, k = 1, \cdots, M \mid \vec{r}(t) = 0\}.$$

Now everyone knows this formula, but it is rather difficult to give a precise reference. I am going to take the average of the above formula over all configurations C

$$< \sum_{n=1}^{\infty} e^{-\lambda_n^{(C)}t} >_{(C)} = \frac{1}{(\sqrt{2\pi t})^3}\int dr < \text{Prob.}\{\cdots\} >_{(C)}.$$

The above averages are integrals over an M dimensional product space and we have used the physicists' notation for average. On the right-hand side we have interchanged the order of integration and taken the average inside. The more interesting interchange on the right is between the average over all configurations and the probability. The probability is just a measure, and therefore, just the integral of the indicator function of a set in function space. So the probability followed by the average represents two integrations, the integration over the paths and the integration over the centers of the spheres. When we interchange, doing the average over configurations first, we take the point of view that $\vec{r}(\tau)$ is fixed. And given a path we want to average over all of the centers; however, given a path it is easy to interpret conditions within the probability sign for a fixed path. The condition $\vec{r} + \vec{r}(\tau) \notin S_k$ means that the centers of the spheres S_k must lie outside the Wiener sausage, so here is the appearance of the Wiener sausage. Now, of course, in this case the path must return to the origin, and you see that the Wiener sausage is really a "Wiener bagel".

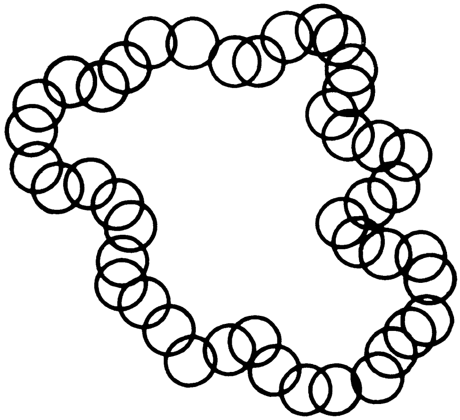

Fig. 2

Given a path, what is the probability that none of the spheres S_k lie on the Wiener sausage? It is $(1 - |W_\delta(t)|/|\Omega|)^M$.

Therefore, the right-hand side of the above average over all configurations becomes

$$\frac{1}{(\sqrt{2\pi t})^3}\int_\Omega d\vec{r}\, E\left\{\left[1-\frac{|W_\delta(t)|}{|\Omega|}\right]^M, \quad \vec{r}+\vec{r}(\tau)\in\Omega \quad \text{for} \quad 0\leqq\tau\leqq t, \,|\, \vec{r}(t)=0\right\} \tag{12}$$

where the notation is rather unfortunate, but it is the best I can do. If I tried to explain it to you in more detail, I would only confuse you. It is better to remain silent and let everyone stare at it, and then it becomes entirely clear. If one tries to verbalize, then one tends to obfuscate matters, a fact which many philosophers have yet to discover.

Now I ask, how should I let $M \to \infty$ and $\delta \to 0$ in order to get a sensible limit. Remember that I derived my previous results for unrestricted Wiener sausages where the ends could wobble, whereas this is a closed Wiener sausage. However, the analysis is similar and the results remain the same. The key result from before is (10): $(|W_\delta(t)|/t) \to 2\pi\delta$ in probability, as $t \to \infty$. But you see, it is obvious by thinking about it, that if you keep t fixed and let δ go to 0, then by a simple scaling argument it comes out that in probability,

$$\frac{|W_\delta(t)|}{\delta} \to 2\pi t \quad \text{as} \quad \delta \to 0. \tag{13}$$

It is very important to know that this convergence is in probability, i.e., that the measure of the paths for which this is not so is negligible, because in formulas above (e.g. (12)) we are only integrating over a subset of all the paths, namely the paths which up to time t remain in Ω.

Now notice that the formula (12) tells us what a sensible limit must be, i.e., we must let $M \to \infty$ and $\delta \to 0$ in such a way that $M\delta = \alpha$ where α is kept fixed. Hence in this limit

$$\mathrm{E}\left\{\left(1 - \frac{|W_\delta(t)|}{|\Omega|}\right)^M, \vec{r} + \vec{r}(\tau) \in \Omega \mid \vec{r}(t) = 0\right\}, \ 0 \leqq \tau \leqq t$$

$$\to \mathrm{e}^{-(-2\pi\alpha t)/|\Omega|}\,\mathrm{Prob.}\{\vec{r} + \vec{r}(\tau) \in \Omega \mid \vec{r}(t) = 0\}, \ 0 \leqq \tau \leqq t$$

and therefore

$$\lim_{\substack{M\to\infty \\ \delta\to 0 \\ M\delta=\alpha}} < \sum_{n=1}^{\infty} \mathrm{e}^{-\lambda_n^{(C)}t} >_{(C)} = \sum_{n=1}^{\infty} \mathrm{e}^{-(\lambda_n^{(C)} + 2\pi\alpha t/|\Omega|)},$$

and the reader should notice that use has been made of the validity of (13) in probability. By a slightly more complicated calculation, one can show that

$$\lim_{\substack{M\to\infty \\ \delta\to 0 \\ M\delta=\alpha}} < \left(\sum_{n=1}^{\infty} \mathrm{e}^{-\lambda_n^{(C)}t}\right)^2 >_{(C)} = \left(\sum_{n=1}^{\infty} \mathrm{e}^{-(\lambda_n^{(0)} + 2\pi\alpha t/|\Omega|}\right)^2$$

and therefore

$$\lim \sum_{n=1}^{\infty} \mathrm{e}^{-\lambda_n^{(C)}t} = \sum_{n=1}^{\infty} \mathrm{e}^{-(\lambda_n^{(0)} + (2\pi\alpha)/|\Omega|)t}$$

in probability.

Since this holds for *every* $t > 0$, it also follows that for every n $\lambda_n^{(C)} \to \lambda_n^{(0)} + 2\pi\alpha/|\Omega|$ in probability, that is, all the eigenvalues are simply shifted by the same fixed constant, which is sometimes called the Lenz shift. Let me now state the first interesting unsolved problem:

1. In the above analysis I have brutally gone to the limit. Suppose however that we have δ very small and M very large without going to the limit, with $M\delta = \alpha$. Then the eigenvalue $\lambda_1^{(C)}$ is a random variable with a certain distribution, i.e., we have a line width. It would be interesting to know the width, i.e., is it of the order of δ or of the order $\sqrt{\delta}$?

Before I state the second unsolved problem, I have to reformulate slightly our original problem. Now we do not need an arbitrary shape; let me take a box of side L. In this container we again place M spheres at random, but now I will require that $M\delta^3/L^3 = \nu$(constant), i.e., the total volume of impurities is fixed. Again I will solve the same Schrodinger equation. (Because we treated the Schrodinger equation in dimensionless units, the length L is the actual length of the box divided by the deBroglie wave length.) This happens to be the problem of the ideal Bose gas in a container in which you have distributed random impurities. Now if the spheres were actually hard, they would not be allowed to overlap. This introduces a great many complications, so assume for the moment that they are allowed to overlap. Our next problem is the following.

2.1°: If there are no impurities, $M = 0$, then the eigenvalues of the problem have the following asymptotic form, where k, ℓ, and m are integers: $\lambda_{k,\ell,n} \sim (k^2 + \ell^2 + m^2)/CL^2$, C a constant. Consequently, the lowest eigenvalue is 0 and the next eigenvalue is $1/CL^2$. So the difference between the lowest and the next lowest eigenvalues is of the order of $1/L^2$. The problem is to prove that $(\lambda_2^{(C)} - \lambda_1^{(C)})L^3$ converges in probability to infinity as $L \to \infty$. Intuitively this means that impurities will not destroy the spacing of the first two eigenvalues by any order of magnitude.

The much more difficult problem is the following about the Wiener sausage:

2.2°: For the ideal Bose gas problem stated above show that

$$\lim_{t\to\infty} \frac{\log E\{e^{-\nu|W_\delta(t)|}\}}{t^{3/5}}$$

exists and is different from 0. Estimates from below on this logarithm can be given. But this conjecture demands a rather precise estimate, which requires a great deal of information. In case someone does not like Wiener sausages, you could already become a famous man as far as I am concerned if you could answer the discrete version of the same problem. This is because there is a very simple analogue of the Wiener sausage for a discrete random walk. Suppose that in d dimensions you start a random walk. This question is, how many distinct lattice points do you hit. We call this quantity $|W_n|$. The conjecture is that

$$\lim_{n\to\infty} (\log E\{e^{-\nu|W_n|}\})(n^{-(d/d+2)})$$

exists as a non-zero number.

The Inverse Problem and the Gel'fand-Levitan Formula. We now turn to a different question known as the inverse scattering problem. The potential $q(\vec{r})$ is now assumed to be of spherical symmetry $q(\vec{r}) = q(r)$, $r = \|\vec{r}\|$ and we shall be interested only in spherically symmetric solutions of (1) ("S-waves") i.e., solutions of the form $\psi(\vec{r}) = \phi(r)/r$ where $\psi = 0$ at the origin ($r = 0$).

Equation (1) becomes now

$$\mathcal{L}\phi = \phi'' - q(x)\phi = -\lambda\phi \tag{14}$$

(where I have replaced r by x and the coefficient 1/2 of ϕ'' by 1 to conform to standard notation) and we normalize ϕ by requiring that $\phi'(0;\lambda) = 1$ (in addition to $\phi(0;\lambda) = 0$). If $g(x)$ vanishes as $x \to \infty$ $\phi(x;\lambda)$ all, for $\lambda > 0$, have the asymptotic form

$$\phi(x) \sim \alpha(\lambda)\sin(\sqrt{\lambda}\,x + \delta(\lambda)) \tag{15}$$

where $\delta(\lambda)$ are known as the phase shift function.

The inverse scattering problem is to reconstruct the potential q from the phase shift function.

It was shown by Bargman that if there are bound states (i.e., square integrable solutions ϕ for some $\lambda < 0$), the problem was not uniquely soluble, and the next important step was taken by Jost and Kohn (for references and a review, see e.g. the article by Fadeev [3]).

Jost and Kohn have shown that

(a) $\delta(\lambda)$ determines the amplitude $\alpha(\lambda)$,

(b) $\alpha(\lambda)$ determines the spectral function $\rho(\lambda)$ of the differential operator $\mathcal{L}$.

The spectral function (whose existence is a highly non-trivial problem) is a non-decreasing function $\rho(\lambda)$, $-\infty < \lambda < \infty$ such that

$$\int_0^\infty \phi(x;\lambda)\phi(y;\lambda)\,d\rho(\lambda) = \delta(y-x) \tag{16a}$$

and for all f, g in $L_2(0, \infty)$

(16b) $$(\mathcal{L}f, g) = \int_0^\infty \lambda \left[\int_0^\infty f(x)\phi(x;\lambda)\,dx \int_0^\infty g(x)\phi(x;\lambda)\,dx \right] d\rho(\lambda).$$

Under sufficiently general conditions on q the existence (and in many cases uniqueness) of $\rho(\lambda)$ has been shown.

The next, and in a way most crucial, step was taken by Gel'fand and Levitan [4] who showed how $\rho(\lambda)$ determines $q(x)$. Their procedure uses a formula of Marchenko, specifically, the fact that $\phi(x;\lambda)$ can be written in the form

(17) $$\phi(x,\lambda) = \frac{\sin x\sqrt{\lambda}}{\sqrt{\lambda}} + \int_0^x L(x,u)\,\frac{\sin u\sqrt{\lambda}}{\sqrt{\lambda}}\,du,$$

where, remarkably enough, $L(x,u)$ does not depend on λ. They then show that L satisfies the so-called Gel'fand-Levitan equations

(18) $$f(x,\xi) + L(x,\xi) + \int_0^x L(x,u)f(u,\xi)\,du = 0,$$

where f is given explicitly in terms of the spectral function by the formula

$$f(u,\xi) = \int_0^\infty \frac{\sin \mu\sqrt{\lambda}}{\sqrt{\lambda}}\,\frac{\sin \xi\sqrt{\lambda}}{\sqrt{\lambda}}\,d\sigma(\lambda),$$

where $\sigma(\lambda) = \rho(\lambda) - \rho_0(\lambda)$, ρ_0 being the spectral function of the problem with $q \equiv 0$ i.e., $\rho_0(\lambda) = 0$, $\lambda < 0$ and $\rho_0(\lambda) = (2/3\pi)\lambda^{3/2}$. If one makes enough assumptions on σ to make sure f exists and is sufficiently smooth, then the theory of Fredholm integral equations permits one to construct L. Given L, we shall see that one immediately obtains the desired potential function q.

The crux of the matter is the Gel'fand-Levitan equation (18), which is used to construct L.

We will give a probabilistic derivation of (18), and then show how to express q in terms of L. We also will show how to obtain the spectral function σ from the asymptotic amplitude $\alpha(\lambda)$. To simplify matters, I shall assume that there are no bound states.

Probability comes into this problem in the following way. Consider the equation

(19) $$\frac{\partial P}{\partial t} = \frac{\partial^2 P}{\partial x^2} - q(x)P.$$

We extend q to the negative axis by defining it as an even function.

The following mild variation of the Kac-Feynman formula is easily derivable

$$\frac{1}{2}\frac{e^{-(y-x)^2/4t}}{2\sqrt{\pi t}}\ E\left\{e^{-\int_0^t q(y+x(\tau))\,d\tau} \middle| y + x(t) = x\right\}$$
$$-\frac{1}{2}\frac{e^{-(y+x)^2/4t}}{2\sqrt{\pi t}}\ E\left\{e^{-\int_0^t q(-y+x(\tau))\,d\tau} \middle| -y + x(t) = x\right\}$$
$$= \frac{1}{2}\int_0^\infty e^{-\lambda t}\phi(x,\lambda)\phi(y,\lambda)\,d\rho(\lambda).$$

Notice that the left-hand side is a vestige of the method of images. The Gel'fand-Levitan results follow very easily from this, as we shall show below. We would like to set $y = 0$, but this gives $0 = 0$. So we consider a small $y > 0$, divide by y and let y tend to 0. This gives us the following useful formula:

$$\int_0^\infty e^{-\lambda t}\phi(x,\lambda)\,d\rho(\lambda) = \frac{e^{-x^2/4t}}{2\sqrt{\pi t}}\frac{x}{t}\ E\left\{e^{-\int_0^t q(x(\tau))\,d\tau} \middle| x(t) = x\right\}$$
$$(20) \qquad + \frac{e^{-(x^2/4t)}}{2\sqrt{\pi t}}\lim_{y\to 0}\frac{1}{y}\left[E\{e^{-\int_0^t q(y+x(\tau))\,d\tau} \mid y + x(t = x\}\right.$$
$$\left. - E\{e^{-\int_0^t q(-y+x(\tau))\,d\tau} \mid -y + x(t) = x\}\right].$$

We will show that the second term on the right-hand side is of no consequence. Note that if q is identically 0, then $\rho(\lambda)$ is well known, in fact $\rho = (2/3\pi)\lambda^{3/2}$. Therefore, we *assume* that

$$(21) \qquad \rho(\lambda) = \frac{2}{3\pi}\lambda^{3/2} + \sigma(\lambda).$$

We will then need to impose smallness conditions on $\sigma(\lambda)$, involving the existence of certain improper integrals integrated with respect to $|d\sigma(\lambda)|$, as do Gel'fand and Levitan.

We also need the simple formula

$$(22) \qquad e^{-\lambda t} = \frac{1}{2\sqrt{\pi}t^{3/2}}\int_0^\infty \frac{\sin\xi\sqrt{\lambda}}{\sqrt{\lambda}}\xi e^{-\xi^2/4t}\,d\xi.$$

If we substitute from (17) and (21) into (20), a routine calculation, using (22), yields

$$\int_0^\infty e^{-\lambda t}\phi(x;\lambda)\,d\rho(\lambda)$$

$$= \int_0^\infty e^{-\lambda t}\left\{\frac{\sin x\sqrt{\lambda}}{\sqrt{\lambda}} + \int_0^x L(x,u)\frac{\sin u\sqrt{\lambda}}{\sqrt{\lambda}}\,du\right\} d\left(\frac{2}{3\pi}\lambda^{3/2}\right)$$

$$+ \int_0^\infty \left(\int_0^\infty \frac{1}{2\sqrt{\pi}t^{3/2}}\frac{\sin\xi\sqrt{\lambda}}{\sqrt{\lambda}}\,\xi e^{-\xi^2/4t}\,d\xi\right)$$

$$\left\{\frac{\sin x\sqrt{\lambda}}{\sqrt{\lambda}} + \int_0^x \cdots\right\} d\sigma(x)$$

$$= \frac{x}{2\sqrt{\pi}t^{3/2}}\,e^{-x^2/4t} + \int_0^x L(x,u)\frac{u}{2\sqrt{\pi}t^{3/2}}\,e^{-u^2/4t}\,du$$

$$+ \int_0^\infty \frac{e^{-\xi^2/4t}}{2\sqrt{\pi}t^{3/2}}\,\xi\left\{f(x,\xi) + \int_0^x L(x;\lambda)f(u,\xi)\,du\right\} d\xi,$$

and hence after minor changes

$$\int_0^\infty e^{-\lambda t}\phi(x;\lambda)\,d\rho(\lambda) = \frac{x}{2\sqrt{\pi}t^{3/2}}\,e^{-x^2/4t}$$

$$+ \int_0^x \frac{e^{-\xi^2/4t}}{2\sqrt{\pi}t^{3/2}}\,\xi\left\{f(x,\xi) + L(x;\xi) + \int_0^x L(x;u)f(u,\xi)\,du\right\} d\xi$$

$$+ \int_x^\infty \frac{e^{-\xi^2/4t}}{2\sqrt{\pi}t^{3/2}}\,\xi\left\{f(x,\xi) + \int_0^x L(x;u)f(u,\xi)\,du\right\} d\xi$$

$$= \frac{e^{-x^2/4t}}{2\sqrt{\pi}t^{3/2}}\,x\,\mathrm{E}\left\{e^{-\int_0^t q(x(\tau))\,d\tau} \mid x(t) = x\right\}$$

$$+ \frac{e^{-x^2/4t}}{2\sqrt{\pi}\sqrt{t}}\lim_{y\to 0}\frac{1}{y}\left[\mathrm{E}\{e^{-\int_0^t q(y+x(\tau))\,d\tau} \mid y + x(t) = x\}\right.$$

$$\left. - \mathrm{E}\{e^{-\int_0^t q(-y+x(\tau))\,d\tau} \mid -y + x(t) = x\}\right].$$

This can be rewritten in a more convenient form as follows:

$$- x\mathrm{E}\{1 - e^{-\int_0^t q(x(\tau))\,d\tau} \mid x(t) = x\} + t\lim_{y\to 0}\frac{1}{y}[\quad]$$

$$= e^{x^2/4t}\int_0^x e^{-\xi^2/4t}\,\xi\left\{f(x,\xi) + L(x,\xi) + \int_0^x L(x;u)f(u,\xi)\,du\right\}$$

$$+ e^{x^2/4t}\int_x^\infty e^{-\xi^2/4t}\,\xi\left\{f(x,\xi) + \int_0^x L(x;u)f(u,\xi)\,du\right\} d\xi.$$

First consider the second term above. Set $\xi = x + \eta t$ and obtain

$$te^{x^2/4t} \int_0^\infty e^{-(x+\eta t)^2/4t} (x - \eta t) \left\{ f(x, x + \eta t) + \int_0^x L(x; u) f(u, x + \eta t)\, du \right\} d\eta$$

$$= t \int_0^\infty e^{-x\eta/2} e^{-t\eta^2/4} (x + \eta t) \left\{ f(x, x + \eta t) + \int_0^x L(x, u) f(u, x + \eta t)\, du \right\} d\eta$$

$$\sim tx \left\{ f(x, x) + \int_0^x L(x, u) f(u, x)\, du \right\} \frac{2}{x}.$$

The first term, i.e.,

$$e^{x^2/4t} \int_0^x e^{-\xi^2/4t} \xi \left\{ f(x, \xi) + L(x, \xi) + \int_0^x L(x, u) f(u, \xi)\, du \right\}$$

is easily shown to diverge (to $+\infty$ or $-\infty$) as $t \to 0$ unless

$$f(x, \xi) + L(x, \xi) + \int_0^x L(x, u) f(u, \xi)\, d\xi \equiv 0,$$

for $\xi < x$. This is the Gel'fand-Levitan integral equation.

Assuming that we can prove the intuitively obvious fact that $\lim_{t\to 0}\lim_{y\to 0} 1/y\,[\quad] = 0$ we obtain

$$-x \lim_{t\to 0} \frac{1}{t} \mathrm{E}\{1 - e^{-\int_0^t q(x(\tau))\, dt} \mid x(t) = x\}$$

$$= 2 \left\{ f(x, x) + \int_0^x L(x; u) f(u, x)\, du \right\} = -2L(x, x)$$

or

$$\lim_{t\to 0} \frac{1}{t} \mathrm{E}\{1 - e^{-\int_0^t q(x(\tau))\, d\tau} \mid x(t) = x\} = \frac{2}{x} L(x; x).$$

It remains to calculate

$$\lim_{t\to 0} \frac{\mathrm{E}\{1 - e^{-\int_0^t q(x(\tau))\, d\tau} \mid x(t) = x\}}{t}$$

$$= \lim_{t\to 0} \frac{1}{t} \mathrm{E} \left\{ \int_0^t q(x(\tau))\, d\tau \mid x(t) = x \right\}.$$

We have

$$\mathrm{E}\left\{\int_0^t q(x(\tau))\,d\tau \mid x(t)=x\right\}$$

$$=\left(\frac{e^{-x^2/4t}}{2\sqrt{\pi t}}\right)^{-1}\int_0^t\int_{-\infty}^{\infty} q(u)\,\frac{e^{-u^2/4t}}{2\sqrt{\pi t}}\,\frac{e^{-(x-u)^2/4(t-\tau)}}{2\sqrt{\pi(t-\tau)}}\,du\,d\tau$$

$$=\int_0^t d\tau\frac{1}{2\sqrt{\pi(\tau/t)(t-\tau)}}\int_{-\infty}^{\infty} q(u)\exp\left\{-\frac{(u-x(\tau/t)(t-\tau))^2}{(4(\tau/t)(t-\tau)}\right\}du$$

$$=\int_0^t d\tau\,\frac{1}{2\sqrt{\pi}}\int_{-\infty}^{\infty} q\left(x\frac{\tau}{t}+v\sqrt{(\tau/t)(t-\tau)}\right)e^{-v^2/4}\,dv$$

$$=t\int_0^1 d\theta\,\frac{1}{2\sqrt{\pi}}\int_{-\infty}^{\infty} q(x\theta+v\sqrt{\theta(1-\theta)}\sqrt{t})\,e^{-v^2/4}\,dv$$

$$\sim t\int_0^1 q(x\theta)\,d\theta=t\,\frac{1}{x}\int_0^x q(u)\,du$$

(continuity of q has been assumed). Finally, $L(x;x)=(1/2)\int_0^x q(u)\,du$ the Gel'fand-Levitan result which gives the potential as twice the derivative of $L(x,x)$.

Before we go on, let me emphasize that I do not claim that the above represents the best method for deriving the Gel'fand-Levitan theory. The rigorous establishment of all the results we have used is rather difficult. However, we have shown that the Gel'fand-Levitan theory now fits into the same general setting that contains "other analytic results". Thus the Gel'fand-Levitan theory which had previously sat to the side, is now integrated into the general theory.

I shall now show that if one knows $\alpha(\lambda)$ then one can determine $\rho(\lambda)$. To begin, we return to the formula immediately preceding (20) and set $x=y$. This gives the formula

$$\frac{1}{\sqrt{\pi t}}\,\mathrm{E}\{e^{-\int_0^t q(x+x(\tau))\,d\tau}\mid x(t)=0\}$$

$$-\frac{e^{-x^2 t}}{\sqrt{\pi t}}\,\mathrm{E}\{e^{-\int_0^t q(-x+x(\tau))\,d\tau}\mid x(t)=2x\} \tag{23}$$

$$=\int^{\infty} e^{-\lambda t}\phi^2(x,\lambda)\,d\rho(\lambda).$$

I have omitted the lower limit from the right-hand side for very definite reasons. Let us supose that q is not necessarily positive.

Then one can show (it is part of the standard lore of elementary quantum mechanics) that if there are solutions ϕ of equation (14) for $\lambda < 0$ that satisfy the asymptotic condition in (15), they must be square integrable. These are known as the bound states of the problem. This allows us to use a lower limit of $-\infty$ in (23) with the understanding that $\rho(\lambda)$ is piecewise constant for negative λ, with jump discontinuities. Now we integrate the above equation from 0 to A with respect to x, divide by A, and consider the behavior as $A \to \infty$. It is extraordinarily easy to see what happens for $\lambda < 0$, that is, in the case of bound states. Since ϕ is square integrable, the average of the integral of ϕ^2 will, of course, go to 0. So the contribution from the bound states disappears in the limit. On the other hand, since ϕ is asymptotically represented by the expression (15), the right-hand side of the expression (23) tends to $(1/2)\int_0^\infty e^{-\lambda t}\alpha^2(\lambda)\,d\rho(\lambda)$, the factor 1/2 representing the average of the function $\sin^2$ on $[-\infty, \infty]$. Previously we have used probabilistic results first and then moved to analytic results. Now we turn this around. On the left-hand side of formula (23), the Brownian motion inside the expectation signs represents a motion starting at x and terminating at 0. But if x is terribly large, it takes you a long while to get to the place where the potential acts. Consequently when we average on x and let $A \to \infty$, the function q plays no part whatsoever, and we can replace the first expected value by 1; the second vanishes upon averaging owing to the factor $\exp(-x^2/4t)$. We thus obtain

$$\frac{1}{2}\int_0^\infty e^{-\lambda t}\,\alpha^2(\lambda)\,d\rho(\lambda) = \frac{1}{2\sqrt{\pi t}} = \frac{1}{2}\int_0^\infty e^{-\lambda t}\,d\left(\frac{1}{\pi}\,\lambda^{1/2}\right),$$

where the last expression is just the representation of the function $1/2\sqrt{\pi t}$ as a Laplace transform. The above equation finally gives us a formula for the spectral function,

$$d\rho(\lambda) = \left(\frac{1}{\pi}\right)\left(\frac{d\lambda}{\alpha^2(\lambda)\lambda^{1/2}}\right).$$

Of course, in the above I did not give a rigorous proof, but it can be made rigorous without too much difficulty.

Finally, let me show you an elementary derivation of (17), the Marchenko representation formula.

We begin with the standard formula

$$\phi(x,\lambda) = \frac{\sin x\sqrt{\lambda}}{\sqrt{\lambda}} + \int_0^x \frac{\sin(x-u)\sqrt{\lambda}}{\sqrt{\lambda}}\,q(u)\phi(u,\lambda)\,du.$$

To make things easier, we follow the physicists' convention of setting $\lambda = k^2$. Now we simply iterate to obtain the following series:

$$\phi(x, k^2) = \frac{\sin kx}{k} + \int_0^x \frac{\sin k(x-u_1)}{k} \frac{\sin ku_1}{k} q(u_1)\, du_1$$
$$+ \int_0^x \frac{\sin k(x-u_1)}{k} q(u_1) \int_0^{u_1} \frac{\sin k(u_1-u_2)}{k} \frac{\sin ku_2}{k}$$
$$\cdot\, q(u_2)\, du_2\, du_1 + \cdots.$$

This series is marvelously convergent. We take the Fourier transform of ϕ, $\int_{-\infty}^{\infty} \phi(x, k^2) e^{i\xi k}\, dk$, and we integrate the series on the right-hand side, term by term. If we define $\epsilon_1 = x - u_1, \epsilon_2 = u_1 - u_2, \cdots$, $\epsilon_r = u_{r-1} - u_r$, $\epsilon_{r+1} = u_r$, then we see that all of the numbers ϵ_i are nonnegative over the respective ranges of integration, and the sum of these numbers adds up to x. Now I did not want to use probability, but just for the heck of it, note that the Fourier transform of these characteristic functions is just the probability density of the random variable $\epsilon_1 x_1 + \epsilon_2 x_2 + \cdots + \epsilon_r x_r + \epsilon_{r+1} x_{r+1}$ where the $x_1, x_2, \cdots, x_r$ are independent random variables uniformly distributed on the interval $[-1, 1]$. So whatever happens, they only add to at most x and therefore the probability density is zero outside the interval $[-x, x]$. Thus

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} \left(\phi(x; k^2) - \frac{\sin kx}{k} \right) e^{i\xi k}\, dk = M(x; \xi)$$

where $M(x; \xi) \equiv 0$ for $|\xi| > x$, and

$$\phi(x; k^2) = \frac{\sin kx}{k} + \int_{-x}^{x} e^{i\xi k} M(x; \xi)\, d\xi$$
$$= \frac{\sin kx}{k} + 2\int_0^x \cos \xi k\, M(x; \xi)\, d\xi$$
$$= \frac{\sin kx}{k} + 2\int_0^x M(x; \xi)\, d\left(-\frac{\sin k\xi}{k} \right)$$
$$= \frac{\sin kx}{k} + \int_0^x \frac{\sin k\xi}{\xi} \left(2\int_0^{\xi} M(x; u)\, du \right) d\xi.$$

This is the Marchenko formula: $L(x, \xi) = 2\int_0^{\xi} M(x; u)\, du$. (Use has been made of the fact that $M(x; x) = 0$.)

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THE ROCKEFELLER UNIVERSITY, NEW YORK, NEW YORK 10021