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Scattering Length and Diffusion

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An expression for an asymptotic property of the Green's function for the diffusion of a particle is obtained. It is shown that this provides (as a special case) a very simple derivation of a previous result of Kac and Luttinger relating the scattering length to a certain Wiener integral.

KEY WORDS: Diffusion; scattering length; path integrals.

1. The purpose of this paper is to obtain an expression for a certain asymptotic property of the Green's function for diffusion. Suppose we have some absorbing material localized near the origin. Let a particle start diffusing at time 0 from a point $\mathbf{r}$, and ask for the probability that at a time t later we find it in a small volume $d\mathbf{r}'$ around $\mathbf{r}'$. This probability is determined by the Green's function in question, and we denote it by $G_t(\mathbf{r}. \mathbf{r}')\, d\mathbf{r}'$. As is well known, G_t satisfies the diffusion equation

$$[\partial G_t(\mathbf{r}, \mathbf{r}')/\partial t] + [-\tfrac{1}{2}\nabla^2 + v(\mathbf{r})]G_t(\mathbf{r}, \mathbf{r}') = 0 \tag{1}$$

and the boundary condition

$$\lim_{t\to 0+} G_t(\mathbf{r}, \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}') \tag{2}$$

δ is the usual Dirac δ function and $v(\mathbf{r})\, d\mathbf{r}$ is the probability per unit time that a particle in $d\mathbf{r}$ around $\mathbf{r}$ is absorbed. (We have chosen units such that the diffusion constant is $\frac{1}{2}$.)

The Green's function may be expressed in terms of a complete orthonormal set of eigenfunctions of the Schrödinger equation with the potential

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$v(\mathbf{r})$ (units such that $\hbar = m = 1$). If $v(\mathbf{r})$ (viewed as a potential energy) possesses no quantum mechanical bound states, then (as is customary in scattering theory) we may write

$$\delta(\mathbf{r} - \mathbf{r}') = \int \frac{d\mathbf{k}}{(2\pi)^3} \psi_k(\mathbf{r})\psi_k^*(\mathbf{r}') \tag{3}$$

where $\psi_k(\mathbf{r})$ is the so-called outgoing wave solution of the Schrödinger equation with energy

$$E = k^2/2 \tag{4}$$

and the asterisk represents complex conjugation. That is, $\psi_k(\mathbf{r})$ is the solution of the Schrödinger equation that satisfies the boundary condition

$$\psi_k(\mathbf{r}) \to \exp(i\mathbf{k}\cdot\mathbf{r}) + f_k(\hat{\mathbf{r}}, \hat{\mathbf{k}})[\exp(ikr)/r], \qquad r \to \infty \tag{5}$$

The quantities $\hat{\mathbf{r}}$ and $\hat{\mathbf{k}}$ are unit vectors in the direction of $\mathbf{r}$ and $\mathbf{k}$, respectively. f_k is known as the scattering amplitude. From (3) we see that G_t is given by

$$G_t(\mathbf{r}, \mathbf{r}') = \int \frac{d\mathbf{k}}{(2\pi)^3} \psi_{\mathbf{k}}(\mathbf{r})\psi_{\mathbf{k}}^*(\mathbf{r}') \exp\left(-\frac{k^2}{2}t\right) \tag{6}$$

since it satisfies the differential equation and the boundary condition.

We shall now prove the following result. Let $G_t^{(0)}$ be the Green's function when $v(\mathbf{r}) = 0$, and let $\mathbf{x}$ and $\mathbf{x}'$ be fixed vectors. Then

$$\lim_{t\to\infty} \sqrt{t}\,(2\pi t)^{3/2}[G_t^{(0)}(\sqrt{t}\,\mathbf{x}, \sqrt{t}\,\mathbf{x}') - G_t(\sqrt{t}\,\mathbf{x}, \sqrt{t}\,\mathbf{x}')]$$
$$= a\left(\frac{1}{x} + \frac{1}{x'}\right) \exp[-\tfrac{1}{2}(x + x')^2] \tag{7}$$

(x is the magnitude of $\mathbf{x}$). The quantity a is the scattering length, defined by

$$a = -\lim_{k\to 0} f_k(\hat{\mathbf{r}}, \hat{\mathbf{k}}) \tag{8}$$

As is shown in elementary discussions of scattering theory, a is independent of the direction $\hat{\mathbf{r}}$, $\hat{\mathbf{k}}$, i.e., it is a constant characterizing the potential $v(\mathbf{r})$.

To obtain (7), we use the representation (6) and (5). For large t we may write (since f_k is zero if v is zero) for the leading term

$$\sqrt{t}\,(2\pi t)^{3/2}[G_t^{(0)}(\sqrt{t}\,\mathbf{x}, \sqrt{t}\,\mathbf{x}') - G_t(\sqrt{t}\,\mathbf{x}, \sqrt{t}\,\mathbf{x}')]$$
$$= -\frac{t^{3/2}}{(2\pi)^{3/2}} \int d\mathbf{k} \exp\left(-\frac{k^2}{2}t\right)$$
$$\times \left\{ f_k(\hat{\mathbf{x}}, \hat{\mathbf{k}}) \frac{\exp(ik\sqrt{t}\,x - i\mathbf{k}\cdot\mathbf{x}'\sqrt{t})}{x} \right.$$
$$\left. + f_k^*(\hat{\mathbf{x}}', \hat{\mathbf{k}}) \frac{\exp(-ik\sqrt{t}\,x' + i\mathbf{k}\cdot\mathbf{x}\sqrt{t})}{x'} \right\} \tag{9}$$

(It is easy to see that the term proportional to $f_k f_k^*$ gives a contribution which goes to zero as t approaches infinity.) The factor $\exp(-\frac{1}{2}k^2t)$ ensures that as $t \to \infty$ the only contribution comes from the neighborhood of $k = 0$. Thus we may use (8). This gives for the right-hand side of (9)

$$a \int \frac{d\mathbf{K}}{(2\pi)^{3/2}} \exp\left(\frac{-K^2}{2}\right) \left[\frac{1}{x} \exp(iKx - i\mathbf{K}\cdot\mathbf{x}') + \frac{1}{x'} \exp(-iKx' + i\mathbf{K}\cdot\mathbf{x})\right]$$

where we have introduced as new integration variables $\mathbf{K} \equiv \sqrt{t}\,\mathbf{k}$. The $\mathbf{K}$ integrals are now elementary and we find (7).

The result (7) can be written somewhat less precisely as follows. Reintroducing $\mathbf{r}$ and $\mathbf{r}'$, we may write, for large r, r', and t,

$$G_t(\mathbf{r}, \mathbf{r}') \sim G_t^{(0)}(\mathbf{r}, \mathbf{r}') - a\left(\frac{1}{r} + \frac{1}{r'}\right) \frac{1}{(2\pi t)^{3/2}} \exp - \frac{(r + r')^2}{2t} \equiv \tilde{G}_t \qquad (10)$$

Using the well-known fact that the unperturbed Green's function $G_t^{(0)}$ is given by

$$G_t^{(0)}(\mathbf{r}, \mathbf{r}') = \frac{1}{(2\pi t)^{3/2}} \exp - \frac{(\mathbf{r} - \mathbf{r}')^2}{2t} \qquad (11)$$

we can show by a simple direct calculation that this expression satisfies

$$[(\partial/\partial t) - \tfrac{1}{2}\nabla^2]\tilde{G}_t(\mathbf{r}, \mathbf{r}') = -2\pi a \delta(\mathbf{r}) G_t^{(0)}(\mathbf{r}, \mathbf{r}') \qquad (12)$$

We have used the standard result

$$\nabla^2(1/r) = -4\pi\delta(\mathbf{r})$$

But (12) is exactly what we would expect on the basis of Fermi's pseudopotential theory.[3] This tells us that if all lengths in the problem (in this case r, r', $\sqrt{t}$) are much greater than the range of the potential, the potential can be replaced by a δ function of strength $2\pi a$ and treated by first-order perturbation theory. With this prescription (12) is equivalent to (1).

2. We now show that our previous result[(2),4] for the scattering length as the expectation value with respect to Wiener measure of a certain functional follows at once from (7). Let us consider the quantity

$$A \equiv \lim_{t\to\infty} \int d\mathbf{r}\, d\mathbf{r}' [G_t^{(0)}(\mathbf{r}, \mathbf{r}') - G_t(\mathbf{r}, \mathbf{r}')](1/2\pi t) \qquad (13)$$

Writing $\mathbf{r} = \sqrt{t}\,\mathbf{x}$, $\mathbf{r}' = \sqrt{t}\,\mathbf{x}'$, we find that (13) becomes

$$A = \lim_{t\to\infty} \frac{1}{(2\pi)^{5/2}} \lim_{t\to\infty} \int d\mathbf{x}\, d\mathbf{x}' \times [G_t^{(0)}(\sqrt{t}\,\mathbf{x}, \sqrt{t}\,\mathbf{x}') - G_t(\sqrt{t}\,\mathbf{x}, \sqrt{t}\,\mathbf{x}')](2\pi t)^{3/2}\sqrt{t} \qquad (14)$$

[3] A nice description of this theory may be found in Ref. 1.

[4] Also see Ref. 3. The results of the present paper are somewhat more general, only requiring no bound states and not $v > 0$. They are also, however, much more heuristic.

Taking the limit under the integral sign (easily justified) and using (7), we find

$$A = \frac{a}{(2\pi)^{5/2}} \int d\mathbf{x}\, d\mathbf{x}' \left(\frac{1}{x} + \frac{1}{x'}\right) \exp - \frac{(x + x')^2}{2} \tag{15}$$

The integral on the right-hand side of (15) is elementary, and we find

$$A = a \tag{16}$$

On the other hand, using the usual relationship[4] between the Green's function of diffusion and an expectation value with respect to Wiener measure, we find at once that the right-hand side of (13) is just

$$\lim_{t\to\infty} (1/2\pi t) \int d\mathbf{r}\, E\left\{1 - \exp\left[-\int_0^t v(\mathbf{r} + \mathbf{r}(t'))\, dt'\right]\right\} = a \tag{17}$$

by (17). $E\{\}$ is the expectation value with respect to Wiener measure of all paths $\mathbf{r}(t')$ that begin at the origin. Equation (17) is our previous result.

Another very similar result may be obtained as follows. Consider

$$\begin{aligned} B &\equiv \lim_{t\to\infty} (1/2\pi t)(2\pi t)^{3/2} \int d\mathbf{r}[G_t^{(0)}(\mathbf{r}, \mathbf{r}) - G_t(\mathbf{r}, \mathbf{r})] \\ &= \lim_{t\to\infty} (1/2\pi) \int d\mathbf{x}[G_t^{(0)}(\sqrt{t}\,\mathbf{x}, \sqrt{t}\,\mathbf{x}) - G_t(\sqrt{t}\,x, \sqrt{t}\,\mathbf{x})](2\pi t)^{3/2}\sqrt{t} \\ &= (a/2\pi) \int d\mathbf{x}\, (2/x) \exp(-2x^2) = a \end{aligned} \tag{18}$$

Again, expressing the Green's functions as Wiener averages,[3] we find that (18) becomes

$$\lim_{t\to\infty} (1/2\pi t) \int d\mathbf{r}\, E\left\{1 - \exp\left[-\int_0^t v(\mathbf{r} + \mathbf{r}(t'))\, dt'\right] \middle| 0\right\} = a \tag{19}$$

where $E\{\ |0\}$ is the expectation value with respect to all paths that begin and end at the origin (conditional Wiener measure).

It is clear that many other relationships of the same general type may be obtained from (7) in a trivial way, but we shall not consider any of these here.

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