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Classical Boundary Conditions as a Technical Tool in Modern Mathematical Physics*

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We review a variety of problems in quantum physics where Dirichlet and Neumann Green's functions enter not as an element in the basic formulation of the problem but as a purely technical tool. Methodology is emphasized.

1. INTRODUCTION

Consideration of problems from electrostatics, electrodynamics, and hydrodynamics led 19th century mathematicians and physicists to study extensively the differential equation

$$(-\Delta + k^2)u = f \qquad \text{in } \Omega$$

with either of the boundary conditions

$$u = 0 \qquad \text{on } \partial\Omega \qquad \text{(Dirichlet)}$$

or

$$\partial u/\partial n = 0 \qquad \text{on } \partial\Omega \qquad \text{(Neumann).}$$

Although there are a limited number of problems of quantum physics which naturally involve finite regions with boundary conditions (hard cores), most quantum problems involve the study of $-\Delta + V$ on all of $\mathbb{R}^3$ or $\mathbb{R}^n$. It would thus appear that the Dirichlet and Neumann boundary conditions are of relevance to the mathematical physicist interested in quantum physics only so far as he felt obligated to talk about them in his courses on classical physics or classical mathematical physics. It is my goal in this paper to try to convince you that this is false, not because classical boundary conditions enter into

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the natural formulation of quantum problems but rather because they can be a useful technical device. Consider the following four problems:

A. *Large coupling constant behavior of* $N(V)$. Let $N(V)$ be the number of bound states (i.e., strictly negative eigenvalues counted up to multiplicity) of $-\Delta + V$. How does $N(\lambda V)$ behave as $\lambda \to \infty$?

B. *Validity of Thomas–Fermi theory.* In what sense is the Thomas–Fermi statistical theory of atoms [11, 33, 13, 22] an approximation to the quantum theory of atoms? In particular, is it asymptotically valid to some regime?

C. *Scattering from singular potentials.* Consider a very singular potential, which for simplicity we suppose has compact support and is positive. We have in mind an example where a single point or a few points are singular so that V is at least bounded away from arbitrarily small balls about each singular points. One would expect on physical grounds that a good scattering theory exists for such systems including both existence and completeness of wave operators. How can one handle the singularities which prevent the use of the "standard" methods [17, 27]?

D. *Weak coupling* $P(\phi)_2$. Since this problem which is taken from constructive quantum field theory is quite technical, I will be somewhat vague in both its formulation and solution. I will state it in terms of "Euclidean field theory" and ask the reader either to accept the fact that there is a connection with quantum field theory, or to go read about it in [24], [30] or [34]. Given a real inner product space, V, the *Gaussian process indexed* by V is a collection of random variables (i.e., measurable functions on a probability measure space), $\phi(v)$, one for each $v \in V$ so that $v \to \phi(v)$ is linear and so that each $\phi(v)$ has a Gaussian distribution with $\text{Exp}(\phi(v)\,\phi(w)) = \langle v, w\rangle$. In the usual sense of isomorphism in probability systems this Gaussian process is uniquely determined. The *free Euclidean field* in n-dimensions is the Gaussian process indexed by $\mathscr{S}(\mathbb{R}^n)$ with inner product

$$(f, g) = \langle f, (-\Delta + 1)^{-1} g\rangle_{L^2}$$

(where we have set an input parameter, the "bare mass," to 1 for convenience). In a natural way, one writes $\phi(f) = \int f(x)\,\phi(x)\,d^n x$, where $\phi(x)$ is a "random distribution." While $\phi(x)^m$ does not make sense (except when $n = 1$), for $n = 2$, there is a natural "renormalized product" $:\phi(x)^m:$ and moreover, if P is a real polynomial which is bounded from below on $\mathbb{R}$, then for any bounded set Λ, one can show that for any $\lambda > 0$, $\exp(-\lambda \int_{x\in\Lambda} :P(\phi(x)):\, d^2)x \equiv \exp(-\lambda U(\Lambda))$ is integrable with respect to the measure $d\mu_0$ defined by the free field Gaussian process. The basic problem is to control

$$\lim_{\Lambda\to\infty} \left[\exp(-\lambda U(\Lambda)\, d\mu_0 / \int \exp(-\lambda U(\Lambda))\, d\mu_0\right]$$

as a measure on some convenient space. (For the expert in quantum field theory, we note that this infinite volume problem is overcome on a perturbative level by the cancellation of disconnected diagrams. It is not so easy on the nonperturbative level.) Once this is controlled in a suitable sense one expects (and indeed one has found!) models of quantum field theories in two space–time dimensions with nontrivial scattering. Since the above is reminiscent of statistical mechanics, it is reasonable to look for analogs of convergent high temperature expansions. The natural expansion in λ is not a suitable expansion, since it is divergent. Can one find a convergent expansion in a suitable regime and thereby control the limit?

These four problems seem to be very different, and indeed, except for the fact that, as we shall see, the solutions of A are quasiclassical and B is by nature quasiclassical, they are very different. But the solutions I shall sketch or hint at (due to Martin [23], Lieb and Simon [20], Deift and Simon [9], and Glimm *et al.* [12], respectively), all depend critically on the use of the classical boundary conditions.

Next, let me give a precise description of the operator solution of the D and N problems which will be useful below. We use the following basic fact about using quadratic forms to define unbounded operators (see [10, 17, 25] for more details): A *closed, positive, quadratic form*, a, on a Hilbert space, $\mathscr{H}$, is a sesquilinear form $a(\circ, \circ)$ on a dense subspace $\mathbb{Q}(a)$ so that: (i) $a(\phi, \phi) \geqslant 0$ for all $\phi \in \mathbb{Q}(a)$, and (ii) $\mathbb{Q}(a)$ with the inner product $(\psi, \phi)_a = a(\psi, \phi) + (\psi, \phi)$ is a Hilbert space. The fundamental fact is that given any such form there is a unique self-adjoint operator, A with $D(|A|^{1/2}) = \mathbb{Q}(a)$, and $a(\phi, \psi) = (|A|^{1/2}\phi, |A|^{1/2}\psi)$.

Given any open subspace, Ω, in $\mathbb{R}^n$ we define two operators $-\Delta_\Omega^{\mathrm{D}}$ and $-\Delta_\Omega^{\mathrm{N}}$ on $L^2(\Omega)$ as follows. Let

$$H^1(\Omega) = \{f \in L^2(\Omega) \mid \text{the distributional gradient gradient } Df \text{ is in } L^2\},$$
$$H_0^1(\Omega) = \text{Closure of } C_0^\infty(\Omega) \text{ in } H^1(\Omega).$$

Both H^1 and H_0^1 are dense in $L^2(\Omega)$, and the inner product $f, g \to \langle Df, Dg\rangle_{L^2}$ on both defines closed, positive quadratic forms. The associated operators are denoted $-\Delta_\Omega^{\mathrm{D}}$ and $-\Delta_\Omega^{\mathrm{N}}$. They solve the classical boundary value problems in the following sense: If Ω is nice enough (say a cube or a bounded region with smooth boundary) and f is nice enough (say C^∞ in a neighborhood of Ω) then $u = (-\Delta_\Omega^{\mathrm{D}} + k^2)^{-1}f$ (resp. $(-\Delta_\Omega^{\mathrm{N}} + k^2)^{-1}f$) for $k > 0$ ($k \geqslant 0$ if Ω is bounded in the D case) solves $(-\Delta + k^2)u = f$ with $u \restriction \Omega = 0$ (resp. $\partial u/\partial n \restriction \Omega = 0$). For further discussion of the operator description of the classical boundary value problems see [8, 21, 27].

A final remark about the "ancient history" of the methods we describe. Like so much in the arsenal of the mathematical physicist. the methods in Sections 2 and 3 go back to Hermann Weyl, who invented them in his study

[25] of the problem which Mark Kac has labeled "Can you hear the shape of a drum?" [16]. (See also Courant and Hilbert [5].) Their earliest use in quantum mechanical problems seems to be by Lieb [36] and Robinson [37], whose work served as motivation for some of those who solved the problems discussed here.

2. Decoupling

Let Ω_1 and Ω_2 be disjoint open sets, and let $\Omega = \Omega_1 \cup \Omega_2$. Then clearly there are natural isomorphisms:

$$L^2(\Omega) \cong L^2(\Omega_1) \oplus L^2(\Omega_2),$$
$$H^1(\Omega) \cong H^1(\Omega_1) \oplus H^1(\Omega_2),$$
$$H_0^{\,1}(\Omega) \cong H_0^{\,1}(\Omega_1) \oplus H_0^{\,1}(\Omega_2).$$

Because of the uniqueness of the association of operators and forms, we have that under this isomorphism

$$-\Delta_\Omega{}^Y = -\Delta_{\Omega_1}^Y \oplus -\Delta_{\Omega_2}^Y \tag{1}$$

for $Y = \mathrm{D}, \mathrm{N}$. Equation (1) describes the fact that "a Dirichlet or Neumann boundary decouples" for the usual setup is one where Ω_1 and Ω_2 are the sets obtained by starting with a connected open set Ω_3 and removing a closed set of measure zero. For example, let $\mathscr{B}$ be the set of line segments between nearest neighbor in the lattice $\mathbb{Z}^2$ in $\mathbb{R}^2$. Let $\Omega_{\mathscr{B}} = \mathbb{R}^2 \backslash \bigcup_{B \in \mathscr{B}} B$ and let $-\Delta^{\mathscr{B}}$ be the associated Dirichlet Laplacian. Let, on $L^2(\mathbb{R}^2) = L^2(\Omega_{\mathscr{B}})$,

$$-\Delta^{\mathscr{B}} = \bigoplus_\alpha -\Delta_\alpha, \tag{2}$$

where $-\Delta_\alpha$ is the Dirichlet Laplacian in a square K_α. Let $d\mu_{\mathscr{B}}$ be the measure associated to the Gaussian process indexed by $\mathscr{S}(\mathbb{R}^2)$ with covariance $(-\Delta^{\mathscr{B}} + 1)^{-1}$. Then for $f_1, ..., f_k \in C_0^{\infty}$, the limit

$$\lim_{\Lambda\to\infty} \int \pi\phi(f_i)\, e^{-U(\Lambda)}\, d\mu \Big/ \int e^{-U(\Lambda)}\, d\mu_{\mathscr{B}} \Big] \tag{3}$$

trivially exists. For, by (2), $d\mu_{\mathscr{B}}$ is a product measure, a product of measures for each K_α, so the quantity in (3) is independent of Λ once ${}_n\bigcup \operatorname{supp} f \subset$ some union of K_α's $\subset \Lambda$. The idea that Glimm *et al.* [12] use to solve Problem D is to expand $\int \pi\phi(f_i)\, e^{-U(\Lambda)}\, d\mu_0 / \int \cdots d\mu_0$ in a series in which (3) is the first term. The other terms of the series all involve $d\mu_{\mathscr{B}\backslash\Gamma}$ defined in the obvious way where Γ is a *finite* subset of $\mathscr{B}$. For each term the $\Lambda \to \infty$ is trivial by decoupling analogous to (2). The hard part is now to obtain estimates on the series proving convergence of their series uniform in Λ. Except for one aspect of these estimates, to which we return in Section 4, we will not describe these rather technical estimates.

3. Bracketing

To describe the next technical device in the D–N arsenal, we begin with a definition.

Definition. Let a, b be quadratic forms which are bounded from below (i.e., $a + c1$ is positive for some c). We say that $a \leqslant b$ if and only if (i) $Q(a) \supset Q(b)$, and (ii) $a(\phi, \phi) \leqslant b(\phi, \phi)$ for all $\phi \in Q(b)$.

There is a simple intuition which allows one to understand the domain condition, (i). Namely, one should think of defining $a(\phi, \phi) = \infty$ for all $\phi \notin Q(a)$. Then (ii) for all ϕ extended to include $\phi \notin Q(b)$ expresses (i).

The basic fact about ordering of the quadratic forms associated with D and N boundary conditions is the following: Let Ω be an open set and let $\{\Omega_i\}_{i=1}^{N}$ (N may be infinite) be a family of disjoint open subsets of Ω so that $\Omega \backslash \bigcup \Omega_i$ has measure zero. (Think of obtaining the Ω_i from Ω by removing some surfaces.) Let $\Omega' = \bigcup \Omega_i$. Then $L^2(\Omega')$ and $L^2(\Omega)$ are naturally isomorphic. The point is that

$$-\Delta_{\Omega}{}^{\mathrm{D}} \leqslant -\Delta_{\Omega'}^{\mathrm{D}}, \tag{4}$$

$$-\Delta_{\Omega'}^{\mathrm{N}} \leqslant -\Delta_{\Omega}{}^{\mathrm{N}}, \tag{5}$$

and, in particular, if $\Omega = \mathbb{R}^n$,

$$-\Delta_{\Omega'}^{\mathrm{N}} \leqslant -\Delta \leqslant -\Delta_{\Omega'}^{\mathrm{D}}. \tag{6}$$

The name "Dirichlet–Neumann bracketing" that I like to use for this circle of ideas comes from (6). To check (4) and (5), we need only note that $H^1(\Omega) \subset H^1(\Omega')$ (at first sight, one might think equality occurs, but consider a function discontinuous across the boundary $\Omega \backslash \Omega'$) and that $H_0{}^1(\Omega') \subset H_0{}^1(\Omega)$ since $C_0{}^\infty(\Omega') \subset C_0{}^\infty(\Omega)$ (functions in $C_0{}^\infty(\Omega')$ must vanish near $\Omega \backslash \Omega'$ so this inclusion is also usually strict). Since the forms are all equal *where finite* (4) and (5) result.

The usefulness of the bracketing inequalities comes from the fact that they imply inequalities on eigenvalues. For let

$$\mu_n(a) = \max_{\phi_1, \ldots, \phi_{n-1}} \left[\min_{\psi \in Q(a) \cap [\phi_1, \ldots, \phi_{n-1}]^\perp} a(\phi, \phi) \right].$$

Clearly, if $a \leqslant b$, then $\mu_n(a) \leqslant \mu_n(b)$. The point is that if the operator, A, associated to a has n or more eigenvalues at the bottom of its spectrum, then $\mu_n(a)$ is the nth eigenvalue, and, if it does not, then $\mu_n(A)$ is the bottom of the continuous spectrum. (See, e.g., [27] for this version of the Weyl min–max principle.) To demonstrate the way to use the tools described, let us give Martin's solution of Problem A:

THEOREM 1. *Let V be in $C_0^\infty(\mathbb{R}^n)$. Then*

$$\lim_{\lambda\to\infty} N(\lambda V)/\lambda^{n/2} = \frac{\tau_n}{(2\pi)^n}\int (V_-(x))^{n/2}\, d^n x,$$

where V_- is the negative part of V, and τ_n is the volume of the unit ball in $\mathbb{R}^n$.

Remarks. 1. By different methods Titchmarsh [38], Birman and Borzov [1], and Tamura [32] have proved this result. Using a simple approximation argument [2, 31] and the recently proved bound $N(V) \leqslant c_n \| V \|_{n/2}^{n/2}$; $n \geqslant 3$ obtained independently by Cwiekel [6], Lieb [19], and Rosenbljum [28], one can extend this result from $C_0^\infty(\mathbb{R}^n)$ to $L^{n/2}(\mathbb{R}^n)$ if $n \geqslant 3$.

2. The beautiful aspect of this result is its interpretation as a quasi-classical limit. For $\tau_n \int (V_-(x))^{n/2}\, d^n x$ is the volume of phase space where $p^2 + V(x) \leqslant 0$. The factor of $(2\pi)^{-n}\lambda^{n/2}$ is effectively h^{-n} since $-\Delta + \lambda V = \lambda(-\lambda^{-1}\Delta + V)$ means that $N(\lambda V)$ is the number of bound states in a system with $\hbar = \lambda^{-1/2}$ i.e. $h = 2\pi\hbar = 2\pi\lambda^{-1/2}$.

Proof. Fix $a > 0$ and consider the decomposition of $\mathbb{R}^n$ into "standard" a-cubes (i.e., cubes of volume a^n with points $\mathbf{n}a$, $\mathbf{n} \in \mathbb{Z}^n$ at their centers). Let $V_a^\pm$ be the functions obtained by replacing V by its $\substack{\max\\ \min}$ in each cube so that $V_a^- \leqslant V \leqslant V_a^+$. Let $-\Delta_a^\pm$ be the Laplacian with $\substack{D\\ N}$ boundary conditions. By (6),

$$-\Delta_a^- + \lambda V_a^- \leqslant -\Delta + \lambda V \leqslant -\Delta + \lambda V_a^+$$

so that

$$n(-\Delta_a^- + \lambda V_a^-) \leqslant N(\lambda V) \leqslant n(-\Delta_a^+ + \lambda V_a^+),$$

where $n(a) \equiv \#$ of negative eigenvalues of A, the operator associated to a. Let $v_a^\pm(\alpha)$ be the value of $V_a^\pm$ in the cube K_α. Then, by decoupling

$$\begin{aligned} n(-\Delta_a^- + \lambda V_a^-) &= \sum_{\{\alpha \mid v_a(\alpha)<0\}} n(-\Delta_\alpha^{\mathrm{N}} + \lambda v_a^-(\alpha)) \\ &\sim \frac{\lambda^{n/2}\tau_n}{(2\pi)^n} \sum_{\{\alpha\mid v_a^-(a)<0\}} a^n (v_\alpha^-(\alpha))]^{n/2} \\ &= \frac{\lambda^{n/2}\tau_n}{(2\pi)^n}\int_{(V_a^-(x)<0)} | V_a^-(x)|^{n/2}\, d^n x, \end{aligned}$$

where we have used the result of an "exact" calculation of the number of eigenvalues that $-\Delta_\alpha^N$ has below $-\lambda v_a^-(\alpha)$ for λ large—this calculation is counting the number of lattice points inside a large sphere. This shows that

$$\underline{\lim}\, N(\lambda V)/\lambda^{n/2} \geqslant \frac{c^n}{(2\pi)^n} \int_{(V_a^-(x)<0)} | V_a^-(x)|^{n/2}\, d^n x,$$

so taking $a \to 0$ we obtain

$$\underline{\lim}\, N(\lambda V)/\lambda^{n/2} \geqslant \frac{\tau^n}{(2\pi)^n} \int (V_-(x))^{n/2}\, d^n x.$$

A similar calculation with $+$ superscripts completes the proof. ∎

Since the Thomas–Fermi theory is a quasiclassical theory also, it is not too surprising that ideas, similar to the above, with additional technical complications lead to the following result of Lieb and Simon [20] which solves Problem B.

THEOREM 2. *Fix h and the mass, m, of the electron. Let E_Q^Z denote the ground state energy of a Z electron quantum mechanical atom about an infinitely heavy nucleus of charge Z with Coulomb form (and the Pauli principle). Let E_{TF}^Z be the corresponding Thomas–Fermi energy. (It is known that $E_{\mathrm{TF}}^Z = Z^{7/3} E_{\mathrm{TF}}^1$.) Then*

$$\lim_{Z\to\infty} (E_Q^Z / E_{\mathrm{TF}}^Z) = 1.$$

For results on the density, on molecules, etc., and for the detailed proof, see [20].

4. CONNECTION WITH WIENER PATH INTEGRALS

A final useful technique in exploiting Dirichlet boundary conditions is its connection with Wiener path integrals. I want to describe briefly the method and illustrate them by giving a proof of the technical estimates of Deift and Simon used in their solution of problem C and in sketching the idea behind one of the detailed estimates of Glimm *et al.*

We begin with a brief description of Weiner integrals. See also [3, 14, 15, 26]. In Section 1, we described Gaussian processes. The one-dimensional Wiener process consists of jointly Gaussian random variables $q(t)$, one for each $t \geqslant 0$ with

$$\mathrm{Exp}(q(t)\, q(s)) = \min(t, s),$$

[that is, we form a vector space of finite sums of the form $\sum_{i=1}^n a_i \delta_{t_i}$ with $(\sum_{i=1}^n a_i \delta_{t_i}, \sum_{j=1}^m b_j \delta_{s_j}) = \sum_{i,j} \bar{a}_i b_j \min(t_i, s_j)$, and set $q(t) = \phi(\delta_t)$]. The n-

dimensional process $\mathbf{q}(t)$ ($\mathbf{q}$ an n-tuple of random variables) consists of n independent copies of the one-dimensional process. The reader can check that

$$\text{Prob}(\mathbf{q}(t) = \mathbf{a}) = (2\pi t)^{-n/2} \exp(-|\,\mathbf{a}\,|^2/4t),$$

which links the Weiner integral to the integral kernel of the operator $e^{t\Delta}$ which is $(2\pi t)^{-n/2} \exp(-|\,x - y\,|^2/4t)$.

Now, one can introduce a concrete version of the space on which the q's live so that the $\mathbf{q}(t)$ are all continuous functions (since this involves fixing an uncountable number of functions everywhere, it involves a choice), that is, one can find a probability measure $d\mu_0$ on the continuous paths ω with $\omega(0) = 0$ so that the $\omega(t)$ have the distribution of the abstract Weiner process.

It is useful to introduce families of additional measures as follows: $d\mu$ is a measure on all paths obtained by writing ω as a pair $(\omega(0), \omega - \omega(0))$ and putting Lebesque measure on the first factor and $d\mu_0$ on the second factor. Thus

$$e^{t\Delta}(x, y) = \mu\{\omega \mid \omega(0) = x,\, \omega(t) = y\},$$

and a measure $d\mu_{\mathbf{x},\mathbf{y},t}$ of these paths with $\omega(0) = \mathbf{x}$, $\omega(t) = \mathbf{y}$ of total mass $(2\pi t)^{-n/2} \exp(-|\,x - y\,|^2/4t)$ defined essentially by the condition that

$$\mu_{\mathbf{x},\mathbf{y},t}(\omega \mid \omega(t_1) = z_1, \ldots, \omega(t_{n-1}) = z_{n-1}\} = \mu\{\omega \mid \omega(t_i) = z_i\,,\, i = 0, \ldots, n\},$$

where $t_0 = 0$. $t_n = t$, $z_0 = x$, and $z_n = y$.

One value of the Weiner measure is that one has the Feynman–Kac formula,

$$e^{-t(-\Delta+V)}(x, y) = \int \exp\left(-\int_0^t V(\omega(s))\,ds\right) d\mu_{x,y,t}(\omega).$$

The connection of all this with Dirichlet boundary conditions is that

Theorem 3. *For any arbitrary open set* Ω,

$$[\exp(t\Delta_\Omega{}^{\mathrm{D}})](x, y) = \mu_{x,y,t}\{\omega \mid \omega(s) \in \Omega,\ \textit{all}\ 0 \leqslant s \leqslant t\}.$$

We give a proof of this result in the Appendix. So far as I know, this is the first proof (however, see [39]) of this fact for arbitrary open sets, although the result is well known for sufficiently nice sets [3]. (We should remark that to the probabilist, Theorem 3 is essentially a *definition* of $-\Delta_\Omega{}^{\mathrm{D}}$; from this point of view we prove the equality of the probabilist's definition and the analyst's definition in Section 1.)

To describe the solution of Problem C, we must recall some scattering theory. Given a self-adjoint operator, A, $P_{\mathrm{ac}}(A)$ denotes the projection onto the absolutely continuous subspace for A. Given another self-adjoint operator,

B, one says that the wave operators $\Omega^{\pm}(A, B)$ *exist* if and only if $s\text{-lim}_{t\to\mp\infty} e^{itA}e^{-itB}P_{ac}(B) \equiv \Omega^{\pm}(A, B)$ exist and that they are complete if and only if $\operatorname{Ran}\Omega^{\pm}(A, B) = P_{ac}(A)$. The following is a standard result in scattering theory (see, e.g., [17] or [27]):

THEOREM 4. *Let A and B be self-adjoint operators. Let F be a strictly monotone decreasing C^2 function on $\mathbb{R}$. If $F(A) - F(B)$ is trace class, then $\Omega^{\pm}(A, B)$ exists and is complete.*

Remark. Because the hypothesis is symmetric in A and B, it suffices to prove existence since existence of both $\Omega^{\pm}(A, B)$ and $\Omega^{\pm}(B, A)$ implies completeness.

We can now give the Deift–Simon [9] solution of Problem C:

THEOREM 5. *Let V be a positive function of compact support which is L^1 on compact subsets avoiding G, a closed set of measure zero. Let $H = -\Delta + V$ as a sum of quadratic forms. Let $H_0 = -\Delta$. Then $\Omega^{\pm}(H, H_0)$ exists and is complete.*

Remarks. 1. One is not limited to either compact support or positive potentials; see [9].

2. The argument we give is somewhat simpler from a technical point of view then that in [9].

Proof. We will show that $e^{-H} - e^{-H_0}$ is trace class. Let S be a large sphere containing the support of V. Let H_0' (resp. H') be the Laplacian with Dirichlet boundary conditions on S. We will show that the three operators $e^{-H'} - e^{-H_0'}$, $e^{-H} - e^{-H'}$, $e^{-H_0} - e^{-H_0'}$ are all trace class. The first is easily seen to be trace class by using decoupling. For letting B be the inside of the sphere and E the outside,

$$e^{-H'} - e^{-H_i'} = (e^{-H'} - e^{-H_0'}) L^2(B) \oplus 0$$

on $L^2(\mathbb{R}^n) = L^2(B) \oplus L^2(E)$. But on $L^2(B)$, $e^{-H_0'}$ is trace class by a direct calculation, and $e^{-H'}$ is trace class since $H' \geqslant H_0'$.

As for the second and third operator, it suffices to show that the six operators, $e^{-A/2}(1 + x^2)^{-n}$ for ($A = H, H', H_0, H_0'$) and $e^{-A/2} - e^{-A'/2}(1 + x^2)^n$ for $A = H, H_0$), are Hilbert–Schmidt. For example,

$$\begin{aligned} e^{-H} - e^{-H'} &= [e^{-H/2}(1 + x^2)^{-n}][1 + x^2)^n(e^{-H/2} - e^{-H'/2})] \\ &\quad + [(e^{-H/2} - e^{-H'/2})(1 + x^2)^n][(1 + x^2)^{-n} e^{-H'/2}]. \end{aligned}$$

Now, if A and B are operators with integral kernels a and b so that $0 \leqslant a(x, y) \leqslant b(x, y)$ and B is Hilbert–Schmidt, then A is Hilbert–Schmidt. Of the four operators $e^{-H_0}(1 + x^2)^{-n}$, the one with the largest kernel is

$e^{-H_0}(1 + x^2)^{-n}$, and of the two operators $(e^{-A/2} - e^{-A'/2})(1 + x^2)^n$, the one with $A = H_0$ has the largest kernel, and all kernels are positive. These assertions all follow from the Weiner integral formulation discussed above. For example

$$(e^{-H/2} - e^{-H'/2})(x, y) = \int_{\omega \text{ crossing } S} \exp\left(-\int_0^{1/2} V(\omega(s))\, ds\right) d\mu_{x,y,\frac{1}{2}}$$

$$\leqslant \int_{\omega \text{ crossing } S} d\mu_{x,y,\frac{1}{2}} = (e^{-H_0/2} - e^{-H_0'/2})(x, y).$$

We have therefore reduced the proof to showing that $e^{-H_0/2}(1 + x^2)^{-n} \equiv R_1$ and $(e^{-H_0/2} - e^{-H_0'/2})(1 + x^2)^{+n} \equiv R_2$ are Hilbert–Schmidt. Now the integral kernel of R_1 is

$$\pi^{-1/2} \exp(-| x - y |^2/2)(1 + y^2)^{-n}$$

is easily seen to be square integrable by a change of variables. To prove that R_2 is Hilbert–Schmidt, it certainly suffices to prove that

$$(e^{-H_0/2} - e^{-H_0'/2})(x, y) \leqslant Ce^{-ax^2} \tag{7}$$

(for then by symmetry, it is less than $Ce^{-a(x^2+y^2)/2}$). Equation (7) follows from the following for all $x \in E$:

$$(e^{-H_0/2} - e^{-H_0'/2})(x, y) \leqslant e^{-H_0/2}(x, \tilde{x}), \tag{8}$$

where $\tilde{x}$ is the point on S closest to x. To prove (8), let P be the plane tangent to S through $\tilde{x}$. There are two cases to consider. If y lies on the other side of P from x, then $| x - y | \geqslant | x - \tilde{x} |$ so

$$(e^{-H_0/2} - e^{-H_0'/2})(x, y) \leqslant e^{-H_0/2}(x, y) \leqslant e^{-H_0/2}(x, \tilde{x}).$$

If y is on the same side of P as x, let y' be the image of y under reflection in P, and let H_1 be the Laplacian with Dirichlet boundary conditions on P. Then, on the one hand

$$e^{-H_1/2}(x, y) = e^{-H_0/2}(x, y) - e^{-H_0/2}(x, y')$$

by the method of images, while on the other hand

$$(e^{-H_0/2} - e^{-H_0'/2})(x, y) = \int_{x,y,\frac{1}{2}} \{\omega \mid \omega(s) \text{ crosses } S\}$$

$$\leqslant \mu_{x,y,\frac{1}{2}}\{\omega \mid \omega(s) \text{ crosses } P\}$$

$$= (e^{-H_0/2} - e^{-H_1/2})(x, y),$$

since a path cannot go from x to y and cross S without crossing P. Thus $e^{-H_0/2}(x, y) - e^{-H'/2}(x, y) \leqslant e^{-H_0/2}(x, y) \leqslant e^{-H_0/2}(x, \tilde{x})$. ∎

Remark. One can also prove (8) using potential theory (maximum principle) ideas. Both maximum principle and image methods are useful in the study of Dirichlet B.C.

We conclude by describing one of the Glimm–Jaffe–Spencer [12] estimates. Following the notation in Section 2, let Γ be a subset of $\mathscr{B}$ and let $-\Delta^\Gamma$ be the Laplacian with Dirichlet boundary conditions on ${}_{\mathscr{B}\backslash\Gamma}\bigcup B$. Let $C^\Gamma = (-\Delta^\Gamma + 1)^{-1}$. The higher-order terms in the Glimm–Jaffe–Spencer series involve multiple differences of the form

$$\sum_{\Gamma \subset S \subset \tilde{\Gamma}} (-1)^{|\tilde{\Gamma}/S|} C^S(x, y) \equiv (\delta_{\tilde{\Gamma},\Gamma} C)(x, y),$$

where $\tilde{\Gamma}\backslash\Gamma$ is finite and $|\tilde{\Gamma}\backslash S| \equiv \#$ of elements of $\tilde{\Gamma}\backslash S$. One needs to prove that $\delta_{\tilde{\Gamma},\Gamma}C$ gets small as $x - y$ goes to infinity and also if $\tilde{\Gamma}\backslash\Gamma$ has prices far from x or y or each other. Now $C = \int e^{-t} B_t$, where $B_t^\Gamma = \exp(t\Delta^\Gamma)$. Moreover, each difference in $\delta_{\tilde{\Gamma},\Gamma}$ forces the paths to cross a segment in $\tilde{\Gamma}\backslash\Gamma$, i.e.,

$$\delta_{\tilde{\Gamma},\Gamma} B_t = \mu_{x,y,t}(\omega \mid \omega \text{ crosses each segment in } \tilde{\Gamma}\backslash\Gamma).$$

In this way, Glimm, Jaffe, and Spencer are able to estimate $\delta_{\tilde{\Gamma},\Gamma}C$. An alternate method to these estimates using potential theory in place of path integrals has been found by Cooper and Rosen [4].

APPENDIX: Identifying Dirichlet Boundary Conditions and Wiener Exclusion

In this section, we give a proof of Theorem 3, based, in part, on ideas of Klauder [18]; see also [7, 29]. Since this Appendix is intended for experts, we freely use various results about quadratic forms and about Wiener measure.

Choose bounded open sets $\Omega_1, \ldots$ in Ω so that $\bar{\Omega}_i \subset \Omega_{i+1}$ and $\bigcup_i \Omega_i = \Omega$. Choose $f_i \in C_0^\infty$ so that $f_i \restriction \Omega_i = 1$, $\operatorname{supp} f_i \subset \Omega_{i+1}$, and $0 \leqslant f_i \leqslant 1$. Define a function V on Ω by

$$V(x) = \sum_i |\operatorname{grad} f_i(x)|^2 + [\operatorname{dist}(x, \partial\Omega]^{-3}.$$

On $L^2(\Omega)$, define the operator $H(\lambda)$ for $\lambda > 0$ as that associated to the quadratic form on $H^1(\mathbb{R}^3) \cap L^2(\Omega) \cap Q(V) \equiv M$, with $(\phi, H(\lambda)\phi) = (\nabla\phi, \nabla\phi) + \lambda(\phi, V\phi)$. We first claim that M is contained and dense in $H_0^1(\Omega)$. For $\phi \in M$ implies that $\nabla\phi \in L^2$. Let $\phi_i = f_i\phi$. Then clearly $\phi_i \to \phi$ in L^2. Moreover, since $(\phi, V\phi) < \infty$, $(\operatorname{grad} f_i)\phi \to 0$ in L^2 so

$$\operatorname{grad} \phi_i = \operatorname{grad} \phi + (\operatorname{grad} f_i)\phi \to \operatorname{grad} \phi.$$

Thus $\phi_i \to \phi$ in $H^1(\Omega)$. Since the ϕ_i's can easily be approximated by $C_0^\infty(\Omega)$ functions, ϕ is in $H_0^1(\Omega)$. Density is obvious since $C_0^\infty(\Omega) \subset M$. It thus follows by general principles [7, 29] that $H(\lambda) \to -\Delta_\Omega^{\rm D}$ in strongly resolvent sense so that [25], $e^{-tH(\lambda)} \to \exp(-t\Delta_\Omega^{\rm D})$ strongly for any $t > 0$. Now let V_n be defined on $\mathbb{R}$ by

$$\begin{aligned} V_n(x) &= V(x) \qquad \text{if} \quad x \in \Omega, \text{ and } V(x) \leqslant n \\ &= n \qquad \text{if} \quad x \notin \Omega \text{ or } V(n) \geqslant n. \end{aligned}$$

Then by a small extension of the monotone convergence theorem for forms [10, 17] (the extension involves the fact that $H(\lambda)$ is not densely defined),

$$\begin{aligned} (-\Delta + \lambda V_n + E)^{-1}\phi &\to (H(\lambda) + E)^{-1}\phi \qquad \text{if} \quad \phi \in L^2(\Omega), \\ &\to 0 \qquad \text{if} \quad \phi \notin L^2(\Omega). \end{aligned}$$

From this result and the Feynman–Kac formula for $(-\Delta + \lambda V_n)$ we conclude that

$$e^{-tH(\lambda)}(x, y) = \int_{\{\omega \mid \omega(s) \in \bar{\Omega},\ \text{a.e. } s\}} \exp\left(-\lambda \int_0^t V(x(\Omega)\, ds\right) d\mu_{x,y,t}(\omega).$$

Now using the fact that V has a $\operatorname{dist}(x, \partial\Omega)^{-3}$ singularity and that a.e. ω is Hölder continuous of order $\frac{1}{2} - \epsilon$, we see that $\int_0^t | V(w(s))| \, ds$ is infinite for a.e. ω with $\omega(s) \in \partial\Omega$ for some s. Thus we can conclude that

$$e^{-tH(\lambda)}(x, y) = \int_{\{\omega \mid \omega(s) \in \Omega,\ \text{all } s\}} \exp\left(-\lambda \int_0^t V(\omega(s))\, ds\right) d\mu_{x,y,t}(\omega).$$

Taking $\lambda \downarrow 0$ and using the fact that $\int_0^t V(\omega(s)) < \infty$ for any continuous path staying strictly with Ω, we complete the proof. ∎

Note added in proof. The methods of this lecture have been applied in a very interesting way in J. Combes, R. Schrader and R. Seiler, *Ann. Phys.* **111** (1978), 1–18.

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