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Statistical properties of many particle eigenfunctions

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Abstract
Wavefunction correlations and density matrices for few or many particles are derived from the properties of semiclassical energy Green functions. Universal features of fixed energy (microcanonical) random wavefunction correlation functions appear which reflect the emergence of the canonical ensemble as $N \to \infty$. This arises through a little known asymptotic limit of Bessel functions. Constraints due to symmetries, boundaries and collisions between particles can be included.

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1. Introduction

The standard tools of quantum chaos investigations include random matrix theory and periodic orbit theory (Gutzwiller trace formula), the Van Vleck–Morette–Gutzwiller propagator and many techniques and phenomena derived from these approaches. Standing somewhat to the side as an inspired insight is Berry's conjecture, which loosely stated is the idea that as $\hbar \to 0$ eigenstates will be indistinguishable from superpositions of infinitely many (local) plane waves with random amplitude, direction and phase, but with a fixed wavelength appropriate to the local kinetic energy. In two dimensions, these assumptions result in strictly Gaussian statistics of the eigenfunctions and the autocorrelation function $\langle \psi^*(\vec{x})\psi(\vec{x}+\vec{R})\rangle = J_0(ka)$, where k is the local wave number and $|\vec{R}| = a$. An equivalent result exists for systems with disorder [1] cementing the connection between Berry's conjecture and disordered systems.

The Berry random plane wave (RPW) [2] hypothesis is free of any specific dynamical information, except the fixed total energy, which defines the 'ensemble' (i.e. microcanonical). The perspective developed here suggests that by extending the RPW hypothesis we can conveniently accommodate many other constraints, incorporating information about real systems. In fact this program has already begun, with Berry's inclusion of the presence of nearby hard walls [3], and Bies and Heller's soft boundary results [4], and multiple hard

walls [5]. Related work by Urbina and Richter [6] and one of us [7] may also be viewed in this light.

The idea of random waves subject to constraints is not confined to one particle in two dimensions. Indeed, Berry gave the N-dimensional formula for free particles in his 1977 paper [8]. Since the underlying idea in the RPW hypothesis is uniform randomness within a quantum context, i.e. the underpinning of quantum statistical mechanics, we must encounter some familiar territory as the RPW hypothesis is extended to the large-N limit. In 1994, Srednicki had suggested that the Berry random wave hypothesis was indeed a foundation for quantum statistical mechanics [9], and showed that the appropriate canonical ensemble was reached for large N, depending on particle statistics. The present paper shows more specifically what happens as the number of particles increases, through a nonstandard and apparently unpublished asymptotic form for Bessel functions (we have not been able to find it in the literature, although it 'ought' to be there), which encodes the equivalence of the canonical and microcanonical ensembles of statistical mechanics. In making the connections to quantum statistical mechanics one also needs procedures for incorporating constraints, which are an essential aspect of the theory. Thus, our procedures for generalizing the RPW to include constraints, mentioned above, are an essential new feature, since the constrained eigenstates are no longer random in Berry's (and Srednicki's) original sense.

Given a continuum at energy E, such as in an enclosure with walls very far away, we can perform the average over all random waves as a trace, i.e.

$$\langle \psi^*(\vec{x})\psi(\vec{x}')\rangle = \mathrm{Tr}[\delta(E-H)|\vec{x}\rangle\langle\vec{x}'|], \tag{1}$$

which immediately yields Berry's result, apart from normalization which we choose differently here. However, a trace over a basis is independent of any unitary transformation on that basis, so it does not matter whether we use a trace over a complete set of random waves or simple local plane waves; both give $J_0(ka)$ for the case of one free particle in two dimensions. In this way, the imaginary part of the retarded Green function $-\frac{1}{\pi}\,\mathrm{Im}[G^+(E)] = \delta(E-H)$ becomes central, formally convenient and equivalent to Berry's RPW hypothesis.

2. Preliminaries

We begin by reviewing the well-known formalism to establish context and notation. The Green function completely characterizes a quantum system, whether it is interacting or not, or has few or many degrees of freedom. The retarded Green function G^+, i.e.

$$G^+ = \mathcal{P}\frac{1}{E-H} - \mathrm{i}\pi\delta(E-H), \tag{2}$$

where $\mathcal{P}$ stands for the principal value of the integral, is the basis for wavefunction statistics and density matrix information, through the following relations, with a convenient choice of normalization:

$$\langle \psi(\mathbf{x})\psi^*(\mathbf{x}')\rangle = -\frac{1}{\pi}\,\mathrm{Im}\langle\mathbf{x}|G^+|\mathbf{x}'\rangle/\rho(E) \tag{3}$$

$$= \langle\mathbf{x}|\delta(E-H)|\mathbf{x}'\rangle/\rho(E), \tag{4}$$

where

$$\rho(E) = \mathrm{Tr}[\delta(E-H)] \tag{5}$$

and where $\langle\cdots\rangle$ stands for the average over the degeneracies. We take these degeneracies to be of dimension up to $ND-1$, where N is the number of particles and D is the spatial

dimension each particle lives in. (We use boldface notation, e.g. $\mathbf{x}$ for the $N \times D$ degrees of freedom.) If true degeneracies do not exist in a particular system, we can artificially open the system up to a continuum. For example, a two-dimensional closed billiard does not have a degeneracy, but it acquires one if we open a hole in it and let it communicate with the outside unbounded 2D space. Of course this changes the billiard properties, and the size of the hole might be problematic, but in fact we shall never really have to open a system up in this way. The quantity $\delta(E - H)$ then implies the average over all scattering wavefunctions at fixed energy E.

There are other interpretations which can be put on the average correlation $\langle\psi(\mathbf{x})\psi^*(\mathbf{x}')\rangle$; for example, we can imagine a large number of potentials which differ in some far away place, and in a way so as to all have an eigenvalue at a particular energy. Then, the average has the interpretation of the average over this 'disorder' ensemble. A slightly different procedure is advocated by Richter *et al*, wherein an energy average is taken [6]. Another interpretation can be applied to individual eigenstates in a closed system, assuming they are at least locally uniform in their properties, by taking the average over different points of origin $\mathbf{x}$. This is particularly appropriate when the analogous classical system is chaotic, as mentioned above [2]. We will be evaluating the Green functions semiclassically in what follows, restricting the time over which the contributing trajectories propagate.

The wavefunction correlation is equal to the coordinate space matrix element of the constant energy density matrix

$$\langle\psi(\mathbf{x})\psi^*(\mathbf{x}')\rangle = \langle\mathbf{x}|\delta(E - H)|\mathbf{x}'\rangle/\rho(E) = \rho(\mathbf{x}, \mathbf{x}', E). \tag{6}$$

Reduced density matrices can also be derived from wavefunction correlations, e.g.

$$\tilde{\rho}(\vec{x}_1, \vec{x}_1', E) = \int \mathrm{d}\vec{x}_2\, \mathrm{d}\vec{x}_3 \cdots \mathrm{d}\vec{x}_N \rho(\vec{x}_1, \vec{x}_2, \ldots; \vec{x}_1', \vec{x}_2, \ldots; E), \tag{7}$$

the one-particle reduced density matrix.

We can approach the correlations via Fourier transform from the time domain, since

$$\delta(E - H) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}Et/\hbar}\, \mathrm{e}^{-\mathrm{i}Ht/\hbar}\, \mathrm{d}t. \tag{8}$$

Thus, the statistics, density matrices and correlations are derivable without further averaging by knowing the time propagator.

In the following, we define the Green function propagator $G(\mathbf{x}, \mathbf{x}', t)$ and the retarded Green function propagator $G^+(\mathbf{x}, \mathbf{x}', t)$ as

$$G(\mathbf{x}, \mathbf{x}', t) = \langle\mathbf{x}|\, \mathrm{e}^{-\mathrm{i}Ht/\hbar}|\mathbf{x}'\rangle, \qquad G^+(\mathbf{x}, \mathbf{x}', t) = \frac{-\mathrm{i}}{\hbar}\Theta(t)\langle\mathbf{x}|\, \mathrm{e}^{-\mathrm{i}Ht/\hbar}|\mathbf{x}'\rangle, \tag{9}$$

where $\Theta(t)$ is the Heaviside step function $\Theta(t) = 0, t < 0, \Theta(t) = 1, t > 0$. It is very rewarding to expand the propagator in semiclassical terms, involving short time (zero length) and longer trajectories. We take $G_{\mathrm{direct}}(\mathbf{x}, \mathbf{x} + \mathbf{r}, t) = \langle\mathbf{x}|\exp[-\mathrm{i}Ht/\hbar]|\mathbf{x} + \mathbf{r}\rangle$, the very short-time semiclassical propagator, which for N particles each in D dimensions reads

$$G_{\mathrm{direct}}(\mathbf{x}, \mathbf{x} + \mathbf{r}, t) \approx \left(\frac{m}{2\pi\,\mathrm{i}\hbar t}\right)^{ND/2} \mathrm{e}^{\mathrm{i}mr^2/2\hbar t - \mathrm{i}V(\mathbf{x}+\frac{\mathbf{r}}{2})t/\hbar}, \tag{10}$$

where $r^2 = |\mathbf{r}|^2$.

It is not difficult to cast the Fourier transform of this short-time version to fit the definition of a Hankel function, i.e.

$$G^{+}_{\rm cl}(\mathbf{x}, \mathbf{x}+\mathbf{r}, E) = \frac{-\mathrm{i}}{\hbar}\int_0^\infty \left(\frac{m}{2\pi \mathrm{i}\hbar t}\right)^{ND/2} \mathrm{e}^{\mathrm{i}mr^2/2\hbar t - \mathrm{i}V(\mathbf{x}+\frac{\mathbf{r}}{2})t/\hbar}\,\mathrm{e}^{\mathrm{i}Et/\hbar}\,\mathrm{d}t$$
$$= -\frac{\mathrm{i}m}{2\hbar^2}\left(\frac{k^2}{2\pi kr}\right)^d H_d^{(1)}(kr), \tag{11}$$

where $d = ND/2-1$, $k = k(\mathbf{x}+\mathbf{r}/2, E)$, $H_d^{(1)}(kr) = J_d(kr)+\mathrm{i}N_d(kr)$ is the Hankel function of order d and J_d is the regular Bessel function of order d. The wave vector k varies with the local potential, i.e. $\hbar^2 k(\mathbf{x}, E)^2/2m = E - V(\mathbf{x})$. Here, using only the extreme short-time version of the propagator, we must suppose $\mathbf{r}$ is not large compared to significant changes in the potential, but this restriction can be removed by using the full semiclassical propagator rather than the short-time version. For the case of one particle in two dimensions, $d = 0$, and we recover Berry's original result for one particle in 2D, $\langle\psi^*(\vec{x})\psi(\vec{x}+\vec{r})\rangle \propto J_0(kr)$.

According to the short-time approximation, for any N,

$$\langle\psi(\mathbf{x})\psi^*(\mathbf{x}+\mathbf{r})\rangle \approx -\frac{1}{\pi}\frac{\mathrm{Im}\big[G^{+}_{\rm cl}(\mathbf{x}, \mathbf{x}+\mathbf{r}, E)\big]}{\rho(E)} = \frac{1}{\rho(E)}\frac{m}{2\pi\hbar^2}\left(\frac{k^2}{2\pi kr}\right)^d J_d(kr), \tag{12}$$

where $k = k(\mathbf{x}, E)$. This result includes interparticle correlations through the potential $V(\mathbf{x})$ and the spatial dependence of $k = k(\mathbf{x}, E)$; the diagonal $r = 0$ limit (following section) is equivalent to classical statistical mechanics. The implications of this for the non-diagonal short-time Green function are intriguing. The way r is defined, it does not matter whether one particle is off diagonal ($\mathbf{x}_i \neq \mathbf{x}_{i'}$) or several or all of them. For given r, the Green function will be the same, apart from changes in the potential $V(\mathbf{x}+\mathbf{r}/2)$.

It is interesting that although the short-time Green function is manifestly semiclassical, the energy form, e.g. equation (12), is obtained by an exact Fourier transform of the semiclassical propagator rather than by stationary phase.

3. Diagonal limit

The diagonal ($r \to 0$) N-body Green function is obtained using the asymptotic form

$$\lim_{r\to 0} J_d(kr) = \frac{1}{\Gamma(d+1)}\left(\frac{kr}{2}\right)^d \approx \frac{1}{\sqrt{2\pi d}}\left(\frac{ekr}{2d}\right)^d; \tag{13}$$

we obtain

$$-\frac{1}{\pi}\mathrm{Im}\big[G^{+}_{\rm cl}(\mathbf{x}, \mathbf{x}, E)\big] \approx \frac{m}{2\pi\hbar^2}\frac{1}{\Gamma(d+1)}\left(\frac{k^2}{4\pi}\right)^d \approx \frac{m}{2\pi\hbar^2}\frac{1}{\sqrt{2\pi d}}\left(\frac{ek^2}{4\pi d}\right)^d, \tag{14}$$

where the second form uses Stirling's approximation, $n! \sim n^n\,\mathrm{e}^{-n}\sqrt{2\pi n}$, and is appropriate below when we consider large N. We note that this behaves as $k^{2d} \sim (E - V(\vec{x}))^d$. This factor is familiar with the computation of the classical density of states. Tracing over all $\vec{x}$ results in

$$\int \mathrm{d}\mathbf{x}\frac{m}{2\pi\hbar^2}\frac{1}{\Gamma(d+1)}\left(\frac{k^2}{4\pi}\right)^d = \int \frac{\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{p}}{h^{ND}}\,\delta(E - H_{\rm cl}(\mathbf{p}, \mathbf{x})) = \rho_{\rm cl}(E), \tag{15}$$

i.e. the classical density of states. The association of the short-time propagator with the classical Hamiltonian and classical density of states is well known. The Berry RPW hypothesis, the short-time propagator and the classical or Weyl (sometimes called Thomas–Fermi) term in the quantum density of states are all closely related.

The quantum spacial integral is over all coordinates, so how does the classical partition function emerge if the classical integral is only over classically allowed coordinates? For forbidden positions, k is imaginary and can be written as, say, $\mathrm{i}\kappa$. An identity for Hankel functions can then be used $\left(\mathrm{i}^{n+1}H_n^{(1)}(\mathrm{i}x) = \frac{2}{\pi}K_n(x)\right)$ to show that the Green function is real so that the imaginary part is zero, explaining why the integral is only over classically allowed positions.

As long as $\mathbf{r} = 0$ (i.e. diagonal Green function) the results obtained within the short-time propagator approximation for any quantity in the presence of a potential (*including* interparticle potentials such as atom–atom interactions) will be purely classical. Since we will be discussing the equivalence of the results from the different ensembles for $\mathbf{r} \neq 0$, it is useful to recall how the classical coordinate space densities in the different ensembles can be shown to coincide since this corresponds to the $\mathbf{r} = 0$ case.

The normalized phase-space density in the microcanonical ensemble and the phase-space density in the canonical ensemble are given by

$$\rho_{\mathrm{cl}}(\mathbf{p}, \mathbf{x}, E) = \frac{1}{\rho_{\mathrm{cl}}(E)}\delta(E - H_{\mathrm{cl}}(\mathbf{p}, \mathbf{x})) \tag{16}$$

and

$$\rho_{\mathrm{cl}}(\mathbf{p}, \mathbf{x}, \beta) = \frac{1}{Q_{\mathrm{cl}}(\beta)}\,\mathrm{e}^{-\beta H_{\mathrm{cl}}(\mathbf{p},\mathbf{x})}, \tag{17}$$

respectively. The density of states and partition function are of course the normalization factors so that

$$\rho_{\mathrm{cl}}(E) = \int \mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{p}\,\delta(E - H_{\mathrm{cl}}(\mathbf{p}, \mathbf{x})), \tag{18}$$

$$Q_{\mathrm{cl}}(\beta) = \int \mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{p}\,\mathrm{e}^{-\beta H_{\mathrm{cl}}(\mathbf{p},\mathbf{x})}. \tag{19}$$

Integrating each phase-space density over momentum space allows us to compare the coordinate space densities

$$\rho_{\mathrm{cl}}(\mathbf{x}, E) = \frac{p^{2d}}{\int \mathrm{d}\mathbf{x}\,p^{2d}}, \tag{20}$$

$$\rho_{\mathrm{cl}}(\mathbf{x}, \beta) = \frac{\mathrm{e}^{-\beta V(\mathbf{x})}}{\int \mathrm{d}\mathbf{x}\,\mathrm{e}^{-\beta V(\mathbf{x})}}, \tag{21}$$

with $p = \sqrt{2m(E - V(\mathbf{x}))}$.

Using the relationship between E and β, $E - \langle V\rangle = \frac{ND}{2\beta}$, where $\langle V\rangle$ is the ensemble average of the potential in one of the statistical ensembles, the coordinate space density becomes

$$p^{2d} = (2m(d+1)/\beta)^d \left(1 + \frac{(\langle V\rangle - V(\mathbf{x}))\beta}{d+1}\right)^d. \tag{22}$$

In the limit $N \to \infty$ ($d \to \infty$), this is

$$p^{2d} = (2m(d+1)/\beta)^d\,\mathrm{e}^{(\langle V\rangle - V(\mathbf{x}))\beta}, \tag{23}$$

$$\frac{p^{2d}}{\int \mathrm{d}\mathbf{x}\,p^{2d}} = \frac{\mathrm{e}^{-V(\mathbf{x})\beta}}{\int \mathrm{d}\mathbf{x}\,\mathrm{e}^{-V(\mathbf{x})\beta}}. \tag{24}$$

This is one of the standard ways of establishing a connection between the ensembles [10].

Since the diagonal Green function gives classical results, we can use it to study classical properties. For example, we can enquire about the average two-particle spacing distribution $\rho_E(r_{12})$ or the probability density for a single particle $P_E(\vec{x}_1)$ starting with the short-time semiclassical Green function and the results will coincide with classical microcanonical statistical mechanics. This statement holds for all N. Similarly, in the large-N limit the canonical ensemble results for these quantities must emerge. This point becomes more interesting for the non-diagonal case, considered next.

4. Link to the canonical ensemble

4.1. Bessel functions become Gaussians

As yet we have found nothing too surprising or useful beyond standard classical statistical mechanics. This changes when we consider the large-N limit for the non-diagonal Green function, $\mathbf{r} \neq 0$. Taking the large-N limit of equation (12), we are confronted with a new question about Bessel functions. The large-d limit of $J_d(x)$ is indeed well known, but this is not yet sufficient for our purposes. It reads

$$\lim_{d\to\infty} \frac{J_d(kr)}{(kr)^d} = \frac{1}{2^d\Gamma(d+1)} \approx \frac{1}{\sqrt{2\pi d}} \left(\frac{e}{2d}\right)^d. \tag{25}$$

This is the standard formula given in the usual references. Equation (25) should be the first term in a power series for $J_d(kr)$ in kr. Another standard result is the power series expansion, valid for all d and kr

$$J_d(kr) = \sum_{m=0}^{\infty} \frac{(-1)^m}{m!\Gamma(m+d+1)} \left(\frac{kr}{2}\right)^{2m+d}. \tag{26}$$

We actually require a different asymptotic result. What make our demands unusual is that, assuming we want the energy to increase in proportion to the number of particles (appropriate to many applications of the large-N limit), then $k \sim \sqrt{E} \sim \sqrt{N} \sim \sqrt{d}$; this means that for fixed r, the combination (kr) increases as $\sqrt{d}$ as $d \to \infty$. If the argument of the Bessel function increases without bound along with its order, some new considerations come into play. We find the desired form using equation (26), after summing a series recognized as that of a Gaussian Taylor expansion,

$$\lim_{d\to\infty} \frac{1}{(kr)^d} J_d(kr) = \frac{1}{2^d d!} \sum_{m=0}^{\infty} \frac{1}{m!} \left(\frac{-k^2r^2}{4(d+1)}\right)^m = \frac{1}{2^d d!} \mathrm{e}^{-k^2r^2/(4(d+1))}, \tag{27}$$

where again $\hbar^2k^2/2m = E - V(\mathbf{x})$. Note that as $d \to \infty$, the argument of the Gaussian holds fixed because of the factor of $d+1$ in the denominator of that argument. Figure 1 illustrates the convergence to the Gaussian as N increases. The asymptotic limit in equation (27) is not in the usual references, although related results have been given for N-bead polymer random chain end-to-end distributions [11]. The connection between the path integral for the propagator and polymer chains is well known [12].

It is interesting that a Gaussian emerges from Bessel functions in the large-N limit. We can put equation (27) together with equations (12) and (4), and express the result, as $N \to \infty$,

$$\langle \psi(\mathbf{x})\psi^*(\mathbf{x}+\mathbf{r})\rangle = \rho(\mathbf{x}, \mathbf{x}', E) \to \frac{1}{\rho(E)} \frac{m}{2\pi\hbar^2 d!} \left(\frac{k^2}{4\pi}\right)^d \mathrm{e}^{-k^2r^2/4(d+1)}. \tag{28}$$

For noninteracting particles moving in zero potential but confined to volume V, the short-time approximation becomes exact and k is constant. For this system, the wavefunction

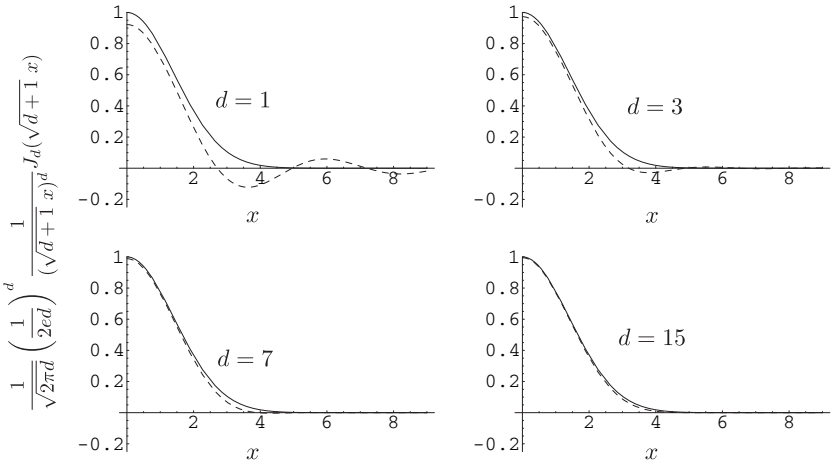

Figure 1. As N increases, the combination $\frac{1}{x^d} J_d(x)$, where $d = ND/2 - 1$, approaches a Gaussian. This is the key link between the quantum microcanonical and canonical ensembles.

correlation becomes

$$\langle \psi(\mathbf{x})\psi^*(\mathbf{x}+\mathbf{r})\rangle = \rho(\mathbf{x}, \mathbf{x}', E) \to \frac{1}{V^N} \mathrm{e}^{-k^2 r^2/4(d+1)}. \tag{29}$$

Something familiar is emerging, here derived in the unfamiliar context of fixed energy (microcanonical ensemble). For a comparison, we recall the standard result for the ideal gas at temperature T [13]:

$$\frac{\langle \mathbf{x}|\mathrm{e}^{-\beta H}|\mathbf{x}+\mathbf{r}\rangle}{\mathrm{Tr}[\mathrm{e}^{-\beta H}]} = \rho(\mathbf{x}, \mathbf{x}', \beta) = \frac{1}{V^N} \mathrm{e}^{-\pi r^2/\lambda^2}, \tag{30}$$

where $\lambda = h/\sqrt{2\pi m \kappa T}$ is the thermal wavelength. Indeed for the free particle case, k is fixed by E and $\langle K\rangle = D/2N\kappa T = \hbar^2 k^2/2m$, where K is the kinetic energy and κ is Boltzmann's constant,

$$\mathrm{e}^{-k^2 r^2/4(d+1)} = \mathrm{e}^{-\pi r^2/\lambda^2}. \tag{31}$$

The canonical ensemble result for the propagator has 'dropped out' of the asymptotic large-N limit of a microcanonical Green function, at least for noninteracting particles, and an unusual asymptotic form for the Bessel function has emerged as the link. With some caveats, the statement

$$\delta(E - H) \sim \mathrm{e}^{-\beta H} \tag{32}$$

has a meaning in the large-N limit, where it is understood that E grows as N, and a temperature is extracted. At a qualitative level, equation (32) merely expresses the known equivalence of the ensembles. In the case of an interaction potential, the relation between E and temperature is of course problematical.

4.2. Interacting particles—short time limit

We can say more about interacting particles using only the short-time propagator introduced above. Longer time events will be discussed in section 6. The short-time approximation to the correlation function for large N, which is equal to the matrix elements of the density operator in coordinate space using our normalization (equation (28)), is given by

$$\rho_{\mathrm{cl}}(\mathbf{x}, \mathbf{x}', E) = \frac{1}{\rho(E)} \frac{m}{2\pi\hbar^2 d!} \left(\frac{k^2}{4\pi}\right)^d \mathrm{e}^{-k^2 r^2/4(d+1)}, \tag{33}$$

with $\hbar k = \sqrt{2m\left(E - V\left(\frac{\mathbf{x}+\mathbf{x}'}{2}\right)\right)}$ and $r = |\mathbf{x} - \mathbf{x}'|$. Again, the Gaussian form of this expression arises from the asymptotic limit of the Bessel function. In the interacting case this can again be brought into the same form as the equivalent expression at constant temperature:

$$\rho_{\mathrm{cl}}(\mathbf{x}, \mathbf{x}', \beta) = \frac{1}{Z(\beta)} \left(\frac{m}{2\pi\beta\hbar^2}\right)^{d+1} \mathrm{e}^{-\frac{mr^2}{2\hbar^2\beta} + V(\frac{\mathbf{x}+\mathbf{x}'}{2})\beta}. \tag{34}$$

In order to make the connection, we must identify the energy with a certain temperature. This relationship between E and β is

$$E - \langle V \rangle = \frac{ND}{2\beta}, \tag{35}$$

where $\langle V \rangle$ is the ensemble average of the potential in one of the statistical ensembles. Using this relationship in equation (33) gives

$$\rho_{\mathrm{cl}}(\mathbf{x}, \mathbf{x}', E) = \frac{1}{\rho(E)} \frac{m}{2\pi\hbar^2 d!} \left(\frac{k^2}{4\pi}\right)^d \mathrm{e}^{-\frac{mr^2}{2\hbar^2\beta}} \mathrm{e}^{-\frac{m(\langle V \rangle - V)r^2}{2\hbar^2(d+1)}}. \tag{36}$$

In order for equation (36) to be equivalent to equation (34), the term with $\langle V \rangle - V$ must be negligible. This is true for configurations of particles which possess the typical (and vastly most probable) total kinetic energy. Since the typical total kinetic energy is by far the most probable, nearly all points in configuration space lead to small values of $\langle V \rangle - V$, and that term is negligible almost always. The remaining terms in equations (36) and (34) are shown to be the same by the equivalence of the classical ensembles as shown in section 3.

It is also telling to trace over the coordinates of all but one of the interacting particles, given by a coordinate $\vec{y}$. We thus seek the reduced density matrix, diagonal or off diagonal in $\vec{y}$. The trace over many coordinates will be overwhelmingly dominated (in the large-N limit) by the most probable total kinetic energy for all the particles. Then, we find

$$\rho_{\mathrm{cl}}(\vec{y}, \vec{y}', \beta) \sim \lambda^{-3N-2} \mathrm{e}^{-\pi r^2/\lambda^2}, \tag{37}$$

where $r^2 = |\vec{y} - \vec{y}'|^2$ and $\lambda = h/\sqrt{2\pi m\kappa T}$. Thus, the quantum-mechanical single-particle Green function and density matrix make sense as their imaginary time counterparts in the $N \to \infty$ limit, in accordance with the well-known results for the canonical ensemble.

4.3. Large-N limit and Boltzmann averaged Green functions

Even though it is a necessary consequence of the equivalence of the ensembles, it is interesting to establish the generality of the Boltzmann average over the energy of a noninteracting subsystem in the following way. Suppose $N - M$ particles are no longer interacting with the remaining M particles, but their states are correlated by having been in contact in the past with the total energy fixed at E. In the time domain and in an obvious notation, we have

$$G_N^+(\mathbf{y}, \mathbf{z}; \mathbf{y}', \mathbf{z}', t) = \mathrm{i}\hbar G_{N-M}^+(\mathbf{y}, \mathbf{y}', t) G_M^+(\mathbf{z}, \mathbf{z}', t). \tag{38}$$

Then, the Fourier convolution theorem can be applied to the Fourier transform into the energy domain, i.e.

$$G_N^+(\mathbf{y}, \mathbf{z}; \mathbf{y}', \mathbf{z}', E) = \frac{\mathrm{i}\hbar}{2\pi} \int_{-\infty}^{\infty} G_{N-M}^+(\mathbf{y}, \mathbf{y}', E - E') G_M^+(\mathbf{z}, \mathbf{z}', E')\, \mathrm{d}E', \tag{39}$$

which incidentally leads to some rather unlikely looking identities for Bessel functions; the reader may easily generate them. Our purpose is served if, focusing on the subsystem of M

particles, we trace over the $N-M$ **y**-coordinates. This gives

$$\mathrm{Tr}_{\mathbf{y}}\left[G^{+}_{N-M}(E-E')\right] \sim \lim_{\mathbf{y}'\to\mathbf{y}} -\frac{m}{2\hbar^2} \times\left(\frac{1}{\Gamma(d_{N-M}+1)}\left(\frac{{k_{N-M}}^2}{4\pi}\right)^{d_{N-M}} + \mathrm{i}\frac{\Gamma(d_{N-M})}{\pi^{d_{N-M}+1}|\mathbf{y}'-\mathbf{y}|^{2d_{N-M}}}\right) \tag{40}$$

times a volume factor, in the case of an ideal gas. The second term is not a function of E'. Therefore, the integral of it times $G_M(\mathbf{z},\mathbf{z}',E)$ is proportional to $\delta(\mathbf{z}'-\mathbf{z})$. As long as $\mathbf{z}\neq\mathbf{z}'$ that term is zero. Neglecting all unimportant (for this argument) factors, this leaves

$$\mathrm{Tr}_{\mathbf{y}}\left[G^{+}_{N-M}(E-E')\right] \propto (E-E')^{d_{N-M}} = E^{d_{N-M}}\left(1-\frac{E'}{E}\right)^{d_{N-M}} \sim E^{d_{N-M}}\,\mathrm{e}^{-\beta E'}, \tag{41}$$

with of course $\beta = 1/\kappa T$. In arriving at equation (41), we used $E = \frac{D}{2}N\kappa T$ for the case of particles embedded in D dimensions. Finally, we arrive at

$$\mathrm{Tr}_{\mathbf{y}}\left[G^{+}_{N}(E)\right] \propto \int_{-\infty}^{\infty} \mathrm{e}^{-\beta E'} G^{+}_{M}(\mathbf{z},\mathbf{z}',E')\,\mathrm{d}E' = G^{+}_{M}(\mathbf{z},\mathbf{z}',\beta) \tag{42}$$

in the large-N limit. This establishes the generality of the Boltzmann average over the subsystem energy for large N. This discussion establishes again the connection between the canonical and microcanonical ensembles, however in a way not involving the Bessel functions and their asymptotic form, so it is less general than other results in this paper valid for any N.

4.4. Stationary phase canonical limit

It is also possible to recover the Gaussian form in equation (28) by carrying out the integral in equation (11) by stationary phase, provided the real factor involving t in the denominator is taken into the exponent, as $-ND/2\log t$, i.e.

$$G^{+}_{\mathrm{cl}}(\mathbf{x},\mathbf{x}+\mathbf{r},E) = \frac{-\mathrm{i}}{\hbar}\int_0^{\infty}\left(\frac{m}{2\pi\mathrm{i}\hbar}\right)^{ND/2} \mathrm{e}^{\mathrm{i}mr^2/2\hbar t - \mathrm{i}V(\mathbf{x}+\frac{\mathbf{r}}{2})t/\hbar + \mathrm{i}Et/\hbar - ND/2\log t}\,\mathrm{d}t. \tag{43}$$

The complex stationary phase point t^* in the large-N limit becomes $t^* = -\mathrm{i}ND\hbar/(2(E-V))$, yielding the same result as in equation (28), with $\hbar^2 k(\mathbf{x},E)^2/2m = E - V(\mathbf{x})$, and making this another route between the quantum microcanonical and canonical ensembles. Since the positions are arbitrary we cannot however identify the *average* kinetic energy with $E-V$, and thus without further averaging we cannot associate t^* with any inverse temperature. It is interesting nonetheless that there is a complex time t^* appropriate to every position $\mathbf{x}$, even if that time is not related to the temperature. For an ideal gas the stationary phase time is $t^* = -\mathrm{i}\hbar/\kappa T = -\mathrm{i}\beta\hbar$, after making the identification $E = D/2N\kappa T$. A discussion about traces over most of the coordinates and the recovery of the usual temperature through $\langle K\rangle = D/2N\kappa T$ proceeds as in section 4.2.

5. Constraints

In the large-N limit the ergodic hypothesis is strongly motivated, but statistical mechanics does not presuppose that ergodicity is unchecked; rather constraints are always present, such as walls and boundaries which control volume. Ergodicity is then defined with respect to these constraints. The guiding idea in this paper, i.e. the extended Berry RPW hypothesis, is that eigenstates of the full system are 'as random as possible, subject to prior constraints'. In this way, thermodynamic constraints arise naturally. The real time, real energy (microcanonical)

semiclassical Green function approach not only automatically generates the averages required to get appropriate wavefunction statistics, but also provides a natural way to include many constraints such as walls, symmetries and even the existence of collisions between particles by going beyond the short time limit term to include returning (not necessarily periodic) trajectories. The semiclassical ansatz for these extended problems in the presence of constraints is

$$G(\mathbf{x}, \mathbf{x}', t) \approx G_{\text{direct}}(\mathbf{x}, \mathbf{x}', t) + \sum_j G_j(\mathbf{x}, \mathbf{x}', t), \tag{44}$$

where $G_j(\mathbf{x}, \mathbf{x}+\mathbf{r}, t)$ is a semiclassical (Van Vleck–Morette–Gutzwiller) Green function

$$G_j(\mathbf{x}, \mathbf{x}'; t) = \left(\frac{1}{2\pi \mathrm{i}\hbar}\right)^{ND/2} \left|\mathrm{Det}\left(\frac{\partial^2 S_j(\mathbf{x}, \mathbf{x}'; t)}{\partial \mathbf{x} \partial \mathbf{x}'}\right)\right|^{1/2} \exp\left(\mathrm{i}S_j(\mathbf{x}, \mathbf{x}'; t)/\hbar - \frac{\mathrm{i}\pi \nu_j}{2}\right) \tag{45}$$

corresponding to the jth trajectory contributing to the path from $\mathbf{x}$ to $\mathbf{x}+\mathbf{r}$, and $G_{\text{direct}}(\mathbf{x}, \mathbf{x}+\mathbf{r}, t)$ is given by equation (10). The short-time term $G_{\text{direct}}(\mathbf{x}, \mathbf{x}+\mathbf{r}, t)$ is singled out as the shortest contributing trajectory: supposing $\mathbf{r}$ to be small compared to distances to walls, etc, we still have a short time, ballistic trajectory as quite distinct from trajectories which have travelled some distance away and come back. There are cases where this separation is not clean; for such cases we can adjust notation accordingly. Note that since a trace over all positions is not being taken, there is no appearance semiclassically of periodic orbits as the only surviving contributors. 'Closed' orbits however can play a large role semiclassically, a fact recognized long ago by Delos [14].

5.1. N particles and a wall

A very useful example is provided by a plane Dirichlet wall felt by all the particles (e.g. $\psi(\vec{x}_1, \vec{x}_2, \ldots, \vec{x}_N) = 0$ for $y_i = 0, i = 1, \ldots, N$), as in a gas confined by a rigid container. The Green function and eigenfunctions must vanish if one or more particles approaches this wall. We can use the method of images, generalized to N particles, if the particles are noninteracting. (The interacting case can in principle be handled by semiclassical trajectory techniques which we bring up in the next section.)

The Green function $G_{\text{wall}}(\mathbf{x}, \mathbf{x}')$ will consist of the shortest distance contribution for which all particles take a direct path from $\mathbf{x}$ to $\mathbf{x}'$, plus paths where one particle has bounced off the wall, paths where two particles have, etc. These histories are included automatically if we apply the symmetrization operator which imposes the image reflections. This operator can be written as

$$\mathcal{R} = \prod_i^N (1 - R_i) = 1 - \sum_i R_i + \sum_{i<j} R_i R_j - \cdots, \tag{46}$$

where R_i is the operator for reflection about the $y = 0$ axis for the ith particle. Applied to the Green function $G(\mathbf{x}, \mathbf{x}+\mathbf{r}, t)$, considered as a function of the coordinates in $\mathbf{x}$ in the absence of the wall, $\mathcal{R}$ yields the series

$$G_{\text{wall}}(\mathbf{x}, \mathbf{x}', t) = G_{\text{direct}}(\mathbf{x}, \mathbf{x}', t) - \sum_i G_i(\mathbf{x}, \mathbf{x}', t) + \sum_{i<j} G_{ij}(\mathbf{x}, \mathbf{x}', t) - \cdots, \tag{47}$$

where $G_i(\mathbf{x}, \mathbf{x}', t)$ corresponds to the ith particle getting from $\vec{x}_i$ to $\vec{x}_i'$ by bouncing off the wall while the others take direct paths, etc. The Fourier transform gives an analogous equation for $G_{\text{wall}}(\mathbf{x}, \mathbf{x}', E)$. The effect of the symmetrization is to create Green function sources reflected across the wall and given proper sign, in the manner familiar from the method of images. The short-time path is shown by the direct path solid line in figure 2, corresponding to the

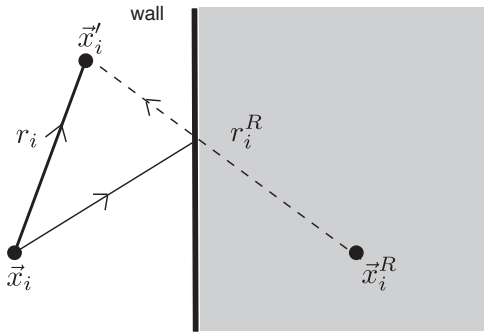

Figure 2. A short and a bouncing path for a particle propagating near a wall. The bounce contribution, if viewed by the image method, is equivalent to a contribution of opposite sign coming from the reflected point $\vec{x}^R$ with the wall removed.

term $G_{st}(\mathbf{x}, \mathbf{x}', t)$. The bounce path is equivalent to a source reflected across the wall with an opposite sign, i.e. the method of images. Define

$$-\frac{1}{\pi}\operatorname{Im}\left[G^+_{st}(\mathbf{x}, \mathbf{x}+\mathbf{r}, E)\right] = \frac{m}{2\pi\hbar^2}\left(\frac{k^2}{2\pi}\right)^d \frac{J_d(kr)}{(kr)^d} \equiv a(k)F_d(kr), \tag{48}$$

then

$$-\frac{1}{\pi}\operatorname{Im}\left[G^+_{\text{wall}}(\mathbf{x}, \mathbf{x}', E)\right] = a(k)\left(F_d(kr) - \sum_i F_d(kr_i) + \sum_{i<j} F_d(kr_{ij}) - \cdots\right). \tag{49}$$

This is the general result for any N. It would appear to be difficult to take it further, since all the distances, e.g.

$$r_{ij} = \sqrt{\sum_{m\neq i,j} |\vec{x}_m - \vec{x}'_m|^2 + \left|\vec{x}_i^R - \vec{x}'_i\right|^2 + \left|\vec{x}_j^R - \vec{x}'_j\right|^2}, \tag{50}$$

where $\vec{x}_j^R$ are the reflected jth particle coordinates, involve square roots. However, if we use the large-N asymptotic form, we find, using $F_d(kr) \to \exp[-k^2r^2/4(d+1)]/2^d d!$,

$$-\frac{1}{\pi}\operatorname{Im}[G_{\text{wall}}(\mathbf{x}, \mathbf{x}', E)] = \frac{a(k)}{2^d d!}\prod_i^N \left(\mathrm{e}^{-\gamma r_i^2} - \mathrm{e}^{-\gamma (r_i^R)^2}\right) = \frac{a(k)}{2^d d!}\,\mathrm{e}^{-\gamma r^2}\prod_i^N \left(1 - \mathrm{e}^{-\gamma \Delta_i^2}\right), \tag{51}$$

where $\gamma = k^2/4(d+1) = \pi/\lambda^2$ and $\Delta_i^2 = \left(r_i^R\right)^2 - r_i^2$. Since r_i is the 'direct' distance from $\vec{x}_i$ to $\vec{x}'_i$, (see figure 2), Δ_i^2 records the distance change upon reflection of the ith particle. We note that Δ_i^2 (and thus the Green function) vanishes as any particle approaches a wall in either $\mathbf{x}$ or $\mathbf{x}'$. It is also simple to see that the single-particle density $\rho(\vec{x})$ in this noninteracting case becomes, for large N,

$$\rho(\vec{x}) = \rho_0\left(1 - \mathrm{e}^{-4\gamma x^2}\right), \tag{52}$$

where x is the distance to the wall and ρ_0 is the density far from the wall.

Formulae (49) and (51) generalize Berry's result [15] for the wavefunction squared of one particle in two dimensions near a wall, namely

$$\langle|\psi(\vec{x})|^2\rangle = \frac{(1 - J_0(k|\vec{x}^R - \vec{x}|))}{\int \mathrm{d}\vec{x}(1 - J_0(k|\vec{x}^R - \vec{x}|))}. \tag{53}$$

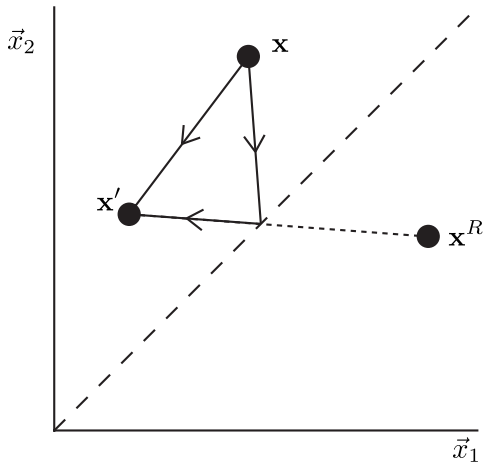

Figure 3. The particle symmetry or antisymmetry condition is equivalent to requiring mirror symmetry or antisymmetry across the $\vec{x}_i = \vec{x}_j$ (hyper)plane. This corresponds to having additional contributions from the images of the particles reflected over the symmetry planes.

The Gaussian we get for large N has a very simple interpretation. First, we note that for noninteracting systems in the canonical ensemble we can write the total density matrix as a product of one-particle density matrices. This is essentially the form of equation (51), since we can write each one-particle density matrix as

$$\rho(\vec{x},\vec{x}',\beta) = \mathrm{e}^{-\gamma|\vec{x}-\vec{x}'|^2/N}\frac{\left(1-\mathrm{e}^{-\gamma(|\vec{x}^R-\vec{x}'|^2-|\vec{x}-\vec{x}'|^2)}\right)}{\int \mathrm{d}\vec{x}\left(1-\mathrm{e}^{-\gamma|\vec{x}^R-\vec{x}|^2}\right)} \to \frac{\left(1-\mathrm{e}^{-\gamma|\vec{x}^R-\vec{x}|^2}\right)}{\int \mathrm{d}\vec{x}\left(1-\mathrm{e}^{-\gamma|\vec{x}^R-\vec{x}|^2}\right)}, \tag{54}$$

where the second form is the diagonal element. However, equation (54) also arises as the density matrix obtained from the Boltzmann average of Berry's result; i.e. averaging the fixed energy results over a canonical distribution of energies, as can be seen from the integral

$$\frac{\int_0^\infty k(1-J_0(k|\vec{x}^R-\vec{x}|))\,\mathrm{e}^{-\beta\hbar^2k^2/2m}\,\mathrm{d}k}{\int_0^\infty k\,\mathrm{e}^{-\beta\hbar^2k^2/2m}\,\mathrm{d}k} = \left(1-\mathrm{e}^{-m|\vec{x}^R-\vec{x}|^2/2\beta\hbar^2}\right). \tag{55}$$

For $D = 2$ and $N = 1$, a Boltzmann average yields the Gaussian. Indeed this necessarily holds in any number of dimensions, i.e. the appropriate Boltzmann average of $J_d(kr)/(kr)^d$ must yield a Gaussian for any d. In the thermodynamic $N \to \infty$ limit for noninteracting particles, each particle separately is Boltzmann distributed over energy, so the result must be the same as a Boltzmann average of the one particle results for any dimension D and for any constraints.

5.2. Symmetries—fermions and bosons

Particle symmetry is an essential part of the many-body problem. Its effect, like other symmetries, is to generate permutations where the distances have changed due to particle exchange. Figure 3 shows this effect graphically. It is gratifying to see directly that permutations which induce large new distances (coming from remote pairs of particles, where 'remote' is a relative term depending on the temperature) make little contribution. Consider N noninteracting fermions or bosons, we wish to compute the reduced density matrix for

two fermions or bosons. This is a well-known result for $N \to \infty$ [13]. The symmetric or antisymmetric Green function is

$$G_{S/A}(\mathbf{x}, \mathbf{x}+\mathbf{r}, E) = \frac{1}{N!}\sum_n \epsilon_n \frac{-\mathrm{i}m}{2\pi\hbar^2}\left(\frac{k^2}{2\pi}\right)^d \frac{H_d(kr_n)}{(kr)^d}, \tag{56}$$

where $r_n = \sqrt{|\vec{x}_1 - \vec{x}'_{p_1}|^2 + \cdots + |\vec{x}_N - \vec{x}'_{p_N}|^2}$, $\{p_1, \ldots, p_N\}$ is the nth permutation of $\{1, \ldots, N\}$ and $\epsilon_n = 1$ if the parity of the permutation is even and $\epsilon_n = \pm 1$ if the parity of the permutation is odd (with the upper sign for bosons and the lower sign for fermions).

$$\begin{aligned}\langle\psi^*(\vec{x_1}\cdots\vec{x_N})\psi(\vec{x_1}\cdots\vec{x_N})\rangle &= -\frac{1}{\pi}\frac{\mathrm{Im}(G_{S/A}(\mathbf{x}, \mathbf{x}+\mathbf{r}, E))}{\rho(E)} \\ &= \frac{1}{\rho(E)N!}\sum_n \epsilon_n \frac{m}{2\pi\hbar^2}\left(\frac{k^2}{2\pi}\right)^d \frac{J_d(kr_n)}{(kr)^d}.\end{aligned} \tag{57}$$

In the limit that N is large, this becomes

$$\langle\psi^*(\vec{x_1}\cdots\vec{x_N})\psi(\vec{x_1}\cdots\vec{x_N})\rangle = \frac{1}{\rho(E)N!}\sum_n^{N!} \epsilon_n \frac{m}{2\pi\hbar^2 d!}\left(\frac{k^2}{4\pi}\right)^d \mathrm{e}^{-k^2 r_n^2/4(d+1)}. \tag{58}$$

The diagonal component of this with the r_n's written out explicitly is

$$\begin{aligned}\langle\psi^*(\vec{x_1}\cdots\vec{x_N})\psi(\vec{x_1}\cdots\vec{x_N})\rangle &= \frac{m}{2\rho(E)N!\pi\hbar^2 d!}\left(\frac{k^2}{4\pi}\right)^d \\ &\times \sum_n^{N!} \epsilon_n \,\mathrm{e}^{-k^2(\vec{x}_1-\vec{x}_{p1})^2/4(d+1)}\cdots\mathrm{e}^{-k^2(\vec{x}_N-\vec{x}_{pN})^2/4(d+1)}.\end{aligned} \tag{59}$$

Up to the normalization constant this is the constant temperature density matrix for N noninteracting fermions or bosons:

$$\begin{aligned}\langle\psi^*(\vec{x_1}\cdots\vec{x_N})\psi(\vec{x_1}\cdots\vec{x_N})\rangle &= \frac{m}{2\rho(E)N!\pi\hbar^2 d!}\left(\frac{k^2}{4\pi}\right)^d \\ &\times \sum_n^{N!} \epsilon_n \,\mathrm{e}^{-m(\vec{x}_1-\vec{x}_{p1})^2/2\beta\hbar^2}\cdots\mathrm{e}^{-m(\vec{x}_N-\vec{x}_{pN})^2/2\beta\hbar^2}.\end{aligned} \tag{60}$$

Again the identification $E = \frac{D}{2}N\kappa T$ was used. This can be rewritten as an integral over wave vectors

$$\langle|\psi(\mathbf{x})|^2\rangle = A\sum_n^{N!}\epsilon_n \int \mathrm{d}\vec{k}_1\cdots\mathrm{d}\vec{k}_N\,\mathrm{e}^{-\beta\hbar^2 {k_1}^2/2m+\mathrm{i}\vec{k}_1\cdot(\vec{x}_1-\vec{x}_{p1})}\cdots\mathrm{e}^{-\beta\hbar^2 {k_N}^2/2m+\mathrm{i}\vec{k}_N\cdot(\vec{x}_N-\vec{x}_{pN})}, \tag{61}$$

where $A = \frac{m}{2\rho(E)N!\pi\hbar^2 d!}\left(\frac{k^2}{4\pi}\right)^d\left(\frac{\beta\hbar^2}{2\pi m}\right)^{d+1}$ is the normalization constant. Rearranging gives

$$\langle|\psi(\mathbf{x})|^2\rangle = A\sum_n^{N!}\epsilon_n \int \mathrm{d}\vec{k}_1\cdots\mathrm{d}\vec{k}_N\,\mathrm{e}^{-\beta\hbar^2({k_1}^2+\cdots+{k_N}^2)/m}\,\mathrm{e}^{\mathrm{i}(\vec{k}_1-\vec{k}_{p1})\cdot\vec{x}_1}\cdots\mathrm{e}^{\mathrm{i}(\vec{k}_N-\vec{k}_{pN})\cdot\vec{x}_N}. \tag{62}$$

If the volume that the particles are confined to is large but finite, then

$$\begin{aligned}&\int\langle|\psi(\mathbf{x})|^2\rangle\,\mathrm{d}\vec{x}_3\cdots\mathrm{d}\vec{x}_N \\ &\quad= AV^{N-2}\sum_n^{N!}\epsilon_n\int\mathrm{d}\vec{\mathbf{k}}\,\mathrm{e}^{-\beta\hbar^2\mathbf{k}^2/2m}\,\mathrm{e}^{\mathrm{i}(\vec{k}_1-\vec{k}_{p1})\cdot\vec{x}_1}\,\mathrm{e}^{\mathrm{i}(\vec{k}_2-\vec{k}_{p2})\cdot\vec{x}_2}\delta_{\vec{k}_3,\vec{k}_{p3}}\cdots\delta_{\vec{k}_N,\vec{k}_{pN}}.\end{aligned} \tag{63}$$

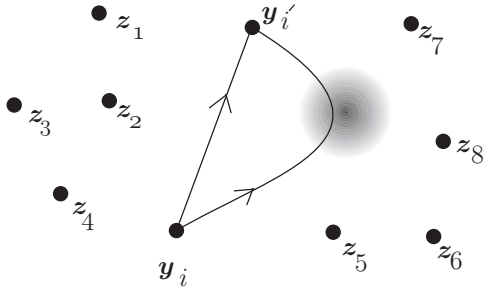

Figure 4. A short ballistic and a colliding path both lead to the same final point for a particle propagating near a localized repulsive potential. The colliding path cannot be treated by the short-time approximation, rather, a Van Vleck Green function is required. In this term, all but the ith particle remain in place.

For fermions if the wave vectors of any two particles are the same, the term is killed by the term with the wave vectors reversed in accordance with the Pauli principle. This leaves only two terms

$$\int \langle|\psi(\mathbf{x})|^2\rangle \, \mathrm{d}\vec{x}_3 \cdots \mathrm{d}\vec{x}_N = AV^{N-2} \sum_n^{N!} \epsilon_n \int \mathrm{d}\mathbf{k}\, \mathrm{e}^{-\beta\hbar^2\mathbf{k}^2/2m}\, \mathrm{e}^{\mathrm{i}(\vec{k}_1-\vec{k}_{p1})\cdot\vec{x}_1}\, \mathrm{e}^{\mathrm{i}(\vec{k}_2-\vec{k}_{p2})\cdot\vec{x}_2}. \tag{64}$$

For bosons there are also only two types of terms, but each is multiplied by the same factor since like terms are added together. Either way, carrying out the integral over $\mathbf{k}$,

$$\int \langle|\psi(\mathbf{x})|^2\rangle \, \mathrm{d}\vec{x}_3 \cdots \mathrm{d}\vec{x}_N = \frac{\left(1 \pm \mathrm{e}^{-m(\vec{x}_1-\vec{x}_2)^2/\beta\hbar^2}\right)}{\int \mathrm{d}\vec{x}_1\, \mathrm{d}\vec{x}_2 \left(1 \pm \mathrm{e}^{-m(\vec{x}_1-\vec{x}_2)^2/\beta\hbar^2}\right)}. \tag{65}$$

This is a well-known result for the density of two noninteracting fermions or bosons.

6. Scattering

A hard wall is a potential energy feature which induces a boundary condition, requiring the wavefunction or Green function to vanish as the wall is approached. Softer potentials do not induce fixed boundary conditions and require a different treatment. A potential may still however be thought of as a constraint: we consider waves as random as possible subject to the existence of a potential, be it fixed or interparticle. In practice, this means we return to the Green function formulation used throughout.

Consider a soft repulsive or attractive potential somewhere in a noninteracting gas. Assuming no boundaries, mutually noninteracting particles can interact with the potential 0 or 1 times. (We assume, for simplicity, that the potential is short ranged. Because of the ergodicity assumption inherent to the random wave hypothesis, the presence of remote walls would actually make no difference.) This circumstance develops along lines very similar to the wall, except that we cannot use the method of images. It illustrates the use of the full semiclassical propagator within this formalism.

Equations (46) and (47) both hold, with the effect of R_i changed to mean 'the ith particle takes the path from initial to final coordinates in which it deflects from the potential, if such a path exists classically'. For N particles, there is a 'direct' term in equation (47) where no particle interacts with the potential, N terms where one of them does, etc. We have, in the simple case shown in figure 4 and in analogy with equation (47),

$$G(\mathbf{x},\mathbf{x}',t) = G_{\rm direct}(\mathbf{x},\mathbf{x}',t) + \sum_i G_{{\rm bounce},i}(\mathbf{x},\mathbf{x}',t) + \sum_{i,j} G_{{\rm bounce},i,j}(\mathbf{x},\mathbf{x}',t) + \cdots, \tag{66}$$

with $G_{\rm direct}(\mathbf{x},\mathbf{x}',t)$ given by equation (10) and, e.g.

$$G_{{\rm bounce},i}(\mathbf{z},\mathbf{y}_i,\mathbf{z}+\mathbf{r},\mathbf{y}_i',t) \approx \left(\frac{m}{t}\right)^{\frac{(N-1)D}{2}} \left(\frac{1}{2\pi {\rm i}\hbar}\right)^{\frac{ND}{2}}$$
$$\times \left|\frac{\partial^2 S_i(\mathbf{y}_i,\mathbf{y}_i';t)}{\partial \mathbf{y}_i \partial \mathbf{y}_i'}\right|^{\frac{1}{2}} {\rm e}^{{\rm i}mr^2/2\hbar t - {\rm i}V(\mathbf{z}+\frac{\mathbf{r}}{2})t/\hbar + {\rm i}S_i(\mathbf{y}_i,\mathbf{y}_i';t)/\hbar - \frac{{\rm i}\pi\nu_i}{2}}. \tag{67}$$

Considering this term where only the ith particle with coordinate $\mathbf{y}_i$ interacts with the potential, we have $N-1$ 'spectator' $\mathbf{z}$ particles, and the propagator becomes a product of the noninteracting Green function for $N-1$ particles and a more complicated Van Vleck semiclassical term for the colliding particle. The noninteracting part contributes a term $(N-1)D/2\log t$ in the exponent along with the one-particle classical action of the ith particle. For sufficiently large N, and tracing over the $\mathbf{z}$ particles, this factor leads again to the usual time condition $t^* = -{\rm i}\beta\hbar$ and a thermal average of the one-particle energy Green function under the Fourier transform from time to energy, as in equation (42):

$$G(\mathbf{y},\mathbf{y}',E) \approx G(\mathbf{y},\mathbf{y}',\beta) = G_{\rm direct}(\mathbf{y},\mathbf{y}',\beta)$$
$$+ \sum_i G_{{\rm bounce},i}(\mathbf{y},\mathbf{y}',\beta) + \sum_{i,j} G_{{\rm bounce},i,j}(\mathbf{y},\mathbf{y}',\beta) + \cdots. \tag{68}$$

$t^* = -{\rm i}\beta\hbar$ becomes the imaginary time over which the action for the $\mathbf{y}$-coordinates are evaluated.

7. Conclusion

Starting with Berry's random plane wave conjecture for chaotic Hamiltonian systems, we have followed its implications for moderate and large numbers of particles N. In the large-N limit, we have necessarily arrived at some familiar territory in statistical mechanics. We have adopted a Green function, semiclassical perspective, arriving at a Gaussian–Bessel function asymptotic result for energy Green functions, providing an *analytic* connection between the quantum microcanonical and canonical ensembles. We have extended the incorporation of constraints into the random wave hypothesis, considering several types of constraints, including walls and interparticle collisions. Indeed, the guiding perspective has been to make quantum waves 'as random as possible subject to known prior constraints'. This must ultimately be equivalent to the ergodic hypothesis of quantum statistical mechanics. The nonstandard methods and perspective used here may possibly lead to new avenues of enquiry, and it is our hope that the semiclassical approach might permit new ways of treating strongly interacting systems.

The next stage in the development of this approach is to consider short-ranged potentials between particles, i.e. interparticle collisions. The first corrections to the free particle limit involve binary collisions, which can be computed semiclassically or using a delta potential appropriate to s-wave scatterers. Again the effect of the other particles will be to provide a thermal reservoir which essentially averages the Green function over a thermal distribution of energies (if N is sufficiently large). We save this for a future paper, where we hope to examine specific potentials and derive two-particle radial distribution functions.

Acknowledgments

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