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General relation between density of states and dwell times in mesoscopic systems

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A relevant relation between the dwell time and the density of states for a three-dimensional system of arbitrary shape with an arbitrary number of incoming channels is derived. This result extends the one obtained by Gasparian and co-workers for the case of a one-dimensional symmetrical potential barrier. We believe that such a strong relation is rich in physical significance because the dwell time is the most widely accepted time measure of a particle's dynamics and the density of states in a given region is one of the most relevant properties of a system in equilibrium.

I. INTRODUCTION

In the controversial field of tunneling times, the dwell time is widely accepted as the average time spent by a particle in a given region of space. This time was postulated by Büttiker in the context of the tunneling time problem;¹ recently, a rigorous derivation of the dwell time was obtained within Feynman's² and Bohm's³ formulations of quantum mechanics. We should also mention that the agreement on the physical significance of the dwell time is not unanimous.^{4,5}

The connection between the dwell time and the density of states in the barrier region was shown by Gasparian and co-workers,^{6,7} for the case of a one-dimensional symmetrical multilayered system. In this paper we will extend this result to an arbitrary three-dimensional region, using a very concise derivation.

We believe that establishing and clarifying the connection between these two quantities is also relevant to the recent work by Wang *et al.*,⁸ whose object is the investigation of the statistics of quasibound states in classically chaotic systems. These authors assume a relation between the energies of quasibound states and the extrema of the dwell time in the system under consideration, which can be addressed using the results we present here.

II. DWELL TIME AND DENSITY OF STATES

Let us consider a region Ω in three-dimensional space, connected with the outside world by N channels. Let a given channel be characterized not only by its spatial location, but also by its particular propagation mode.

We choose as an orthonormal basis for this system the set of stationary state eigenfunctions corresponding to each of these N incoming channels, i.e., $\{|\phi_n(E)\rangle\}$, where $n=1,\ldots,N$. Our basis is continuous and degenerate, so that an appropriate normalization is

$$\langle \phi_n(E') | \phi_m(E'') \rangle = \delta_{nm} \delta(E' - E''); \qquad (1)$$

of course, we also have

$$\sum_{n=1}^{N} \int dE |\phi_n(E)\rangle \langle \phi_n(E)| = \hat{1}.$$
 (2)

We now derive an expression for the dwell time associated with a general wave function in this set. Let us consider a wave packet $|\psi_n(t)\rangle$ incoming from the *n*th channel, such that the probability of finding the particle in Ω vanishes for time approaching $\pm \infty$. $|\psi_n(t)\rangle$ can be written in terms of our basis as

$$|\psi_n(t)\rangle = \int \alpha_n(E) e^{-iEt/\hbar} |\phi_n(E)\rangle dE,$$
 (3)

where $\int |\alpha_n(E)|^2 dE = 1$ so that $|\psi_n(t)\rangle$ is normalized to unity.

The mean dwell time in Ω associated with the wave packet $|\psi_n(t)\rangle$ is^{9,10}

$$\tau_D^{(n)} = \int_{-\infty}^{+\infty} dt \int_{\Omega} |\psi_n(\mathbf{r}, t)|^2 d\mathbf{r}$$
$$= \int_{-\infty}^{+\infty} dt \langle \psi_n(t) | \hat{P}_{\Omega} | \psi_n(t) \rangle, \qquad (4)$$

where \hat{P}_{Ω} in the projection operator onto the region Ω . Substitution of (3) in (4) yields

$$\tau_D^{(n)} = 2 \pi \hbar \int |\alpha_n(E)|^2 \langle \phi_n(E) | \hat{P}_\Omega | \phi_n(E) \rangle dE.$$
 (5)

Therefore the dwell time $\tau_D^{(n)}(E)$ for the stationary state $|\phi_n(E)\rangle$ can be defined as

$$\tau_D^{(n)}(E) = 2 \pi \hbar \langle \phi_n(E) | \hat{P}_\Omega | \phi_n(E) \rangle, \qquad (6)$$

which corresponds to the limit of (5) as $|\alpha_n(E)|^2$ tends to a delta function.

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Equation (6) is equal to the well-known expression postulated by Büttiker,¹ provided the different normalization for the wave function used here is taken into account. In fact, for the wave functions of our basis the incoming probability current is just $(2\pi\hbar)^{-1}$ [the total probability is given in units of inverse energy, according to normalization (1), therefore the probability current is in units of inverse action]. In the Appendix two interesting formulas relating the dwell time (6) to perturbative potential approaches^{2,12} and to the Green's functions for our system are shown.

The local density of states $\rho(\mathbf{r}, E)$ is given by¹¹

$$\rho(\mathbf{r}, E) = \sum_{n=1}^{N} \int \langle \mathbf{r} | \phi_n(E') \rangle \langle \phi_n(E') | \mathbf{r} \rangle \, \delta(E - E') dE',$$
(7)

which, in our case, becomes

$$\rho(\mathbf{r}, E) = \sum_{n=1}^{N} \langle \mathbf{r} | \phi_n(E) \rangle \langle \phi_n(E) | \mathbf{r} \rangle.$$
(8)

The density of states $\rho_{\Omega}(E)$ for the region Ω is just the integral of $\rho(\mathbf{r}, E)$ over Ω ; therefore we obtain

$$\rho_{\Omega}(E) = \sum_{n=1}^{N} \int_{\Omega} \langle \mathbf{r} | \phi_{n}(E) \rangle \langle \phi_{n}(E) | \mathbf{r} \rangle d\mathbf{r}$$
$$= \sum_{n=1}^{N} \langle \phi_{n}(E) | \hat{P}_{\Omega} | \phi_{n}(E) \rangle.$$
(9)

From (6) and (9), one straightforwardly obtains

$$\rho_{\Omega}(E) = \frac{1}{2\pi\hbar} \sum_{n=1}^{N} \tau_{D}^{(n)}(E), \qquad (10)$$

i.e., the density of states in Ω is proportional to the sum of the dwell times in Ω for all incoming channels.

III. COMMENTS

The result of Gasparian and Pollak⁶ can be easily obtained as a particular case of (10). In fact, for a one-dimensional region the number of channels reduces to two (for left and right incoming waves) and for a symmetric potential we have $\tau_D^{(1)}(E) = \tau_D^{(2)}(E) = \tau_D(E)$, so that we can write

$$\rho_{[1\text{dim-sym}]} = \frac{1}{\pi\hbar} \tau_D(E), \qquad (11)$$

which corresponds exactly to Eq. (5) of Ref. 6.

If the region Ω is connected to the outside world by tunneling barriers, so that we have quasibound states in Ω , the density of states and the dwell times associated with all the incoming channels are strongly peaked for energy values corresponding to these quasibound states [actually, for a quasiclosed region, $\rho_{\Omega}(E)$ and the $\tau_D^{(n)}$'s have to be a set of delta functions]. Searching for the peaks in the density of states is therefore a possible way to find the quasibound states. Moreover, formula (10) tells us that, in these conditions, a peak in the dwell time for one of the incoming channels practically implies a peak in the density of states, so that, in order to evaluate the statistics of quasibound states,⁸ it is correct to search for the maxima of the dwell times of all the possible incoming channels.

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APPENDIX: TWO FORMULAS FOR THE DWELL TIME OF STATIONARY STATES

In this appendix we want to demonstrate two formulas which relate the expression (6) for the dwell time to perturbative potential approaches^{2,12} and to the Green's functions for the system under consideration.

Let us apply a perturbative potential V to the region Ω , so that $V\hat{P}_{\Omega}$ is the perturbation operator to be added to the unperturbed Hamiltonian \hat{H} . The new orthonormal basis for this system is $\{|\phi_{n,V}^{\pm}(E)\rangle\}$, where each function is a solution of the equation

$$(E \pm \epsilon - \hat{H} - V\hat{P}_{\Omega}) \left| \phi_{n,V}^{\pm}(E) \right\rangle = 0, \qquad (A1)$$

for $\epsilon \rightarrow 0$ and the *n*th incoming channel.

We want to show that the dwell time expression given by (6) is just the diagonal matrix element of $2i\hbar \partial/\partial V$ evaluated for V=0, i.e.,

$$\tau_{D}^{(n)}(E) = \left[2i\hbar \frac{\partial}{\partial V} \right]_{nn} \bigg|_{V=0}$$
$$= \frac{\langle \phi_{n,V}^{\pm}(E) | 2i\hbar \frac{\partial}{\partial V} | \phi_{n,V}^{\pm}(E) \rangle}{\langle \phi_{n,V}^{\pm}(E) | \phi_{n,V}^{\pm}(E) \rangle} \bigg|_{V=0}.$$
(A2)

Let us point out that both the numerator and the denominator diverge (because the basis is Dirac-normalized). Nevertheless their ratio is finite, as we will show.

We can write¹¹

$$\left|\phi_{n,V}^{\pm}(E)\right\rangle = \left|\phi_{n}(E)\right\rangle \pm V\hat{G}^{\pm}(E)\hat{P}_{\Omega}\left|\phi_{n,V}^{\pm}(E)\right\rangle, \quad (A3)$$

where $\hat{G}^{\pm}(E)$ is a solution of the equation

$$(E \pm \epsilon - \hat{H})\hat{G}^{\pm}(E) = \hat{1}, \qquad (A4)$$

for $\epsilon \rightarrow 0$. Substituting (14) in (13) yields

$$\tau_D^{(n)}(E) = \pm 2i\hbar \frac{\langle \phi_n(E) | G^{\pm}(E) P_{\Omega} | \phi_n(E) \rangle}{\langle \phi_n(E) | \phi_n(E) \rangle} .$$
(A5)

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Since in the right-hand side of this equation is a diagonal matrix element, it has to be real, therefore only the imaginary part of $\hat{G}^{\pm}(E)$ matters. But we know¹¹ that

$$\operatorname{Im}\{\hat{G}^{\pm}(E)\} = \mp \pi \sum_{m=1}^{N} |\phi_m(E)\rangle \langle \phi_m(E)| \qquad (A6)$$

which, substituted in (A5) allows us to write

$$\tau_{D}^{(n)}(E) = 2\pi\hbar \sum_{m=1}^{N} \frac{\langle \phi_{n}(E) | \phi_{m}(E) \rangle \langle \phi_{m}(E) | \hat{P}_{\Omega} | \phi_{m}(E) \rangle}{\langle \phi_{n}(E) | \phi_{n}(E) \rangle}$$
$$= 2\pi\hbar \langle \phi_{n}(E) | \hat{P}_{\Omega} | \phi_{n}(E) \rangle, \qquad (A7)$$

where the last step derives from the orthogonality of the basis. Therefore Eq. (6) is shown to be equivalent to (A2) and (A5).

- ¹M. Büttiker, Phys. Rev. B 27, 6178 (1983).
- ²D. Sokolovski and L.M. Baskin, Phys. Rev. A 36, 4604 (1987).
 ³C.R. Leavens and G.C. Aers, in *Scanning Tunneling Microscopy III*, edited by R. Wiesendanger and H.-J. Güntherodt, Springer
- Series in Surface Sciences Vol. 29 (Springer-Verlag, Berlin, 1993), p. 105.
 ⁴D. Sokolovski and J.N.L. Connor, Phys. Rev. A 47, 4677 (1993).
- ⁵V.S. Olkhovski and E. Recami, Phys. Rep. **214**, 339 (1992).
- ⁶V. Gasparian and M. Pollak, Phys. Rev. B 47, 2038 (1993).
- ⁷V. Gasparian (unpublished).
- ⁸Y. Wang *et al.* (unpublished).
- ⁹W. Jaworski and D.M. Wardlaw, Phys. Rev. A 37, 2843 (1988).
- ¹⁰C.R. Leavens and G.C. Aers, Phys. Rev. B **39**, 1202 (1989).
- ¹¹E.N. Economou, *Green's Functions in Quantum Physics* (Springer-Verlag, Heidelberg, 1979), pp. 10 and 57.
- ¹²G. Iannaccone and B. Pellegrini, Phys. Rev. B 49, 16 548 (1994).