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Spontaneous transitions in quantum mechanics

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Abstract. The problem of spontaneous pair creation in static external fields is reconsidered. A weak version of the conjecture proposed by Nenciu (1980 *Commun. Math. Phys.* **76** 117–28) is stated and proved. The method reduces the proof of the general conjecture to the study of the evolution associated with the time-dependent Hamiltonian, $H_\epsilon(t)$, of a vector which is the eigenvector of $H_\epsilon(t)$ at some given time. A possible way of proving the general conjecture is discussed.

1. Introduction

We reconsider in this paper the problem of spontaneous pair creation in static external fields. In the original version [4], the problem was addressed to high-energy physicists. The experimental test was done by comparing the theoretical predictions with the experimental results coming from heavy ion collision experiments. As is stated in [5], there was no agreement between the two results, one of the possible causes being the large effects of non-adiabatic processes.

Over the past few years, experimental results have shown that the transport properties of semiconductors with high symmetry may change drastically if a certain critical value of the external electric field is exceeded. A particular example is a quasi-one-dimensional semiconductor, cooled down below the Peierls transition temperature. It is known that, below this critical temperature, a gap opens in the single-particle excitation spectrum. Moreover, the experimental results [3] show the existence of a threshold value of the applied electric field where the transport properties change drastically. The two elements: existence of the gap in the one-particle Hamiltonian spectrum and the existence of a critical value of the applied electric field, above which the conductivity is practically reduced to zero, are strong arguments for the idea that we are faced here with the phenomenon of spontaneous pair creation. We agree that there are many theories which, more or less, explain this phenomenon. While most of them involve interacting quantum fields, our hope is that an effective potential can be written down such that, for applied electric fields above the threshold value, the over-critical part of the conjecture [4] applies. If this is true, then there may be another way to test the theory experimentally, this time, with better control on the time variations of the external fields and so, on the non-adiabatic processes. In some situations, the threshold value of the electric field can be small. This means that, experimentally, we are not enforced to switch off the applied field (to protect the sample). This shows one of the qualitative differences between the two experimental settings: in heavy ion collisions, the quantum system is perturbed by the electric fields produced during the collisions so we have no control on the ‘switch on’ or ‘switch off’ of the interaction. In contradistinction, for a semiconductor with low critical value of the electric field, we have total control on how slowly the interaction is introduced and switched off.

Because of a technical difficulty, in [5], the definition of over-critical external fields was slightly modified in order to prove the existence of the over-critical external fields. We propose another approach of the problem which avoids this technical difficulty. However, this does not mean that the problem of spontaneous pair creation is solved, but, in the light of the latter observation, the new approach seems to be more appropriate for the problem of spontaneous pair creation in semiconductors.

2. Description of the problem

Because the results in scattering problems involving periodic Schrödinger operators are much poorer than for those involving Dirac operators, we will treat the problem at the level of first quantization. We show that, above the critical value of the interaction, electrons can spontaneously transit between two different energetic bands. If the scattering operator can be implemented in the second quantization, this result is equivalent to spontaneous pair creations of electrons and holes.

For simplicity, we will discuss here the case of a self-adjoint operator, H_0 , defined on some dense subspace $\mathcal{D}(H_0)$ of the Hilbert space \mathcal{H} , the spectrum of which consists of two absolute continuous, bounded, disjoint parts. We denote the lower and upper parts by σ_- and σ_+ respectively. Let $H_\lambda = H_0 + \lambda V$ be the perturbed operator, where we assume that $\mathcal{D}(H_\lambda) = \mathcal{D}(H_0)$, $\mathcal{D}(H_0) \subset \mathcal{D}(V)$ and the perturbation leaves σ_- and σ_+ unchanged. Our interest is in the case when, as λ increases, some eigenvalues emerge from σ_+ and move continuously to σ_- , and there is a critical value, λ_c , at which the lowest eigenvalue touches σ_- and then it disappears in the lower continuum spectrum. We study the scattering problem of pair (H_0, H_λ) in the adiabatic switching formalism for both cases: $\lambda < \lambda_c$ and $\lambda > \lambda_c$.

Let us consider a function, $\varphi : \mathbb{R} \rightarrow \mathbb{R}_+$, $\varphi \in C^\infty$ such that

$$\varphi(s) = \begin{cases} 1 & |s| < 1 \\ 0 & |s| > 2 \end{cases} \quad (1)$$

and, for a pair of positive numbers, $\varepsilon = (\varepsilon_1, \varepsilon_2)$, we consider the adiabatic switching factor:

$$\varphi_\varepsilon(s) = \begin{cases} \varphi(\varepsilon_1 s) & s < 0 \\ \varphi(\varepsilon_2 s) & s \geq 0. \end{cases} \quad (2)$$

One can consider that ε_1 controls the ‘switch-on’ process and ε_2 controls the ‘switch-off’ process. Note that φ_ε is also of C^∞ . For the time-dependent Hamiltonian $H_{\varepsilon,\lambda}(t) = H_0 + \lambda \varphi_\varepsilon(t)V$, and the time-independent Hamiltonian $H_\lambda = H_0 + \lambda V$, we denote by

$$W_{\varepsilon,\lambda}^\pm = s - \lim_{T \rightarrow \pm\infty} U_{\varepsilon,\lambda}^*(T, 0) e^{-iT H_0} \quad (3)$$

and

$$W_\lambda^\pm = s - \lim_{T \rightarrow \pm\infty} e^{iT H_\lambda} e^{-iT H_0} \quad (4)$$

the adiabatic and static Moller operators. The notation $U_{\varepsilon,\lambda}(T, T')$ stands for the propagator corresponding to $H_{\varepsilon,\lambda}(t)$. We suppose that, for $\lambda \in [0, \lambda_0]$, $\lambda_0 > \lambda_c$, these operators exist, the adiabatic Moller operators converge strongly to the static operators. In addition, we consider that the static Moller operators are locally complete on σ_- , i.e. $\text{Range}[P_{H_\lambda}(\sigma_-)W_\lambda^\pm] = P_{H_\lambda}(\sigma_-)\mathcal{H}$. We will discuss later why the situation is different in the case when the Moller operators are only weakly complete (in the sense of [7]). With these assumptions, one can define the unitary scattering matrix $S_\lambda = (W_\lambda^-)^\dagger \times W_\lambda^+$ and the adiabatic version,

$S_{\varepsilon,\lambda} = (W_{\varepsilon,\lambda}^-)^\dagger \times W_{\varepsilon,\lambda}^+$. It is known [2] that the adiabatic scattering operator converges weakly to the static scattering operator in the adiabatic limit, $\varepsilon \rightarrow 0$.

Let us denote by $P_{H_\lambda}(\Omega)$ the spectral projection of H_λ corresponding to some $\Omega \subset \mathbb{R}$. The spontaneous excitations (transfer from $P_{H_0}(\sigma_-)$ to $P_{H_0}(\sigma_+)$ and vice versa) are denied by the fact that the scattering matrix S_λ commutes with the unperturbed Hamiltonian and consequently $P_{H_0}(\sigma_\pm) S_\lambda P_{H_0}(\sigma_\mp) \equiv 0$. The key observation is that $S_{\varepsilon,\lambda}$ does not commute with the unperturbed Hamiltonian and, because $S_{\varepsilon,\lambda}$ goes weakly to the static scattering operator, we still have a chance for $\lim_{\varepsilon \rightarrow 0} \|P_{H_0}(\sigma_\pm) S_\lambda P_{H_0}(\sigma_\mp)\| > 0$. Indeed, it was proven in [5] that this is the case if one considers a discontinuous switching factor, φ_δ , with $\lim_{\delta \rightarrow 0} \varphi_\delta$ a smooth function. Moreover, it was shown that

$$\lim_{\varepsilon_1 = \varepsilon_2 \rightarrow 0} \|P_{H_0}(\sigma_\pm) S_{\varepsilon,\lambda} P_{H_0}(\sigma_\mp)\| = 1 - o(\delta) \tag{5}$$

provided $\lambda > \lambda_c$. We will prove in the next section that

$$\lim_{\varepsilon_1 \rightarrow 0} \lim_{\varepsilon_2 \rightarrow 0} \|P_{H_0}(\sigma_\pm) S_{\varepsilon,\lambda > \lambda_c} P_{H_0}(\sigma_\mp)\| = 1 \tag{6}$$

but with φ of C^∞ class. As was already pointed out in the previous section, this version may be more appropriate for the case of pair creation in semiconductors.

3. The result

Our main result is:

Theorem 1. *In the conditions enunciated in the previous sections, for $\lambda \in [0, \lambda_0 > \lambda_c]$ and $H(t)$ of C^3 in respect with t (in the sense of [6]), then*

$$\lim_{\varepsilon_1 \rightarrow 0} \lim_{\varepsilon_2 \rightarrow 0} \|P_{H_0}(\sigma_-) S_{\varepsilon,\lambda} P_{H_0}(\sigma_+)\| = \begin{cases} 0 & \text{if } \lambda < \lambda_c \\ 1 & \text{if } \lambda > \lambda_c. \end{cases} \tag{7}$$

Proof. The under-critical part ($\lambda < \lambda_c$) results directly from the adiabatic theorem. In this situation, the order of limits are not important. Note that the under-critical case was proven in full generality for Dirac operators in [4].

We now start the proof of the over-critical part ($\lambda > \lambda_c$) which closely follows [5]. We will denote by $E_g(t)$ and $\psi_g(t)$ the lowest eigenvalue of $H_{\varepsilon,\lambda}(t)$ and one of its eigenvectors. (Without loss of generality, we can suppose that the eigenvalues do not change their order during the switching). Any constant which depends on $\varepsilon_{1,2}$ and goes to zero as $\varepsilon_{1,2}$ goes to zero will be denoted by $o(\varepsilon_{1,2})$. Our task is to find a vector ϕ , $\|\phi\| = 1$, such that

$$\|P_{H_0}(\sigma_-) S_{\varepsilon,\lambda} P_{H_0}(\sigma_+) \phi_\varepsilon\| > 1 - o(\varepsilon_1, \varepsilon_2). \tag{8}$$

Let $\varphi(-s_0) = \lambda_c/\lambda$, $s_0 > 0$, and $0 < \delta < 1$ such that $E_g(-(s_0 + \delta)/\varepsilon_1)$ exists. From the adiabatic theorem applied on $(-2/\varepsilon_2, -(s_0 + \delta)/\varepsilon_1)$ we obtain

$$\|P_{H_0}(\sigma_+) U_{\varepsilon,\lambda}(-2/\varepsilon_1, -(s_0 + \delta)/\varepsilon_1) \psi_g(-(s_0 + \delta)/\varepsilon_1)\| > 1 - o(\varepsilon_1) \tag{9}$$

and we will choose $\phi'_{\varepsilon_1} = U_{\varepsilon,\lambda}(-2/\varepsilon_1, -(s_0 + \delta)/\varepsilon_1) \psi_g(-(s_0 + \delta)/\varepsilon_1)$, where the index ε_1 emphasizes that this vector depends only on ε_1 . Again, from the adiabatic theorem on $(-(s_0 + \delta)/\varepsilon_1, 0)$ we have

$$\|P_{H_\lambda}(\sigma_-) U_{\varepsilon,\lambda}(0, -2/\varepsilon_1) \phi'_{\varepsilon_1}\| > 1 - o(\varepsilon_1). \tag{10}$$

Because W_λ^\pm are complete, there exists $\tilde{\phi}_{\varepsilon_1} \in P_{H_0}(\sigma_-)\mathcal{H}$, $\|\tilde{\phi}_{\varepsilon_1}\| \leq 1$, such that

$$W_\lambda^+ \tilde{\phi}_{\varepsilon_1} = P_{H_\lambda}(\sigma_-) U_{\varepsilon,\lambda}(0, -2/\varepsilon_1) \phi'_{\varepsilon_1}. \tag{11}$$

In fact, $\tilde{\phi}_{\varepsilon_1}$ is given by

$$\tilde{\phi}_{\varepsilon_1} = P_{H_0}(\sigma_-)(W_\lambda^+)^{\dagger} U_{\varepsilon,\lambda}(0, -2/\varepsilon_1) \phi'_{\varepsilon_1}. \tag{12}$$

Thus we can continue:

$$\begin{aligned} & \| P_{H_0}(\sigma_-) e^{iH_0 2/\varepsilon_2} U_{\varepsilon,\lambda}(2/\varepsilon_2, 0) U_{\varepsilon,\lambda}(0, -2/\varepsilon_1) \phi'_{\varepsilon_1} \| \\ & \geq | \langle \tilde{\phi}_{\varepsilon_1}, e^{iH_0 2/\varepsilon_2} U_{\varepsilon,\lambda}(2/\varepsilon_2, 0) U_{\varepsilon,\lambda}(0, -2/\varepsilon_1) \phi'_{\varepsilon_1} \rangle | \\ & \geq | \langle W_\lambda^+ \tilde{\phi}_{\varepsilon_1}, U_{\varepsilon,\lambda}(0, -2/\varepsilon_1) \phi'_{\varepsilon_1} \rangle | \\ & \quad - | \langle [U_{\varepsilon,\lambda}^*(2/\varepsilon_2, 0) e^{-iH_0 2/\varepsilon_2} - W_\lambda^+] \tilde{\phi}_{\varepsilon_1}, U_{\varepsilon,\lambda}(0, -2/\varepsilon_1) \phi'_{\varepsilon_1} \rangle | \\ & = \| P_{H_\lambda}(\sigma_-) U_{\varepsilon,\lambda}(0, -2/\varepsilon_1) \phi'_{\varepsilon_1} \|^2 - | \langle [W_{\varepsilon_2,\lambda}^+ - W_\lambda^+] \tilde{\phi}_{\varepsilon_1}, U_{\varepsilon,\lambda}(0, -2/\varepsilon_1) \phi'_{\varepsilon_1} \rangle | \\ & > 1 - o(\varepsilon_1) - | \langle [W_{\varepsilon_2,\lambda}^+ - W_\lambda^+] \tilde{\phi}_{\varepsilon_1}, U_{\varepsilon,\lambda}(0, -2/\varepsilon_1) \phi'_{\varepsilon_1} \rangle | \end{aligned} \tag{13}$$

by using inequality (10). Finally, choosing $\phi = e^{-iH_0 2/\varepsilon_1} \phi'_{\varepsilon_1}$ it follows from (9) that

$$\| P_{H_0}(\sigma_-) S_{\varepsilon,\lambda} P_{H_0}(\sigma_+) \phi \| > \| P_{H_0}(\sigma_-) e^{iH_0 2/\varepsilon_2} U_{\varepsilon,\lambda}(2/\varepsilon_2, -2/\varepsilon_1) \phi'_{\varepsilon_1} \| - o(\varepsilon_1). \tag{14}$$

Further, from inequality (13)

$$\| P_{H_0}(\sigma_-) S_{\varepsilon,\lambda} P_{H_0}(\sigma_+) \phi_{\varepsilon_1} \| \geq 1 - o(\varepsilon_1) - | \langle [W_{\varepsilon_2,\lambda}^+ - W_\lambda^+] \tilde{\phi}_{\varepsilon_1}, U_{\varepsilon,\lambda}(0, -2/\varepsilon_1) \phi'_{\varepsilon_1} \rangle |. \tag{15}$$

Because $\tilde{\phi}_{\varepsilon_1}$ do not depend on ε_2 , the statement of the theorem follows from the strong convergence of the adiabatic Moller operator to the static Moller operator. \square

Following [1], one can second quantize our problem by considering $P_{H_0}(\sigma_\pm)$ as the spaces of particles and antiparticles (holes). If $S_{\varepsilon,\lambda}$ can be implemented in the Fock space, then one can follow the method of [5] to show that this result is equivalent to spontaneous pair creation.

We want to point out that the local completeness of Moller operators is essentially given in the proof of the above theorem. Supposing that they are only weakly locally complete (i.e. $Ran P_{H_\lambda}(\sigma_-) W_\lambda^- = Ran P_{H_\lambda}(\sigma_-) W_\lambda^+ \neq P_{H_\lambda}(\sigma_-) H_{a.c.}(H_\lambda)$), then the eigenvector $\tilde{\psi}_g(-(s_0+\delta)/\varepsilon_1)$ may be trapped in $P_{H_\lambda}(\sigma_-)[Ran W_\lambda^+]^\perp$ under the evolution U_ε . Unfortunately, it follows from [8] that this is not a rare case. Moreover, because of infinite dimensionality of this subspace, the weak convergence

$$w - \lim_{\varepsilon_1 \rightarrow 0} P_{H_\lambda}(\sigma_-) U_{\varepsilon,\lambda}(0, -1/\varepsilon_1) = 0 \tag{16}$$

cannot be used to show that the vector escapes from $P_{H_\lambda}(\sigma_-)[Ran W_\lambda^+]^\perp$ after a long period of time. The conclusion is that during the ‘switch-on’ process, the eigenvector is most likely trapped and stays in $P_{H_\lambda}(\sigma_-)[Ran W_\lambda^+]^\perp$. Then there is no way of defining a vector similar to $\tilde{\phi}_{\varepsilon_1}$ so the above proof cannot be applied. Because $(W_{\varepsilon,\lambda}^-)^\dagger$ converges only weakly to $(W_\lambda^-)^\dagger$, there is no direct argument against the possibility that the ‘switch-off’ process to bring this vector back to $P_{H_0}(\sigma_+)\mathcal{H}$.

4. Conclusions

The last observation shows that even in this simplified form, the problem of spontaneous transitions is not trivial. A deep question about the subject is under what conditions the same result is true disregarding any order of the limits, in particular, for $\varepsilon_1 = \varepsilon_2$. In the case when Moller operators are complete (or locally complete on σ_-), the result of the last section reduces this problem to the study of $\tilde{\phi}_{\varepsilon_1}$ properties. One might expect that

$$\int_0^\infty dt \|V e^{-itH_0} \tilde{\phi}_{\varepsilon_1}\| < M \quad (17)$$

with M independent of ε_1 in which case it is straightforward that the order of limits is unimportant. To prove a relation like 17, one has to prove that $\tilde{\phi}_{\varepsilon_1}$ belongs to a set of vectors for which the Cook criterion is valid, together with uniform estimates. From the definition of $\tilde{\phi}_{\varepsilon_1}$, one can see that this problem can be reduced to the study of the evolution of the eigenvector $\psi(-(s_0 + \delta)/\varepsilon_1)$, which does not depend on ε_1 . In most cases, the Schwartz space may be chosen as the set of vectors for which the Cook criterion holds. Unfortunately, to prove that the evolution of $\psi(-(s_0 + \delta)/\varepsilon_1)$ belongs to this space is almost impossible. A much easier task is to prove that it belongs to some Sobolev space $W^{k,p}$. If this step is accomplished, we think that $W^{k,p}$ estimates of [9] may be used to complete the proof, at least for large dimensions.

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