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Time Boundedness of the Energy for the Charge Transfer Model

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Abstract. The energy behavior of the time-dependent Schrödinger equation

$$i\frac{\partial}{\partial t}\psi=\frac{-1}{2m}\Delta\psi+\sum_{j=1}^{N}V_j(x-y_j(t))\psi$$

is discussed, where the $y_j(t)$ are trajectories of classical scattering. In particular, we prove that the energy cannot become arbitrarily large as $t\to\infty$.

1. Introduction and Results

The charge transfer model describes a system of one quantum particle, e.g., an electron, and N others, which can be treated classically because they have a much greater mass (see [1–5, 8–10]). We suppose that the trajectories $y_j(t), j=1, \ldots, N$, of the heavy particles are given and cause a time-dependent potential for the first one. So we have to consider the Schrödinger equation

$$\frac{d}{dt}\psi(t)=-iH(t)\psi(t) \tag{1.1}$$

in the Hilbert space $L^2(\mathbb{R}^\nu)$, where $H(t)=H_0+V(t)$, $H_0=-\frac{1}{2m}\Delta$ and

$$V(t)=\sum_{j=1}^{N}V_j(x-y_j(t)).$$

In addition to the self-adjointness of all $H(t)$, $t\in\mathbb{R}$, one needs some smoothness of $V(t)$ for the existence of the time evolution. If the $y_j(t)$ are continuously differentiable and the $\nabla V_j(x)$ are H_0-bounded, then the existence is well known (Theorem X.71 in [7]). This does not include the Coulomb potential $V_j(x)=|x|^{-1}$ for dimension $\nu=3$, which is the most important in the charge transfer model. However, some recent papers ([5, 8, 11]) show that there also exists a time evolution for potentials $V_j(x)$ with singularities like $|x|^{-\frac{3}{2}+\varepsilon}$, $\varepsilon>0$, $\nu=3$.