NON-LINEAR RESPONSE OF SOME QUANTUM SYSTEMS

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We have investigated the non-linear response of some simple quantum systems in order to determine the limits of the validity of the linear-response theory. A general expression for the non-linear response has been given by Tani[1]. We consider here only static perturbations of the system. The expectation value $\langle\hat{B}\rangle_t$ of an observable $\hat{B}$ at time t after the switching on of the perturbation $-F\hat{A}$, where the operator $\hat{A}$ specifies the nature of the perturbation and the scalar F measures its intensity, is according to Tani given by

$$\langle\hat{B}\rangle_t = iF \int_0^t dt' \langle [\exp(i\hat{H}t')\hat{B}\exp(-i\hat{H}t'),\hat{A}]\rangle_0 + \langle\hat{B}\rangle_0 \ . \qquad (1)$$

Here the symbol $\langle\ \rangle_0$ denotes the thermodynamic average over the states of the unperturbed system. The Hamiltonians of the unperturbed and perturbed system are $\hat{H}_0$ and $\hat{H} = \hat{H}_0 - F\hat{A}$, respectively.

First we calculate the polarization $\langle\hat{p}\rangle_t$ of the two-level system in the transverse electric field E. It follows from (1) that

$$\langle\hat{p}\rangle_t = E\frac{p^2}{kT}\frac{w^2}{w^2+\Delta^2}\{1-\cos[2(w^2+\Delta^2)^{1/2}\ t]\};\ \Delta = pE\ , \qquad (2)$$

where 2w is the level splitting and p the matrix element for the induced dipole transitions between both states of the system. In case of the inhomogeneous broadening the oscillating term may be discarded. Non-linear effects become important when $\Delta \geq w$. In the limit $\Delta \to 0$ we regain the Kubo linear response[2].

Next we consider the electric conductivity of the one-dimensional conductor. The tight-binding one-band approximation is used for the electron states of the system. The medium in which the one-dimensional conductor is embeded produces stochastic fluctuations $f_n(t)$ of the local electron energy. The subscript n denotes the site $R_n = na$, where a is a lattice constant, of the particular localized state. The energy fluctuations $f_n(t)$ and $f_{n'}(t)$ at different sites $n' \neq n$ are statistically independent but have the same statistical properties. By using the Tani formula we obtain the following approximate expression for the electron mobility

$$\mu = 2ea^2 \beta w^2 \Gamma/(\Delta^2 + \Gamma^2); \quad \Delta = eaE , \qquad (3)$$

where e is the electron charge, $\beta = 1/kT$, and w is the inter-site tunneling matrix element. Further

$$\Gamma = \int_{-\infty}^{\infty} \overline{f_n(t')f_n(t)}dt' . \qquad (4)$$

The bar over $f_n(t')f_n(t)$ denotes the time average with respect to t. The non-linearity of the response becomes important when $\Delta \geq \Gamma$.

In the end we consider the response to a constant electric field of the electron which moves in a very weak periodic potential. For simplicity reasons only one-dimensional case is discussed. In consequence of the weak periodic potential the energy spectrum of the unperturbed system is split into mini-bands. The motion of the electron is restricted to a particular mini-band if the perturbation due to the external electric field is small. Due to the Bragg reflections at the Brillouin zone boundaries the Bloch oscillations take place when the interaction of the electron with other degreees of freedom of the system, for instance with phonons, is weak. Suc a system shows a very strong non-linear behaviour at relatively low fields. By increasing the electric field we must finally consider also the inter-band transitions. For strong enough fields a complete breakdown of the Bragg reflections take place. One can show[3] that the residual probability for the Bragg reflection at the n-th zone boundary is given by

$$\pi V_n^2/eE\ \left[d\varepsilon(n\pi/a)/dk\right] \qquad (5)$$

and is inversely proportional to the field E. Here $2V_n$ is the energy gap between the (n-1)-th and the n-th band, and $\varepsilon(k) = k^2/2m$ is the energy of the free electron. The number of crossings of the zone boundaries per unit time is proportional to the electron velocity eE in the k-space. Therefore the probability per unit time for the Bragg reflection does not depend on the field. From such considerations one concludes that in case of strong fields the response of the system is again linear although different from the low-field response. Also here the formulation of the problem in terms of the Tani response formula is possible.

References

1) K. Tani, Prog.Theoret.Phys. (Kyoto) 32 (1964),167.
2) R. Kubo, J.Phys.Soc.Japan 12 (1957),570.
3) P. Gosar, Nuovo Cimento 18 (1960), 241.