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Blocking of inter-subspace tunneling by intra subspace inelastic scattering.

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Abstract : In recent years the notion of intrinsic decoherence and dephasing of a particle interacting with its environment is being investigated intensively. This has an important bearing on a plausible causal connection between incoherent c-axis resistivity and high-temperature superconductivity. In our work we study the tunnel supression and incoherent motion of a particle tunneling between two sites. The bosonic excitations of the environment are coupled to only one site inducing on-site spin flips. We show that this on-site spin flip scattering makes the tunnel motion incoherent. In the high-temperature limit incoherent rate or hopping rate has been calculated. We also briefly discuss the renormalization of the effective tunneling by environmental coupling at zero temperature following Wegner's renormalization group procedure.

Keywords: tunneling, incoherence, spin-flip, renormalization

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One of the most interesting and physically realizable low-dimensional system is a strongly correlated metal, with the possibility of electrons escaping into the third direction by a weak tunneling. Generalization to a d-dimensional system with escape into (d+1)th dimension is obvious, when d=0 (quantum dot), d=1(quantum wire) or d=2 (quantum sheet). For an important realization one may consider a class of high-T_c layered cuprates, where metallic 2-dimensional CuO_2-sheets are weakly coupled across the spacer layers of various oxides of Ca, Sr, Bi etc [1, 2]. It has been proposed earlier that the normal state c-axis resistivity (ρ_c) in the highly anisotropic systems is incoherent and is controlled by the ab-plane resistivity (ρ_{ab}) [3, 4, 5]. Indeed in the best single crystal samples both ρ_c and ρ_{ab} are linear in temperature, from T_c (10^2K) right up to 10^3K (far above the Debye temperature) with $\rho_c \propto \rho_{ab}$. This has been attributed to the blocking of already weak inter-planer tunneling ($t_\perp$) by a strong intra-planer scattering rate ($1/\tau_\|$ of electronic origin). This "quantum Zeno efect" was discussed interms of well known spin-boson model Hamiltonian where the tunneling rate is cutoff by its coupling to a bosonic bath after Caldeira and Leggett [2, 6]. In this work we have reexamined this blocking effect through a simple spin-boson model which is **qualitatively different** from the two-state Caldeira-Leggett model, and is more directly related to the problem of blocking of inter-planer tunneling by blocking of intra-planer scattering. Thus, whereas in the usual spin-boson model, the blocking is due to the adiabatic overlap of the two bosonic ground states (displaced Harmonic oscillators) for the particle in two states, that multiplies the electronic tunneling matrix element, in the present case it is the decoherence due to the intra-planar incoherent dynamics that cut-off the inter-planar coherent tunneling - a truely Quantum Zeno effect.

We have considered the model Hamiltonian

$$H = H_S + H_B + H_{SB}, \tag{1}$$

where

$$H_S = V \sum_\sigma (c_{1\sigma}^\dagger c_{2\sigma} + c_{2\sigma}^\dagger c_{1\sigma}), \tag{2}$$

$$H_B = \sum_q \hbar\omega_q (a_q^\dagger a_q + 1/2), \tag{3}$$

$$H_{SB} = \sum_q \alpha_q (a_q + a_q^\dagger)(c_{1\uparrow}^\dagger c_{1\downarrow} + c_{1\downarrow}^\dagger c_{1\uparrow}). \tag{4}$$

Here H_S describes the tunneling between the two sites 1 and 2 and $c_{i\sigma}$, $c_{i\sigma}^\dagger$ are the annihilation and creation operators of the tunneling particle with i and σ being site and spin index. H_B is the harmonic bath Hamiltonian ,a_q,$a_q^\dagger$ are the bosonic annihilation and creation operators, and H_{SB} couples the bath to site 1 inducing the onsite spin flips. Thus, H_S simulates the inter-planar tunneling (conserving spin σ), and H_{SB} models the intra-planar dynamics rendered incoherent by coupling to the bath H_B. The question now addresed is how the on-site incoherent spin-flip dynamics blocks the tunneling rate 1→2 between the sites 1 and 2. For this we first derive the quantum Langevin equations for the system variables and obtain effective incoherent tunneling rate in the high temperature limit. Finally we describe a renormalization group procedure for calculating effective tunnel matrix element at zero temperature.

Quantum Langevin Equations; dynamics in the high temperature limit

To obtain the quantum Langevin equations for the system variables $c_{i\sigma}$ and $c^\dagger_{i\sigma}$. We use the anticommutation relations $\{c^\dagger_{i\sigma}, c_{j\sigma'}\} = \delta_{ij}\delta\sigma\sigma'$, commutation relations $[a_k, a^\dagger_{k'}] = \delta_{kk'}$ for the bath variables and the Heisenberg equation of motion for any operator A, namely $dA/dt = \frac{1}{i\hbar}[A, H]$. We get

$$\begin{aligned}
i\hbar\frac{d(c^\dagger_{i\alpha}c_{j\beta})}{dt} &= V\sum_\sigma c^\dagger_{i\alpha}c_{2\sigma}\delta_{j1}\delta_{\sigma\beta} + V\sum_\sigma c^\dagger_{i\alpha}c_{1\sigma}\delta_{j2}\delta_{\sigma\beta} - V\sum_\sigma c^\dagger_{1\sigma}c_{j\beta}\delta_{i2}\delta_{\sigma\alpha} \\
&- V\sum_\sigma c^\dagger_{2\sigma}c_{j\beta}\delta_{i1}\delta_{\sigma\alpha} + \sum_q \alpha_q(a_q + a^\dagger_q)c^\dagger_{i\alpha}c_{1\downarrow}\delta_{j1}\delta_{\beta\downarrow} \\
&- \sum_q \alpha_q(a_q + a^\dagger_q)c^\dagger_{1\uparrow}c_{j\beta}\delta_{i1}\delta_{\alpha\downarrow} \\
&+ \sum_q \alpha_q(a_q + a^\dagger_q)c^\dagger_{i\alpha}c_{1\uparrow}\delta_{j1}\delta_{\beta\downarrow} - \sum_q \alpha_q(a_q + a^\dagger_q)c^\dagger_{1\downarrow}c_{j\beta}\delta_{i1}\delta_{\alpha\uparrow}. \quad (5)
\end{aligned}$$

Here i , j and α, β takes on values 1,2 and $\uparrow$, $\downarrow$ respectively with all possible combinations.

$$\frac{da_q}{dt} = -\frac{i}{\hbar}\alpha_q(c^\dagger_{1\uparrow}c_{1\downarrow} + c^\dagger_{1\downarrow}c_{1\uparrow}) - i\omega_q a_q, \quad (6)$$

$$\frac{da^\dagger_q}{dt} = \frac{i}{\hbar}\alpha_q(c^\dagger_{1\uparrow}c_{1\downarrow} + c^\dagger_{1\downarrow}c_{1\uparrow}) + i\omega_q a^\dagger_q. \quad (7)$$

Eqs. (6) and (7), being linear, can be readily solved. We then substitute the formal solutions of $a^\dagger_q(t)$ and $a_q(t)$ (which involve initial values of variables $a^\dagger_q(0)$ and $a_q(0)$ at time t=0) in eqn(5). If one assumes the Ohmic spectral density for bath variables, i.e., $\rho(\omega) = \frac{\pi}{2}\sum_q \frac{4\alpha_q^2}{\hbar^2}\delta(\omega - \omega_q) = \alpha\omega$, α being the coupling constant or Kondo parameter, we get Markovian quantum Langevin equations (for the details see [7]).

$$
\begin{aligned}
i\hbar\frac{d(c^{\dagger}_{i\alpha}c_{j\beta})}{dt} &= V\sum_{\sigma}c^{\dagger}_{i\alpha}c_{2\sigma}\delta_{j1}\delta_{\sigma\beta}+V\sum_{\sigma}c^{\dagger}_{i\alpha}c_{1\sigma}\delta_{j2}\delta_{\sigma\beta}-V\sum_{\sigma}c^{\dagger}_{1\sigma}c_{j\beta}\delta_{i2}\delta_{\sigma\alpha} \\
&- V\sum_{\sigma}c^{\dagger}_{2\sigma}c_{j\beta}\delta_{i1}\delta_{\sigma\alpha}+\left\{F(t)-\frac{i\eta}{\hbar}\left[c^{\dagger}_{1\downarrow}c_{2\uparrow}-c^{\dagger}_{2\uparrow}c_{1\downarrow}+c^{\dagger}_{1\uparrow}c_{2\downarrow}-c^{\dagger}_{2\downarrow}c_{1\uparrow}\right]\right\} \\
&\left[c^{\dagger}_{i\alpha}c_{1\downarrow}\delta_{j1}\delta_{\beta\downarrow}-c^{\dagger}_{1\uparrow}c_{j\beta}\delta_{i1}\delta_{\alpha\downarrow}+c^{\dagger}_{i\alpha}c_{1\uparrow}\delta_{j1}\delta_{\beta\downarrow}-c^{\dagger}_{1\downarrow}c_{j\beta}\delta_{i1}\delta_{\alpha\uparrow}\right], \qquad (8)
\end{aligned}
$$

where $F(t)$ is

$$F(t)=\sum_{q}\alpha_q(a_q(0)e^{-i\omega_q t}+a^{\dagger}_q(0)e^{i\omega_q t}). \qquad (9)$$

As the operators $a_q(0), a^{\dagger}_q(0)$ of the bath are distributed in accordance with the statistical equilibrium distribution for given temperature T, $F(t)$ is referred as Langevin operator noise term. The statistical properties of $F(t)$ can be obtained using the equlibrium distribution for bath varaibles togther with the Ohmic spectral density. Owing to the operator nature of the random Langevin force $F(t)$, it is difficult to solve for the expectation values of site occupancy using equations (8). However in the high temperature limit (made precise in the ref. [7]), one can treat $F(t)$ as a classical c-number random variable. One can readily verify that in the classical limit taking $\hbar \to 0$, the nonequal time commutator of $F(t)$ vanishes and the autocorrelation of the Gaussian random force $F(t)$ becomes

$$\langle F(t)F(t')\rangle = \eta kT\delta(t-t'), \qquad (10)$$

where η is the dissipation coefficient and is related to Kondo parameter α ($\eta = (\hbar\alpha/2)$ [7]. Henceforth we set $\hbar$ to be unity. With the use of Novikov's theorem [7] for the functionals of Gaussian variables we can compute the expression for the averaged quantum expectation value for the occupation probability of a particle on site 2, $n_2(t){=}< \sum_\sigma c^{\dagger}_{2\sigma}c_{2\sigma} >$ (<...> brackets denotes the average over the stochastic variable $F(t)$), subject to the initial condition that the system was prepared initially at t=0 on the site 1. For this we have solved the set of coupled linear equations and the final result is

$$
\begin{aligned}
n_2(t) &\equiv < \sum_{\sigma} c^{\dagger}_{2\sigma}c_{2\sigma} > \\
&= \frac{4V^2}{b}\left\{\frac{e^{-t\frac{a+b}{2}}}{a+b}-\frac{e^{-t\frac{a-b}{2}}}{a-b}\right\}+\frac{1}{2} \qquad (11)
\end{aligned}
$$

where $a{=}\eta k_B T$ and $b{=}\sqrt{(\eta k_B T)^2-16V^2}$.

In the absence of environment coupling (η=0), the particle executes the coherent tunneling oscillations between the two sites with frequency $2V$, namely

$n_2(t)$=(1/2)(1 − $cos(2Vt)$). As the coupling (or temperature) is increased thermally induced onsite spin-flip scattering destroys the coherence and $n_2(t)$ approaches the equlibrium value 1/2 in the asymptotic time limit. The rate of tunneling decreases rapidly as η (the strength of coupling to bath) increases. Indeed, the exponetial in the expression for $n_2(t)$ can be approximated for $\eta k_B T >> V$ to give the incoherent tunneling rate $\sim (4V^2/\eta k_B T)$, that decreases monotonically with increasing η. In this regime $n_2(t)$ exhibits no oscillations and approaches monotonically the value 1/2. The particle hops randomly (incoherently) with no fixed tunneling period and the motion becomes overdamped. This is in agreement with the result obtained by Kumar and Jayannavar [3]. Thus we have established that onsite spin flip scattering decreases the incoherent tunnel rate.

Flow equations for effective tunnel matrix element.

In this section using continuous unitary transformation introduced recently by Wegner [8], we obatin flow equations for the coupling parameters in the Hamiltonian H . In this approach the Hamiltonain is diagonalised by continuous infinitesimal unitary transformation starting from the original Hamiltonain, H(l=0)= H and terminating with a diagonal Hamiltonain with renormalized coupling constants as $l \to \infty$. Here l is the flow parameter labelling the tunneling rate $V(l)$ and coupling constant $\alpha_k(l)$ under the transformation. The flow equations can be written in a differential form

$$\frac{dH}{dl} = [\eta(l), H(l)] \,, \quad H(l=0) = H, \tag{12}$$

where η is the generator of the infinitesimal unitary transformation, it is an anti-hermitain operator that depends on H and therefore implicitly on the flow parameter l. Wegner proposed to choose $\eta(l) = [H_d(l), H(l)]$, where $H_d(l)$ is the appropriate diagonal part of $H(l)$. However, there are several possibilites to choose η so that $H(\infty)$ becomes diagonal. We have made the following ansatz for η,

$$\eta(l) = -\sum_{kx} \eta_{kx}(l)(a_k + a_k^\dagger)(c_{2\uparrow}^\dagger c_{1\downarrow} + c_{2\downarrow}^\dagger c_{1\uparrow} - c_{1\uparrow}^\dagger c_{2\downarrow} - c_{1\downarrow}^\dagger c_{1\uparrow})$$
$$+ \sum_{ky} \eta_{ky}(l)(a_k^\dagger - a_k)(c_{1\uparrow}^\dagger c_{1\downarrow} + c_{1\downarrow}^\dagger c_{1\uparrow}) + \sum_{kz} \eta_{kz}(l)(a_k^\dagger - a_k)(c_{2\uparrow}^\dagger c_{2\downarrow} + c_{2\downarrow}^\dagger c_{2\uparrow}), \tag{13}$$

where η_{kx},η_{ky} and η_{kz} are coefficients to be determined. The flow equations for the parameter of the original Hamiltonian generates interactions not contained in the original Hamiltonian which are quadratic in the bath operators. We have neglected them, as one usually expects them to be unimportant for low lying excitation of the systems at T=0 [9]. Following closely the procedure given in [9] we finally obtain the flow equations of the effective tunnel matrix elemnt $V(l)$, for Ohmic spectral density of bath (the details will be published elsewhere) and is given by

$$\frac{dV(l)}{dl} = -\alpha \int_0^{\omega_c} \omega^2 exp\left(2\int_0^l \frac{4V^2(l) - (\omega)^2}{V(l)} \omega dl\right) d\omega. \quad (14)$$

where ω_c is an upper cutoff freequency of harmonic bath. We have verified that $V(0) > 0$ initially, $V(l)$ decreases monotonically to zero as $l \to \infty$, indicating the complete suppression of tunneling between two sites. This is a simple case of orthogonal catastrophe. Thus at zero temperature on-site spin flip scattering suppresses the tunneling.

In conclusion we have shown that onsite spin-flip scattering induced by environment makes tunnel motion incoherent. The intra-site spin-flip scattering blocks the inter-site tunneling. The calculated incoherent tunnel rate in the high temperature limit is in agreement with earlier known results. At zero temperature the tunnel motion is suppressed.

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