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Nonadiabatic effect in a quantum charge pump

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Nonadiabatic effects in a quantum charge pump are studied through the exact solution of a time-dependent Schrödinger equation and the noninteracting Anderson impurity model. An approximate solution to the interacting Anderson model in the large Coulomb repulsion limit is also presented. The nonadiabatic corrections are rigorously found to die off exponentially as the pumping frequency goes to zero. Moreover, the semiclassical rate equation is derived when the temperature is higher than the energy quantum of the pumping frequency. Finally, nonadiabatic heating in the system is discussed.

Recently, there has been tremendous interest in the realization and improvement of quantum charge pumps and electron turnstiles.[1–7] One important application of such quantum charge transfer devices is for a practical standard for electric current measurements. This would require a precision of the order of one part in 10^8. The present accuracy of such devices is about one part in 10^4, which is a very good start though still quite far from the goal. Several factors may affect the precision: thermal excitations, uncontrolled movement of impurities, and nonadiabatic effects. In an experiment one is also faced with the problem of precisely measuring a small current (typically <1 nA), but this is something not intrinsic to the quantum devices. In the present paper we address the question of nonadiabatic effects.

The most important step in a cycle of quantized charge pumping is to precisely trap a certain number of electrons with an evolving potential configuration. It has been shown that this can be done in the adiabatic limit and at sufficiently low temperatures.[3] In Fig. 1 we illustrate a model process of trapping one electron. An electron gas is confined to the left side of the infinite potential wall. A potential barrier grows slowly, creating a potential well between the barrier and the wall. The region to the right of the barrier is also supposed to be confined laterally. As the barrier grows, a resonant energy level begins to form in the potential well. The width of the resonant level is initially broad, but becomes narrower as the barrier becomes higher and wider. Eventually, when the barrier becomes so high that there is negligible amount of tunneling through the barrier, we obtain a sharp level (to be denoted as $|\psi_0\rangle$ with energy ϵ_0) localized inside the potential well. If such a level lies below the Fermi energy, and thermal equilibrium is maintained with the gas, then we have one electron (per spin) trapped in the well at sufficiently low temperatures. When Coulomb repulsion energy is taken into consideration, it is possible that only a single electron may stay in the level with an energy below the Fermi energy and become trapped.[8,9]

To deal with nonadiabatic effects, we need to solve the time-dependent problem. We first make some general remarks using the noninteracting Schrödinger equation. We assume that the system was initially in equilibrium when the barrier was low or flat, with the occupied states being $\{|\psi_k(t_0)\rangle, E_k < E_F\}$. These states will evolve to $|\psi_k(t)\rangle$ at time t. The probability of occupying at time t the trapping state $|\psi_0\rangle$ is then given by the following formula:

$$N_0(t) = \int_{E_k<E_F} dk\, |\langle \psi_0|\psi_k(t)\rangle|^2 = 1 - \int_{E_k>E_F} dk\, |\langle \psi_0|\psi_k(t)\rangle|^2 , \quad (1)$$

where the measure dk is appropriately chosen according to the normalization of the initial states, and the second equality follows from the completeness of the states $\{|\psi_k(t)\rangle\}$ with all possible energies. The overlap in (1) may be expanded in terms of the adiabatic states $\{|\psi_q^a(t)\rangle\}$, defined as the eigenstates of the Hamiltonian at time t with energy E_q, yielding

$$N_0(t) = 1 - \int_{E_k>E_F} dk \left| \int dq\, \langle \psi_0|\psi_q^a(t)\rangle \times \langle \psi_q^a(t)|\psi_k(t)\rangle \right|^2 . \quad (2)$$

When the barrier becomes large, a resonance occurs near

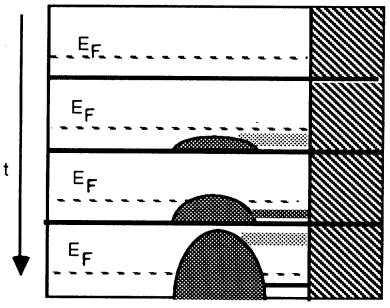

FIG. 1. The formation and narrowing of a resonant level in the potential well to the right of the growing barrier. If thermal equilibrium is maintained with the Fermi sea on the left, one electron (per spin) will be trapped with probability one in the level and in the potential well.

ϵ_0 with a narrow width δ. This means that only those adiabatic states with $|E_q-\epsilon_0|\lesssim\delta$ are going to contribute appreciably in the above integral. On the other hand, when the Hamiltonian changes with a time scale of $1/\gamma$, the overlap $\langle\psi_q^a(t)|\psi_k(t)\rangle$ will be small unless $|E_k-E_q|\lesssim\gamma$; the overlap generally decreases exponentially with increasing $|E_k-E_q|/\gamma$ when the latter becomes large. In the above expressions and hereafter, we take the convention of $\hbar=1$. These considerations show that when $E_F-\epsilon_0\gg\delta+\gamma$, $N_0(t)-1$ is very small.

We have solved exactly a one-dimensional model with a δ-function barrier potential whose strength behaves as $V(t)=V_0+V_1e^{\gamma t}$. The important dimensionless parameters are

$$\tilde{\gamma}=2m\gamma a^2,\quad \tilde{V}_0=2maV_0,\quad \zeta=ka\ , \tag{3}$$

where a is the width of the potential well between the barrier and the wall, and k is now the wave number of an initial state. The trapping state $|\psi_0\rangle$ is at $\zeta=\pi$. We find that N_0 depends on time only through $V(t)$, and we plot N_0 as a function of the time-dependent barrier strength for several values of $\tilde{\gamma}$ in Fig. 2. At large values of $\tilde{\gamma}$ the average occupation tries to maintain its initial value, while in the adiabatic limit it monotonically grows to 1.

To see the $\tilde{\gamma}$ dependence of the nonadiabatic correction, we have calculated the overlap at time $t=+\infty$ for small $\tilde{\gamma}$, which is found to be

$$|\langle\psi_0|\psi_k\rangle|^2=\zeta\left[\frac{4\pi\sin(\zeta)}{\tilde{\gamma}|1+i\tilde{V}_0(\sin\zeta/\zeta)e^{i\zeta}|}\right]^2 e^{-\tilde{\gamma}_0/\tilde{\gamma}}\ , \tag{4}$$

where the exponent is given by

$$\tilde{\gamma}_0=\pi(\zeta^2-\pi^2)+2\pi|\zeta^2-\pi^2| +2\,\mathrm{Im}\int_{\zeta^2}^{\pi^2}d\alpha\ln\left[i\frac{\tilde{V}_0}{2}+\frac{\sqrt{\alpha+i\tilde{\gamma}/2}}{1-\exp(i2\sqrt{\alpha+i\tilde{\gamma}/2})}\right]. \tag{5}$$

In the above integral, we should choose the branch with $\mathrm{Im}[\sqrt{\alpha+i\tilde{\gamma}/2}]\geq 0$ and with the phase of the argument of ln lying in $[-\pi/2,\pi/2]$. When $\tilde{V}_0\gg 1$, the above results simplify to

$$|\langle\psi_0|\psi_k\rangle|^2=(16\pi^2\zeta^3/\tilde{V}_0^2\tilde{\gamma}^2)e^{-2\pi|E(k)-\epsilon_0|/\gamma}\ , \tag{6}$$

where $E(k)=k^2/2m$ is the energy of the initial state, and $\epsilon_0=\pi^2/2ma^2$ is the energy of the trapping state. As expected, the overlap decreases exponentially with the energy difference scaled by γ. When $\tilde{V}_0$ is not large, the overlap still decreases exponentially as the energy difference increases, but the exponent is a more complicated function. In the limit of $\tilde{V}_0=0$, we find that

$$\tilde{\gamma}_0=\begin{cases}2\pi(\pi^2-\zeta^2)-\frac{4}{3}(\pi^3-\zeta^3) & \text{for } \zeta<\pi\\ \frac{4}{3}(\pi^3-\zeta^3) & \text{for } \pi<\zeta<2\pi\\ \cdots\ .\end{cases} \tag{7}$$

The conclusion of this study is that $N_0(t=+\infty)-1$ is exponentially small when $E_F-\epsilon_0$ is large compared with γ. Further study shows that the occupation of higher states in the potential well is exponentially small if their energies are higher than the Fermi energy by an amount much larger than γ. Similar results are also found in a numerical solution of the problem with a square barrier potential.

For a real system, we have to take the very important Coulomb repulsion in the potential well into account. To make the problem tractable, we will use the time-dependent Anderson impurity model to represent our system. We first would like to see whether the essential results of the potential barrier problem can be faithfully reproduced by the noninteracting version of the Anderson model: $H=\sum_{k,\sigma}\epsilon_{k\sigma}c_{k\sigma}^\dagger c_{k\sigma}+\sum_\sigma\epsilon_\sigma(t)c_\sigma^\dagger c_\sigma+\sum_{k,\sigma}V_{k\sigma}(t)(c_{k\sigma}^\dagger c_\sigma+c_\sigma^\dagger c_{k\sigma})$, where $c_{k\sigma}^\dagger$ creates an electron in the kth state in the Fermi sea, and $c_\sigma^\dagger$ creates an electron in the potential well. Assuming the couplings V_k decrease from finite initial values to zero as time goes to infinity, we obtain the occupation number $N_\sigma(t)=\langle c_\sigma^\dagger(t)c_\sigma(t)\rangle$ (in the Heisenberg picture) as

$$N_\sigma(t)=\int(d\omega/\pi)f(\omega-E_f)|g_\sigma(\omega,t)|^2\ , \tag{8}$$

where $f(\omega)=1/[1+\exp(\omega)/k_BT]$, and

$$g_\sigma(\omega,t)=\int_{-\infty}^{t}d\tau\,A_\sigma(\tau)\exp\left[-\int_\tau^t dt'A_\sigma^2(t')\right] \times\exp\left[i\int_0^\tau[\epsilon_\sigma(t')-\omega]dt'\right], \tag{9}$$

with $A_\sigma^2(t)=\Delta\sigma(t)$ being the width of the resonant level of spin σ. In the derivation of the above formulas we have also used a separable time dependence of the coupling $V_{k\sigma}(t)=u_\sigma(t)v_{k\sigma}$, and have made the wide band approximation with

$$\sum_k|v_{k\sigma}|^2\delta(\epsilon_{k\sigma}-\omega)=\Delta_\sigma/\pi\ , \tag{10}$$

independent of ω.[10] Thus, explicitly, $A_\sigma(t)=u_\sigma(t)\sqrt{\Delta_\sigma}$.

We first discuss the nonadiabatic correction to the occupation number at large time. In the zero temperature limit, to simulate the coupling $A_\sigma(t)$ between the level and the external environment in the δ-function potential

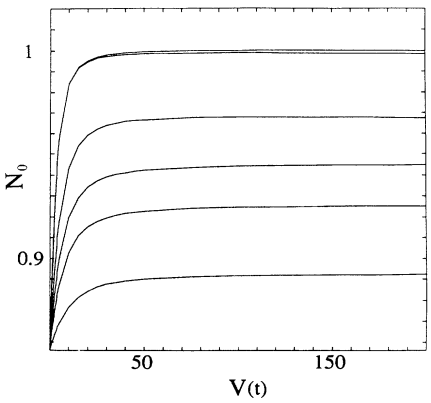

FIG. 2. N_0 as a function of the time-dependent barrier strength. From top to bottom, $\tilde{\gamma}=0$ (adiabatic), 9, 25, 36, 49, and 100, respectively. The Fermi level is at $\zeta=4$.

model, we take $A_\sigma(t)=\Delta_0^{-1/2}(1+w_1e^{\gamma t})^{-1}$ and $\epsilon_\sigma(t)=\epsilon_0$. The integral in (9) can be evaluated in the limit of $\gamma/\Delta_0\ll 1$ by the steepest-descent method, with the result $|g(\omega,\infty)|^2=(\pi/\gamma)(\Delta_0/\omega)^{3/2}e^{-A_0/\gamma}$, where the exponent A_0 equals $2\pi|\omega-\epsilon_0|$ for $|\omega-\epsilon_0|/\Delta_0\gg 1$, and it becomes a more complicated function of ω when the inequality is not satisfied. This behavior of the exponent is quite similar to that in the δ-potential model. Substituting the above expression back to (9), we find that $N_\sigma(\infty)-1\propto e^{-2\pi\epsilon_{f0}/\gamma}$ with $\epsilon_{f0}=E_f-\epsilon_0$.

At finite temperature, the correction due to the thermal excitation is $\propto e^{-\beta\epsilon_{f0}}$ ($\beta=1/k_BT$) and becomes the dominant contribution to the error of trapping electrons if $\gamma\beta<1$. Here we present a complete solution for the semiclassical limit of $\gamma\beta\ll 1$. Using the Fourier transform of the Fermi function $f(\omega)$, we can rewrite the right-hand side of (9) as

$$\int_{-\infty}^{t}d\tau\,h(\tau)\left\{h(\tau)-2k_BT\int_{-\infty}^{\tau}ds\,h(s)\frac{\sin\int_s^\tau[\epsilon_\sigma(t')-E_F]dt'}{\sinh[\pi k_BT(\tau-s)]}\right\}, \tag{11}$$

where $h(\tau)$ stands for $A_\sigma(\tau)\exp[-\int_\tau^t dt'\,A_\sigma^2(t')]$. Under the condition $\gamma\beta\ll 1$, $h(s)$ and $\epsilon_\sigma(t')$ in (11) are slowly varying and their arguments may be replaced by τ because of the relatively sharp peak due to the sinh function.[11] The resulting s integral can be trivially carried out, yielding

$$N_\sigma(t)=\int_{-\infty}^{t}d\tau\,2\Delta(\tau)\exp\left[-\int_\tau^t dt'2\Delta(t')\right]\tilde{f}(\epsilon_\sigma(\tau),\Delta(\tau)), \tag{12}$$

where $\Delta(t)=A_\sigma^2(t)$, and

$$\tilde{f}(\tilde{\epsilon},\tilde{\Delta})=(1/\pi)\int_{-\infty}^{\infty}f(\omega-E_f)\{\Delta/[\Delta^2+(\omega-\tilde{\epsilon})^2]\}d\omega\ . \tag{13}$$

The result (12) can be alternatively obtained from the rate equation

$$\dot{N}_\sigma(\tau)=2\Delta(\tau)[\tilde{f}(\epsilon_\sigma(\tau),\Delta(\tau))-N_\sigma(\tau)]\ , \tag{14}$$

which reduces to the usual semiclassical form with $\tilde{f}$ replaced by f only when $\beta\Delta\to 0$.

In the preceding discussions, we neglected electron-electron interactions in order to simplify the derivation of nonadiabatic corrections. We now address the problem of nonadiabatic effects in the presence of Coulomb repulsion in the trapping state by including the Hubbard interaction term U in the Anderson model:

$$H=\sum_{k,\sigma}\epsilon_{k\sigma}c_{k\sigma}^\dagger c_{k\sigma}+\epsilon_\sigma(t)c_\sigma^\dagger c_\sigma+\sum_{k,\sigma}V_{k\sigma}(t)(c_{k\sigma}^\dagger c_\sigma+c_\sigma^\dagger c_{k\sigma})+Un_\uparrow n_\downarrow\ . \tag{15}$$

The interacting model has no exact solution even in the static case. Here we apply the approximate results of Kasai and Okiji,[12] developed in the context of charge transfer scattering of atoms by metal surfaces. The approximation should be valid above the Kondo temperature.[13] To simplify matters again, we are only going to study the large-U limit. It is then easy to derive from Eqs. (46)–(48) of Ref. 12 the following result:

$$dn(t)/dt=-\Delta(t)[3n(t)-2]+\int_{-\infty}^{t}dt'[2-n(t')]\Sigma(t,t')\ , \tag{16}$$

where $n(t)=n_\uparrow(t)+n_\downarrow(t)$ and

$$\Sigma(t,t')=\frac{2}{\beta}\Delta^{1/2}(t)\Delta^{1/2}(t')\frac{\sin[\epsilon_{f0}(t-t')]}{\sinh[(\pi/\beta)(t-t')]}\times\exp\left[-\int_{t'}^{t}\Delta(\tau)d\tau\right]\ .$$

We are interested in the nonadiabatic correction to the occupation number at large time. By setting $\eta(t)=n(t)-1$, we write the above equation for $\eta(t)$ as

$$d\eta(t)/dt=-3\Delta(t)\eta(t)-\int_{-\infty}^{t}\Sigma(t,t')\eta(t')dt'+B(t)\ , \tag{17}$$

where $B(t)=\int_{-\infty}^{t}\Sigma(t,t')dt'-\Delta(t)$. Equation (17) can be solved by finding a Green function satisfying Eq. (17) but with the term $B(t)$ replaced by $\delta(t-t_0)$. By defining

$$G(t,t_0)=A(t,t_0)\exp\left[\int_{t_0}^{t}\Omega(t')dt'\right]$$

for $t>t_0$ and $G(t,t_0)=0$ for $t\le t_0$, we can write the solution as

$$\eta(t)=\int_{t_0}^{t}G(t,t')B(t')dt'\ .$$

The exponent $\Omega(t)$ and the coefficient $A(t,t_0)$ represent the fast and slow varying parts of the Green function, respectively, and can be determined by equating the terms on both sides of the same order in γ.[14] It is found that $\Omega=2\Delta\pm[\Delta(\Delta-2\epsilon_{f0}/\pi)]^{1/2}$ and

$$A(t,t_0)=\frac{1}{2}\left[\frac{[\Omega(t_0)-2\Delta(t_0)][\Omega(t)-\Delta(t)]}{[\Omega(t)-2\Delta(t)][\Omega(t_0)-\Delta(t_0)]}\right]^{1/2}\ .$$

At zero temperature, we can write the solution $\eta(\infty)$ as

$$\eta(\infty)=-\frac{1}{\pi}\int_{\epsilon_{f0}}^{\infty}d\omega\int_{-\infty}^{\infty}\Delta^{1/2}(\tau)G(\infty,\tau)g(\omega,\tau)\times e^{i\omega\tau}d\tau+\text{c.c.}, \tag{18}$$

where t_0 is set to negative infinity and $g(\omega,\tau)$ is defined by (9) with vanishing ϵ_σ. Finally, by using the steepest-

descent method again, we can show that $\eta(\infty)\sim O(e^{-A_0/\gamma})$, where the exponent A_0 is positive and is equal to $\pi\epsilon_{f0}$ for $\epsilon_{f0}/\Delta_0 \gg 1$. Notice that the value of the exponent is just half of that for the noninteracting Anderson model. In other situations, the exponent is a more complicated function of Δ_0 and ϵ_{f0}.

In the semiclassical limit $\gamma\beta \ll 1$, Eq. (16) may be written as

$$\frac{dn(t)}{dt} = -\Delta(t)[(3+\delta\tilde{f})n(t) - 2(1+\delta\tilde{f})] , \tag{19}$$

where $\delta\tilde{f} = \tilde{f}(-\epsilon_{f0},\Delta) - \tilde{f}(\epsilon_{f0},\Delta)$, and we have also assumed $\epsilon_{f0}/\Delta \gg 1$. In the limit of $\beta\Delta \to 0$, we further have $\delta\tilde{f} \to 2f(-\beta\epsilon_{f0}) - 1$, yielding the usual form of the semiclassical rate equation.[11] The occupation number at time infinity is then $1/(1+\frac{1}{2}e^{-\beta\epsilon_{f0}})$.

In summary, we have studied nonadiabatic effects in a quantum charge pump by solving a time-dependent Schrödinger equation and a time-dependent noninteracting Anderson model exactly, and we find that the nonadiabatic corrections to quantized trapping of electrons is in the form of $e^{-A_0/\gamma}$, where $A_0 = 2\pi\epsilon_{f0}$ if the resonant level width is always much less than the spacing between the Fermi energy and the resonant energy. We have also studied the interacting Anderson model in the large-U limit and reached a similar conclusion except that the exponent is reduced by a factor 2. For a typical turnstile device, we have $\epsilon_{f0} \sim 1$ meV. In order for the nonadiabatic correction to be less than 10^{-8}, the pumping frequency $f = \omega/2\pi \simeq \gamma/4\pi$ should be less than ~ 20 GHz. Moreover, when the temperature is much larger than $\hbar\gamma$, semiclassical rate equations are obtained for the occupation number of the resonant level.

Finally, we comment on the overall heating effect in a trapping process. We define $P(t)$ as the time derivative of the difference between the total electron energy at time t and that in the adiabatic state. Following Ref. 15, we obtain the heating power in the small-γ limit as

$$P(t) = \pi \int dE \left[\frac{dq}{dE}\right]^2 \left[-\frac{\partial f(E)}{\partial E}\right] |\langle \psi_q | \dot{H} | \psi_q \rangle|^2 ,$$

where $|\psi_q\rangle$ is an eigenstate of H with energy $E = E_q$. In our δ-potential model, the above formula is reduced to the form

$$P(t) = \frac{1}{\pi}\gamma(\hbar\gamma)\left[\frac{\tilde{V}_1}{\zeta_f}\right]^2 \sin^4\zeta_f \left|1+\tilde{V}\frac{\sin\zeta_f}{\zeta_f}e^{i\zeta_f}\right|^{-4} \times e^{2\gamma t} ,$$

where ζ_f is the Fermi wave number. The total heating energy of the system in a trapping process is found as

$$\delta E = \frac{\tilde{\gamma}}{2\pi}\left[1+\frac{\xi}{2i\zeta_f}\ln\left[\frac{\xi - i\zeta_f}{\xi + i\zeta_f}\right]\right] ,$$

where $\xi = \zeta_f \cot\zeta_f + \tilde{V}_0$ and the angle of $\xi \pm i\zeta_f$ is restricted in $(-\pi,\pi)$. The heating energy is generally proportional to $\tilde{\gamma}$, but diverges at the points $\zeta_f = n\pi$ (n is a positive integer) if the Fermi level approaches them from below. The divergence is due to the high peak of $P(t)$, which is $\propto \varepsilon^{-2}$ and centered at time $t = (1/\gamma)\ln(\zeta_f/\varepsilon)$, where $\varepsilon = n\pi - \zeta_f$. The physical reason for the divergence is that the excitation becomes large when the Fermi energy is close to the resonant level due to the high local density of states there.[16] For a typical value of the heating energy when ζ_f is away from the divergent points, we set $\zeta_f = 3\pi/2$, yielding $\delta E = \hbar\gamma(3\pi/8\tilde{V}_0^2)$ for $\tilde{V}_0 \gg 3\pi/2$, and $\delta E = \hbar\gamma/2\pi$ in the opposite limit. The typical heating power is therefore $\sim\hbar\gamma^2 = 5.3\times10^{-15}$ W for an operating frequency as high as 1 GHz, and the heat must be dissipated in order to maintain the system at its initial temperature.

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[16] Strictly speaking, the expansion of $P(t)$ in powers of γ fails at points $\zeta_f = n\pi$ because of the long lifetime of the resonant levels. In an exact theory, the divergence is expected to be rounded.