

Finite bias conductance of an Anderson level: A source-Liouville Hartree–Fock study

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We address the problem of stationary conductance through an Anderson spin-degenerate level at finite bias. Just as in the Anderson solution, for a finite bias in parameter space (bias, gate voltage, interaction constant, and the couplings to the leads) there exist spin-polarized and non-spin-polarized regions. The transition curve between them is found analytically for the case of symmetric coupling to the left and right leads. We approach the problem by a non-Markovian source-Liouville equation where the two-body interaction self-energies are taken in the Hartree–Fock approximation. © 2005 American Institute of Physics. [DOI: 10.1063/1.1835261]

I. INTRODUCTION

Spontaneous spin polarization in quantum systems conducting coherent currents has recently been experimentally observed.^{1–12} This phenomenon is an important issue for Spintronics, since it may open a possibility to control the spin of a single electron by voltage bias and gate voltage. Apart from this, the theory of this effect attracts recently much interest.^{13–19} Successful explanation of this effect has been obtained within, e.g., the local spin density approximation.^{14–16}

Since the study of realistic systems is a complicated problem, some insight on the physics underlying the spontaneous spin-polarization phenomenon can be taken from the study of the simplest system, i.e., the Anderson spin-degenerate level. The equilibrium case of an Anderson level immersed into a reservoir of free electrons is well studied. On a Hartree–Fock level (the Anderson solution Ref. 20), the level can develop a spin polarization if the two-body interaction constant is large enough. At sufficiently low temperatures this local spin is quenched by surrounding electrons due to the Kondo effect.²¹ The Kondo effect, however, disappears at higher temperatures.¹⁰

The nonequilibrium case of a conducting Anderson model was studied mostly at differential (or infinitely small) biases.^{17,18} Some attention has been paid to a finite bias case,^{19,22} e.g., it was shown that a finite bias can destroy the Kondo screening of the spin. However, the entire picture on what is happening to the Anderson level at finite biases is not yet clear. Therefore, it is highly desirable to possess a solution, analogous to the original Anderson solution, for a general case of finite bias conductance through an Anderson level. In this paper we present such an analytical solution. This solution may be useful for further study of spin polarization in a conducting quantum mesoscopic system, including the study of the Kondo effect at finite biases. The main result is that we find two regimes of the conductance: the regime of a small bias, $U < U_0$, $U_0 = \Gamma/2\sqrt{3}$, where U is the bias and Γ is the width of the level, when the leads split the level together and the spin polarization arises just as in the Anderson solution; and the regime of large bias, $U > U_0$, in

which the level is split only when it is close to one of the chemical potentials in the leads, but not is in between.

II. FORMALISM

We start with defining the Hamiltonian for the total system (central system+ leads) for a general multilevel case,

$$\hat{H} = \sum_n E_n \hat{\psi}_n^\dagger \hat{\psi}_n + \frac{1}{4} \sum_{lkmn} \hat{\psi}_k^\dagger \hat{\psi}_l^\dagger U_{klmn} \hat{\psi}_m \hat{\psi}_n + \sum_{A \subset \alpha} [E_A + V_\alpha(t)] \hat{r}_A^\dagger \hat{r}_A + \sum_{n,A} (g_{nA} \hat{\psi}_n^\dagger \hat{r}_A + \text{H.c.}) \quad (1)$$

Here $\hat{\psi}_n$ is the electron destruction operator in state n of the central system, E_n is “bare” energy of state n , U_{klmn} is the two-body interaction potential in the chosen basis which obeys²⁴

$$U_{klmn} = -U_{klnm} = U_{nmkl}^*, \quad (2)$$

\hat{r}_A 's are the electron destruction operators in the leads, A is an index running over all the quantum states in all the leads which are labeled by a parameter $\alpha = L, R$, E_A is the energy of state A , $V_\alpha(t)$ is the electrostatic potential in lead α , and finally g_{nA} 's are the coupling (tunneling) constants.

The Liouville-type equation for one-particle density matrix

$$\rho(t) \equiv \rho_{ik}(t) = \langle \hat{\psi}_k^\dagger(t) \hat{\psi}_i(t) \rangle, \quad (3)$$

under the assumption that the system is weakly coupled to the leads has the following form (see Ref. 23 for details):

$$\dot{\rho} = -i[h\rho - \rho h^\dagger] + D, \quad (4)$$

where

$$\begin{aligned}
(h\rho)_{xy}(t) &= E_x \rho_{xy}(t) + \frac{1}{2} \sum_{lmn} U_{xlmn} \rho_{nlmy}^{(2)}(t) \\
&+ \sum_{mn} \int dt' \Sigma_{xm}^r(t, t') \rho_{mn}(t') \\
&\times (-iG_{ny}^a(t', t)), \\
(\rho h)_{xy}(t) &= \rho_{xy}(t) E_y + \frac{1}{2} \sum_{lmn} \rho_{xnm}^{(2)}(t) U_{lmny} \\
&+ \sum_{mn} \int dt' (iG_{xm}^r(t', t)) \rho_{mn}(t') \Sigma_{ny}^a(t', t), \\
D_{xy}(t) &= \sum_{mA} \int dt' A_{xy}^A(t, t') n_A(t'), \\
A_{xy}^A(t, t') &= \sum_{mA} [\Sigma_{xm}^{r,A}(t, t') G_{my}^a(t', t) \\
&- G_{xm}^r(t, t') \Sigma_{my}^{a,A}(t', t)].
\end{aligned} \tag{5}$$

Here the tunneling self-energies are defined as

$$\begin{aligned}
\Sigma_{xy}^{r(a)}(t, t') &= \sum_A \Sigma_{xy}^{r(a), A}(t, t'), \\
\Sigma_{xy}^{r(a), A}(t, t') &= g_{xA} G_A^{r(a)}(t, t') g_{Ay},
\end{aligned} \tag{6}$$

where

$$G_A^r(t, t') = -i\theta(t-t') \exp\left(-iE_A(t-t') - i \int_{t'}^t dt'' V_\alpha(t'')\right),$$

$$G_A^a(t', t) = [G_A^r(t, t')]^*$$

are the retarded and advanced Green's functions of reservoir level A , with (in general time-dependent) occupation denoted by $n_A(t)$. We also define

$$\rho_{wxyz}^{(2)}(t) = \langle \hat{\psi}_z^\dagger(t) \hat{\psi}_y^\dagger(t) \hat{\psi}_x(t) \hat{\psi}_w(t) \rangle$$

as the two-particle density matrix, and

$$G_{xy}^{r(a)}(t, t')$$

is the dressed, i.e., exact, retarded (advanced) Green function of the central system.

Equation (4) is not closed since the evolution of the one-particle density matrix depends on the two-particle density matrix. This is due to the fact that the two-body interaction leads to the so-called Bogoliubov chain, i.e., an infinite set of equations where the time evolution of an N -particle density matrix depends on an $(N+1)$ -particle density matrix. In order to obtain a closed system of equations one has to truncate the Bogoliubov chain at some level by factorizing the many-particle density matrix into a product of density matrices of a lesser number of particles. The easiest and most common way to arrive at a tractable system of equations is to factorize the two-particle density matrix by introducing two-body interaction self-energies. We do it in the spirit of the time-dependent Hartree-Fock approximation, i.e., by assuming that the two-particle self-energy is an on-time operator $\hat{\Xi}(t, t') \propto \hat{\Xi}(t) \delta(t-t')$ so that

$$\begin{aligned}
\frac{1}{2} \sum_{lmn} U_{xlmn} \rho_{nlmy}^{(2)}(t) &= \sum_n \Xi_{xn}^r(t) \rho_{ny}(t), \\
\frac{1}{2} \sum_{lmn} \rho_{xnm}^{(2)}(t) U_{lmny} &= \sum_n \rho_{xn}(t) \Xi_{ny}^a(t),
\end{aligned}$$

and that it is a functional of the one-particle density matrix at the same moment t only,

$$\Xi_{xy}^{r(a)}(t) \equiv \Xi_{xy}^{r(a)}(\{\rho(t)\}_{lm}).$$

The retarded Green function now is the solution of the equation

$$\begin{aligned}
\left(i \frac{\partial}{\partial t} - E_x\right) G_{xy}^r(t, t') - \sum_m \Xi_{xm}^r(t) G_{my}^r(t, t') \\
- \int dt'' \sum_m \Sigma_{xm}^r(t, t'') G_{my}^r(t'', t') \\
= \delta_{xy} \delta(t-t') G_{xy}^r(t' + 0^+, t') = -i \delta_{xy}.
\end{aligned} \tag{7}$$

After choosing an approximate form of the two-body self-energy Eqs. (4) and (7) become closed and can be propagated numerically.

As in Ref. 23, we turn to the weak coupling limit so that the tunneling self-energies become diagonal, and we assume that the reservoirs are sufficiently ‘‘homogeneous’’ on the energy scale considered. These assumptions result in

$$\Sigma_{xy}^{r(a)}(t, t') \approx (\Delta E_x \mp i\Gamma_x/2) \delta(t-t') \delta_{xy}, \tag{8}$$

where ΔE_x is the shift of the x -level energy and Γ_x is the coupling rate to all the reservoirs, $\Gamma_x = \sum_\alpha \Gamma_x^\alpha$, where $\Gamma_x^\alpha = 2\pi\sigma^\alpha(E_x) |g_{x,\alpha E_x}|^2$ is the coupling rate of level x to reservoir α and $\sigma^\alpha(E_x)$ is the density of states of the corresponding reservoir at level energy E_x .

Finally, the proposed set of equations takes the form

$$\dot{\rho} = -i[h\rho - \rho h^\dagger] + D, \tag{9}$$

$$h = \delta_{xy} \tilde{E}_x + \Xi_{xy}^r(t),$$

$$D_{xy}(t) = \sum_A \int dt' A_{xy}^A(t, t') n_A(t'),$$

$$\begin{aligned}
A_{xy}^A(t, t') &= \sum_A [\Sigma_{xx}^{r,A}(t, t') G_{xy}^a(t', t) \\
&- G_{xy}^r(t, t') \Sigma_{yy}^{a,A}(t', t)],
\end{aligned}$$

$$G_{xy}^r(t, t') = -iT \exp\left(-i \int_{t'}^t dt'' \hat{h}(t'')\right)_{xy}, \tag{10}$$

where $\tilde{E}_x = E_x + \Delta E_x - i\Gamma_x/2$ are the levels' energies renormalized with respect to the interaction with the reservoirs and T denotes chronological ordering.

One of the possible ways to construct a closed system of equations is to use a time-dependent Hartree-Fock factorization of the two-particle correlation function,

$$\begin{aligned}\rho_{wxyz}^{(2)}(t) &= \langle \hat{\psi}_z^\dagger(t) \hat{\psi}_y^\dagger(t) \hat{\psi}_x(t) \hat{\psi}_w(t) \rangle \\ &\approx \rho_{wz}(t) \rho_{xy}(t) - \rho_{xz}(t) \rho_{wy}(t).\end{aligned}$$

Due to the fermion symmetry of the interaction potential (2) the two terms give equal results and the self-energy becomes

$$\Xi_{xy}^r(t) = \Xi_{xy}^a(t) = \sum_{lm} U_{xlm} \rho_{ml}(t). \quad (11)$$

III. A SINGLE LEVEL BETWEEN TWO LEADS

Now we turn to a spin-degenerate Anderson level. The energy of the level, already renormalized with respect to interaction with the leads, can always be set at zero. The coupling rates of the level to the left and right leads are denoted as Γ^L and Γ^R , respectively ($\Gamma = \Gamma^L + \Gamma^R$). The two-body potential must have, due to fermion symmetry, the Hubbard form

$$\hat{U} = \frac{\Gamma}{2} u \hat{n}_1 \hat{n}_2,$$

where the subscripts 1 and 2 correspond to spin-up and spin-down states, \hat{n} 's are the particle number operators, and we scale the two-body interaction constant by $\Gamma/2$ to get a dimensionless quantity u .

From Eq. (11) one obtains two-body self-energies in the following form:

$$\Xi_{ik}(t) = u \begin{bmatrix} \rho_{22}(t) & -\rho_{12}(t) \\ -\rho_{21}(t) & \rho_{11}(t) \end{bmatrix}_{ik}.$$

One can always choose the direction of spin quantization in such a way that the one-particle density matrix ρ is diagonal at some instant t_0 . At all the following time moments, $t > t_0$, the one-particle density matrix together with the two-body self-energies and consequently with the full retarded and advanced Green's functions of the system will remain diagonal in these states' indices basis. This implies that we can consider only diagonal elements of one-particle density matrix, i.e., the average states' occupations $n_{1,2}(t) = \langle \hat{n}_{1,2} \rangle(t)$.

The equations for n_1 and n_2 become

$$\begin{aligned}\dot{n}_{1(2)}(t) &= -\Gamma n_{1(2)}(t) \\ &+ \int dt' dE \sum_{\alpha} \Gamma^{\alpha} F_{E,1(2)}^{\alpha}(t, t') n_E^{\alpha}(t'), \\ F_{E,1(2)}^{\alpha}(t, t') &= \frac{1}{\pi} \text{Re} \exp \left[-i \left(E - i \frac{\Gamma}{2} \right) (t - t') \right. \\ &\quad \left. - i \int_{t'}^t dt'' (V_{\alpha}(t'') - u n_{2(1)}(t'')) \right].\end{aligned}$$

The occupation numbers $n_E^{L,R}(t)$ in the leads depend on the energy (E) of the states in the leads and in general case vary in time. These equations are valid for time-dependent conductance. However, we are interested here in stationary conductance so that the leads' occupation numbers are time

independent and the electrostatic potentials can be absorbed into chemical potentials in the leads, which we define as μ^L and μ^R .

The resulting equations for the occupations take the form

$$n_1 = f(n_2), \quad n_2 = f(n_1),$$

$$\begin{aligned}f(n) &= \sum_{a=L,R} \int_{-\infty}^{\mu^a} dE \frac{\kappa^a}{\pi} \frac{\Gamma/2}{(E - un)^2 + (\Gamma/2)^2} \\ &= \pi^{-1} \sum_{a=L,R} \kappa^a \cot^{-1}(2\pi un - \mu^a/(\Gamma/2)),\end{aligned} \quad (12)$$

where $\kappa^a = \Gamma^a/\Gamma$, $\kappa^L + \kappa^R = 1$. Equation (12) can be viewed as a generalized Anderson model, suitable for a nonequilibrium (current-carrying) case of interaction with many reservoirs with different chemical potentials μ^a .

Just as in the Anderson model, there are two regions in parameter space: spin-compensated and non-spin-compensated regions. It is convenient to introduce the dimensionless gate voltage V_g defined as the average between the chemical potentials in the leads with opposite sign, $V_g = -(\mu^L + \mu^R)/\Gamma$. (Recall that the level energy is fixed at zero, so that the shift in the leads' energies is equivalent to the opposite shift of a level, i.e., to introduction of a gate voltage.) We also define the dimensionless voltage bias between the leads, which equals the chemical potentials' difference, $U = (\mu^L - \mu^R)/\Gamma$.

The transition surface between these regions is derived in the Appendix and is given for symmetric level ($\kappa^{L,R} = 1/2$) by Eqs. (A4) and (A5).

The transition surface is given in Fig. 1, where it is presented as a family of curves $V_g(u)$ on the gate-voltage interaction-constant plane, $V_g - u$, for different fixed values of the bias U . In the following we discuss the physics underlying this formal solution. For simplicity we will discuss the cases of small and large biases, respectively, in the limits $u \gg u_1(U)$ and $u_2(U) \ll u \ll u_1(U)$ [the threshold parameters $u_1(U), u_2(U)$ are defined by Eqs. (A6) and (A7)]. In these limits the average population of each spin can be given as $[\theta(\mu^L - \varepsilon) + \theta(\mu^R - \varepsilon)]/2$ (Ref. 25), where ε is the "dressed" (i.e., accounting for two-body interactions) energy of the sublevel.

For a finite-width level to start feeling the chemical potentials difference (bias voltage) the bias must exceed some threshold value. This threshold value for bias voltage is found in the Appendix to be equal to $U_0 = 1/\sqrt{3}$. We call $U > U_0$ the large bias case while $U < U_0$ is the small bias case.

Consider first the case of small bias [see Figs. 2(a)–(c)]. The small bias region can also be referred to as Anderson region. The two chemical potentials, which are close enough to each other, split the level in such a way [Fig. 2(b)] that one of the states is occupied and is under both chemical potentials, $n_1 \approx 1$, while the other state, due to two-body interaction, jumps above the chemical potentials and remains unpopulated, $n_0 \approx 0$. The average occupations behaves as in the equilibrium case of equal chemical potentials (Anderson model with a single reservoir with one chemical potential), but there is still a bias in the system so that the current flows.

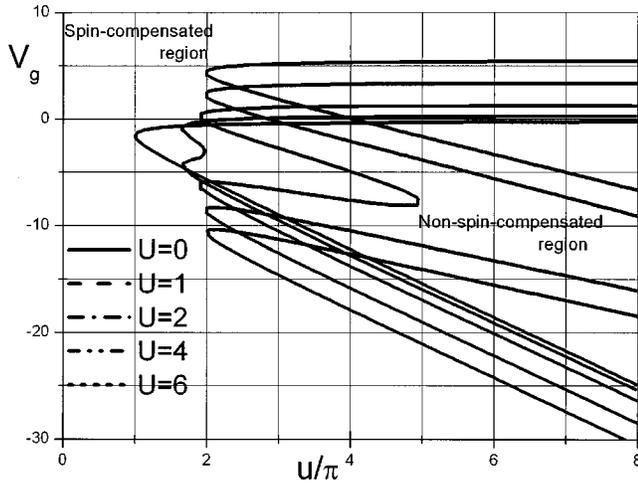


FIG. 1. A family of transition curves between spin-compensated and non-spin-compensated solutions as a function of the gate voltage (V_g)-interaction constant (u) at different biases U .

In the large bias case the two well-separated chemical potentials of the two leads split the level separately [see Figs. 2(d)–2(h)]. As soon as the gate voltage puts the level under the upper chemical potential one of the states saturates acquiring an average occupation $n_1 \approx 1/2$ and starts conducting current [Fig. 2(e)]. This average occupation corresponds to the fluctuations between the occupied and unoccupied lower state in the process of the so-called sequential electron tunneling from one lead to the other. The other state jumps above the potential by $un_1 = u/2$ and is not occupied $n_2 \approx 0$.

With further decrease of the gate voltage the upper level also gets beneath the upper chemical potential, saturates, $n_2 = n_1 \approx 1/2$, and also starts conducting electrons [Fig. 2(f)]. At this point the spin-polarization disappears and both sublevels conduct currents equivalently. With further decrease of V_g we again reach a spin-polarized region [Fig. 2(g)]. In this

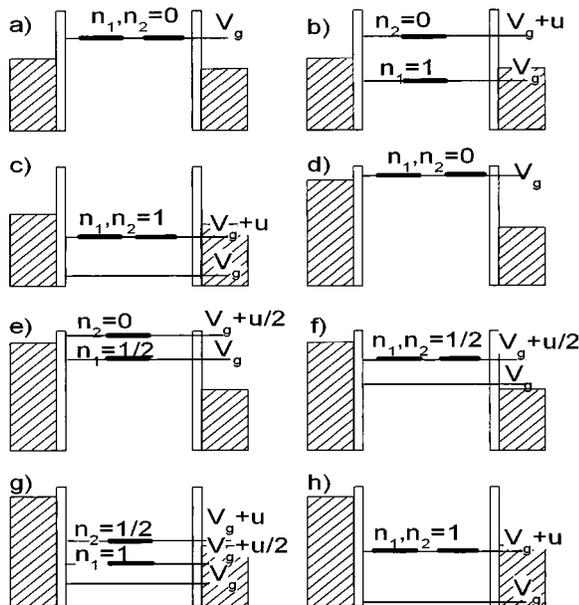


FIG. 2. (a)–(c) Evolution of states populations and energies with decreasing gate voltage V_g for small bias; (d)–(h) the same for the large bias.

region one of the states is beneath both chemical potentials, whereas the upper one is in between them. Now the higher level conducts electrons so that $n_2 \approx 1/2$, while the lower one is populated $n_1 \approx 1$ and is not involved in the conductance process.

Finally, with further decrease of the gate voltage both states get under both chemical potentials so that they are occupied, $n_1 = n_2 \approx 1$, and no current flows through the system [Fig. 2(h)].

In the spin-compensated region the average populations of the spin-up and the spin-down states are the same, $n_1 = n_2$, the system is not spin-polarized and spin-up and spin-down electrons are being transferred from one lead to the other equally. In the non-spin-compensated region the system spontaneously develops a spin-polarization, $n_1 \neq n_2$, and conducts mostly electrons with some chosen spin direction. Actually, the system works as a spin-diode.¹³

CONCLUSION

At sufficiently low temperatures the Kondo effect tends to quenching of spin-polarization in the Anderson level so the validity of our results are restricted to temperatures greater than Kondo temperature. However, that temperature is generally low, e.g., in Ref. 10 it was of order 1 K. Furthermore, as shown in Ref. 20 the voltage bias destroys the Kondo resonance so that in the region of large biases our simple treatment can still be physically valid.

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APPENDIX

Here we derive an equation detailing the boundary between spin-compensated and non-spin-compensated regions in the space of the dimensionless parameters: gate voltage V_g , voltage bias, U , and interaction constant u .

On the boundary between spin-compensated and non-spin-compensated regions the occupations of the sublevels are still equivalent, $n_1 = n_2$, and consequently one of the equations determining the boundary is

$$f(n) = n, \quad (\text{A1})$$

where the function $f(n)$ is given in Eq. (12). The second necessary equation on the transition curve can be obtained by differentiating Eq. (12),

$$\frac{\partial f(n)}{\partial n} = -1. \quad (\text{A2})$$

Equations (A1) and (A2) are an overdetermined system of equations with respect to variable n , so that they determine a surface in the system parameter space.

The equation for this surface can be obtained analytically in the case of a symmetric coupling to the leads, i.e., $\Gamma^L = \Gamma^R$, $\kappa^{L,R} = 1/2$. For the symmetric coupling to the leads the sign of the bias gives only the direction of the current, but plays no role in the average occupations of the spin states. Therefore, it suffices to consider only positive biases.

Equation (A2) reads

$$\frac{u}{2\pi} \sum_{\pm} \frac{1}{1+(z \pm U)^2} = 1, \quad (\text{A3})$$

where for convenience we introduced the additional variable $z = 2\pi un + V_g$. This equation can be solved with respect to variable z . There are four such solutions $\pm z^{>}, \pm z^{<}$:

$$z^{>,<} = \left\{ \frac{u}{2\pi} + U^2 - 1 \pm \left[\left(\frac{u}{2\pi} \right)^2 + 4U^2 \left(\frac{u}{2\pi} - 1 \right) \right]^{1/2} \right\}. \quad (\text{A4})$$

Substituting these solutions into Eq. (A1), one arrives at the four different equations which determine V_g as a function of u and U . The boundary surface is given as

$$V_g = -\frac{u}{2} \pm \left(z^{>,<} + \frac{u}{2\pi} \sum_{\pm} \tan^{-1}(z^{>,<} \pm U) \right). \quad (\text{A5})$$

Eqs. (A5) and (A4) are the exact analytical expressions for the surface boundary between the spin-compensated and non-spin-compensated regions. These equations determine the four different, but connected, branches of one boundary surface. This surface is given in Fig. 1.

The two branches corresponding to the two solutions of Eq. (A3), $\pm z^{<}$, exist only at $U > U_0$, where the threshold value of the bias is $U_0 = 1/\sqrt{3}$, whereas the other two branches always exist. Accordingly, the forms of the curves $V_g(u)$ qualitatively differ before and after the threshold bias. In the small bias case the transition curve $u(V_g)$ [the inverse function to the function $V_g(u)$] is a function with one minimum at the point,

$$u_1(U) = \pi(1 + U^2), \quad V_g^1(U) = -u_1/2. \quad (\text{A6})$$

This point corresponds to the smallest value of interaction constant at which the spin-instability exist, and at which the region of instability on the gate voltage scale shrinks to a point.

The small bias case includes the case of zero bias, i.e., the original Anderson problem. The boundary of spin-polarization instability is given for the Anderson solution as

$$V_g = -\frac{u}{2} \pm \left[\sqrt{\frac{u}{\pi} - 1} + \frac{u}{\pi} \tan^{-1} \left(\sqrt{\frac{u}{\pi} - 1} \right) \right].$$

This expression reproduces the known existence of interaction-constant threshold in the Anderson solution, $u_{Anderson} = u_1|_{U=0} = \pi$.

For large bias, $U > U_0$, the transition curve $u(V_g)$ is a function with two minima and one local maximum between them at point (A6). The coordinates of the two minima are

$$u_2(U) = 4\pi(\sqrt{U^4 + U^2} - U^2),$$

$$V_g^2(U) = -\frac{u_2(U)}{2} \pm (\sqrt{2\sqrt{U^4 + U^2} - U^2 - 1} + \frac{u}{2\pi} \sum_{\pm} \tan^{-1}(\sqrt{2\sqrt{U^4 + U^2} - U^2 - 1} \pm U)). \quad (\text{A7})$$

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