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LETTER TO THE EDITOR

Integro-differential Schrödinger equation for dissipative systems

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Abstract. The canonical treatment of the quantum dynamics of systems with dissipation affected degrees of freedom proceeds within the sum over histories picture of quantum theory. This paper proposes to supplement that approach with a Schrödinger equation approach to the same physics. Starting from a Lagrangian that is of the same form as those obtained by path integration, one can arrive at a quantized Hamiltonian analogue using the standard rules applied to non-dissipative systems. The resulting Hamiltonian is non-diagonal in position representation, so that the corresponding Schrödinger equation is a nonlinear integro-differential equation reminiscent of the Hartree equation. In the case of the normal tunnel junction, with a quasiparticle heat bath, this equation has an exact solution.

Suppose one attempts to give an account of the quantum mechanics associated with the Lagrangian

$$\mathscr{L}(\varphi)=\frac{\dot{\varphi}^2(t)}{2}-V(\varphi(t))+\int R(t-t')D(\varphi(t))D(\varphi(t'))\,\mathrm{d}t'. \tag{1}$$

It was originally shown by [1–3] that $\mathscr{L}$'s of this form could be obtained from models coupling φ to degrees of freedom comprising a heat bath. Upon integrating out the heat bath degrees of freedom, one obtains the quantum analogue of (1) expressed as a path integral

$$\begin{aligned} G(\varphi(\beta),\,\varphi(0)) &= \int \mathscr{D}\varphi\; \mathrm{e}^{-S(\varphi)/\hbar} \\ S(\varphi) &= \int_{\varphi(0)}^{\varphi(\beta)} \mathrm{d}\tau\; \mathscr{L}(\varphi). \end{aligned} \tag{2}$$

This letter will attempt the quantization of (1) using the rules that take one from the dissipation free Lagrangian ($R=0$) to its quantized Hamiltonian analogue and corresponding Schrödinger equation (see equations (17) and (22)). For the sake of having a non-trivial model system, the main ideas will be formulated in the context of the superconducting tunnel junction with quasiparticle fluctuation induced dissipation

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and capacitive charging. The Lagrangian for this system is [3]

$$\mathscr{L}(t)=\frac{\dot{\varphi}^2(t)}{2}+4\int \mathrm{d}t'\ A(t-t')\cos\left(\frac{\varphi(t)-\varphi(t')}{2}\right)+4\int \mathrm{d}t'\ B(t-t')\cos\left(\frac{\varphi(t)+\varphi(t')}{2}\right). \quad (3)$$

Previous attempts to quantize (3), by Schrödinger equation, were based on a slowly varying approximation [3]. Let $\tau=t'-t$ in (3). Expand $\varphi(t+\tau)$ in the Taylor series

$$\varphi(t+\tau)=\sum\left(\frac{\mathrm{d}^m\varphi(t)}{\mathrm{d}t^m}\right)\frac{\tau^m}{m!}. \quad (4)$$

If these time derivatives are small, the cosine terms can also be expanded

$$\begin{aligned}\mathscr{L}&=\mathscr{L}_0+\sum_{r=1}^{\infty}M_r\left(\ldots\frac{\mathrm{d}^k\varphi}{\mathrm{d}t^k}\ldots\right)\\ \mathscr{L}_0&=\frac{\dot{\varphi}^2}{2}+\alpha\dot{\varphi}^2+\beta\cos\varphi\end{aligned} \quad (5)$$

where the M_r terms have φ-derivatives higher than one.

Dropping the M_r terms allows one to quantize $\mathscr{L}_0$ using the usual method.

Classical rules:

(i) define a canonical momentum: $l=\partial\mathscr{L}/\partial\dot{\varphi}$;
(ii) form a classical Hamiltonian: $H=\dot{\varphi}l-\mathscr{L}_0$;
(iii) generate $\dot{F}(l,\varphi)$ through the Poisson bracket $\dot{F}=\{H,F\}$.

Quantizing rules:

(iv) substitute operators φ; $\mathrm{i}(\partial/\partial\varphi)$ for φ; l;
(v) replace Poisson brackets by commutators;
(vi) form Schrödinger equation $H\psi(\varphi)=\varepsilon\psi(\varphi)$.

Problems with this approach arise when one attempts to quantize the next level of approximation following from (5):

$$\mathscr{L}_1=\mathscr{L}_0+\gamma(\ddot{\varphi})^2. \quad (6)$$

Because $\mathscr{L}_1$ contains a second derivative, a new set of quantization rules are required. The most obvious, non-trivial, attempt to quantize involves a new classical Hamiltonian

$$H_1(\varphi,l;\dot{\varphi},k)=l\dot{\varphi}+k\ddot{\varphi}-\mathscr{L}_1(\varphi,\dot{\varphi},\ddot{\varphi}) \quad (7)$$

with new canonical momenta

$$\begin{aligned}l&=\frac{\partial\mathscr{L}_1}{\partial\dot{\varphi}}-k\\ k&=\frac{\partial\mathscr{L}_1}{\partial\ddot{\varphi}}.\end{aligned} \quad (8)$$

Presumably, one could find operator representations for φ, l; $\dot{\varphi}$, k and by substitution in (7) arrive at a quantized H_1.

Although the scheme that takes one from $\mathscr{L}_0$ to quantum theory is standard, the quantization of $\mathscr{L}_1$ requires wholly new concepts in both classical mechanics and its quantization. That the penalty for the inclusion of one higher order in (5), is a complete revision of the standard formalism, seems extravagant. This problem only becomes worse upon the inclusion of ever higher orders. Each additional level of approximation requires the definition of novel canonical momenta whose physical meanings are unclear. The net result is a proliferation of 'basic' rules for treating individual cases. Furthermore, since $\mathscr{L}_0$ is obtained as the lowest rung on the ladder of approximations leading to the 'divergence' above, any attempt to quantize $\mathscr{L}_0$ using standard rules is questionable.

In what follows, (3) will be converted into its quantized Hamiltonian analogue using only one additional rule beyond the six listed above. This rule is obtained by insisting on consistency with a result obtained by field theory techniques. This result (whose derivation is too long for a note) consists of an effective weak coupling Hamiltonian H_{eff}. By insisting that the formalism, to be produced, reduce to H_{eff} in the weak coupling limit, one resolves an ambiguity that would otherwise prevent the recovery of a unique formalism.

Keeping these remarks in mind one can proceed with the quantization of (3). First define canonical momentum $l=\dot{\varphi}$ and form $H=l\dot{\varphi}-\mathscr{L}$:

$$H(0)=\frac{l^2}{2}-\left\{2\int_{-\infty}^{\infty}\mathrm{d}\tau\, A(-\tau)[\mathrm{e}^{-\mathrm{i}\varphi/2}\,\mathrm{e}^{\mathrm{i}\varphi(\tau)/2}+\text{c.c.}]\right.$$
$$\left.+2\int_{-\infty}^{\infty}\mathrm{d}\tau\, B(-\tau)[\mathrm{e}^{-\mathrm{i}\varphi/2}\,\mathrm{e}^{-\mathrm{i}\varphi(\tau)/2}+\text{c.c.}]\right\}. \tag{9}$$

Notice that H is evaluated at $t=0$ so that its quantization proceeds in the Schrödinger representation. The product of exponentials is used because the cosine form does not recover H_{eff}; the 'seventh rule' is thus utilized.

The trick that allows one to express H (equation (9)) in terms of a single canonical momentum, is the use of rule three to give an expression for φ-derivatives:

$$\frac{\mathrm{d}^m\varphi}{\mathrm{d}t^m}=\{H,\{H,\ldots\{H,\varphi\}\ldots\}\}. \tag{10}$$

Putting (10) into (4) and the result into (9) gives a self-consistently defined classical H.

Replacing Poisson brackets by commutators sums (4) exactly:

$$\varphi(\tau)=\mathrm{e}^{\mathrm{i}H\tau}\varphi\,\mathrm{e}^{-\mathrm{i}H\tau} \tag{11}$$

whence the quantized H can be written

$$H=-\frac{1}{2}\frac{\partial^2}{\partial\varphi^2}-\left\{\int_{-\infty}^{\infty}\mathrm{d}\tau\, A(-\tau)[\mathrm{e}^{-\mathrm{i}\varphi/2}\,\mathrm{e}^{\mathrm{i}\varphi(\tau)/2}+\mathrm{e}^{\mathrm{i}\varphi/2}\,\mathrm{e}^{-\mathrm{i}\varphi(\tau)/2}]\right.$$
$$\left.+\int_{-\infty}^{\infty}\mathrm{d}\tau\, B(-\tau)[\mathrm{e}^{-\mathrm{i}\varphi/2}\,\mathrm{e}^{-\mathrm{i}\varphi(\tau)/2}+\mathrm{e}^{\mathrm{i}\varphi/2}\,\mathrm{e}^{\mathrm{i}\varphi(\tau)/2}]+\text{h.c.}\right\}\mathrm{e}^{\mathrm{i}\varphi(\tau)/2}$$
$$=\mathrm{e}^{\mathrm{i}H\tau}\,\mathrm{e}^{\mathrm{i}\varphi/2}\,\mathrm{e}^{-\mathrm{i}H\tau}. \tag{12}$$

Written more compactly, (12) becomes

$$H = H_\varphi - gF(H) \tag{13}$$

where gF is the curly bracket in (12) and g is a dimensionless coupling parameter. In the weak coupling limit, the first iteration of (13) yields: $H_{\text{eff}} = H_\varphi - gF(H_\varphi)$, the field theory result. A further advantage of this approach is that it trivially recovers the field theory result; something out of reach of the slowly varying approach.

One is now in a position to generate a self-consistent slowly varying approximation via

$$e^{iH\tau}\mathcal{O}\, e^{-iH\tau} = \mathcal{O} + i\tau[H, \mathcal{O}] + \ldots.$$

In the weak coupling limit, and to lowest non-trivial order, H_{eff} becomes

$$H^*_{\text{eff}} = -\frac{1}{2}\left[1 + \int_{-\infty}^{\infty} d\tau\ \tau^2(A + A^*)\right]\frac{\partial^2}{\partial\varphi^2} - \left[2\int_{-\infty}^{\infty} d\tau\ (B + B^*)\right]\cos\varphi. \tag{14}$$

By forming $\langle\varphi|H|\varphi'\rangle$, one can obtain a Schrödinger equation via

$$\int d\varphi'\ \langle\varphi|H|\varphi'\rangle\psi_l(\varphi') = \varepsilon(l)\psi_l(\varphi) \tag{15}$$

where

$$\langle\varphi|H|\varphi'\rangle = -\frac{1}{2}\frac{\partial^2}{\partial\varphi^2}\delta(\varphi - \varphi') - \left\{\sum_{l,l'}\int_{-\infty}^{\infty} d\tau\ A(-\tau)\right.$$

$$\left.\times\left[e^{-i\varphi/2}\langle\varphi|\, e^{iH\tau}|l\rangle\langle l|\, e^{i\varphi/2}|l'\rangle\langle l'|\, e^{-iH\tau}|\varphi'\rangle + \ldots\right]\right\}. \tag{16}$$

Unit operators constructed from eigenstates of H have been inserted where useful. Put (16) into (15) to get

$$-2U\frac{\partial^2}{\partial\varphi^2}\psi_l(\varphi) - \int d\varphi'\ K(\varphi, \varphi')\psi_l(\varphi') = \varepsilon(l)\psi_l(\varphi) \tag{17}$$

$$K(\varphi, \varphi') = 2\sum_{l,l'}\psi_l(\varphi)\psi^*_{l'}(\varphi')\int d\varphi''\psi^*_{l'}(\varphi'')\psi_{l'}(\varphi'')$$

$$\times\left[(A_F + A^*_F)\cos\left(\frac{\varphi - \varphi''}{2}\right) + (B_F + B^*_F)\cos\left(\frac{\varphi + \varphi''}{2}\right)\right]$$

where A_F ; B_F are the Fourier transforms of A; B evaluated at frequency $(\varepsilon(l) - \varepsilon(l'))/\hbar$; U is the capacitive charging energy e^2/C.

For the normal tunnel junction, $B_F = 0$ and (17) has an exact plane wave solution $\exp(-il\varphi)$. One obtains a recursive expression for the energy band

$$\varepsilon(l) = 2Ul^2 - \left\{A_F\left(\frac{\varepsilon(l+\frac{1}{2}) - \varepsilon(l)}{\hbar}\right) + A_F\left(\frac{\varepsilon(l-\frac{1}{2}) - \varepsilon(l)}{\hbar}\right) + \text{c.c.}\right\}. \tag{18}$$

This band agrees with bands obtained by other methods [4] in that there is no splitting, but there is a Van-Hove singularity on the first Brillouin zone boundary ($|l| \leqslant \frac{1}{4}$ in a 4π-periodic model).

The main result of this work is a method for quantizing dissipative systems whose classical Hamiltonians are of the form:

$$H(t)=\frac{l^2(t)}{2}+V(\varphi(t))-\int R(t-t')D(\varphi(t))D(\varphi(t'))\,\mathrm{d}t'. \tag{19}$$

(1) Working in Heisenberg representation, replace the D's by:

$$D(\varphi(t))=\mathrm{e}^{\mathrm{i}Ht}D(\varphi)\,\mathrm{e}^{-\mathrm{i}Ht}. \tag{20}$$

Do the same with $l(t)$ and $\varphi(t)$ in V.

(2) Form $\mathrm{e}^{-\mathrm{i}Ht}H(\varphi(t))\,\mathrm{e}^{\mathrm{i}Ht}$ to get the Schrödinger representation:

$$H=-\frac{1}{2}\frac{\partial^2}{\partial\varphi^2}+V(\varphi)-\left\{\int \mathrm{d}\tau\,\frac{R(-\tau)}{2}\,[D(\varphi)\,\mathrm{e}^{\mathrm{i}H\tau}D(\varphi)\,\mathrm{e}^{-\mathrm{i}H\tau}]+\mathrm{h.c.}\right\}$$

$$\tau=t'-t. \tag{21}$$

(3) Follow the procedure above to get a Schrödinger equation:

$$\left[-\frac{1}{2}\frac{\partial^2}{\partial\varphi^2}+V(\varphi)\right]\psi_l(\varphi)-\int \mathrm{d}\varphi'\,K(\varphi,\varphi')\psi_l(\varphi')=\varepsilon(l)\psi_l(\varphi) \tag{22}$$

where K is a function of the other ε's so that the energy spectrum of (22) is recursively defined.

This procedure is easily generalized to systems with multiple degrees of freedom and field degrees of freedom. In the latter case, one obtains Hamiltonian densities of the form:

$$\mathscr{H}=-\frac{1}{2}\frac{\delta^2}{\delta\Phi^2(r)}+V(\Phi(r))-\left\{\int \mathrm{d}^4x\,\frac{R(r,-\tau)}{2}\,[D(\Phi)\,\mathrm{e}^{\mathrm{i}H\tau}D(\Phi)\,\mathrm{e}^{-\mathrm{i}H\tau}]+\mathrm{h.c.}\right\}$$

$$H=\int \mathrm{d}^3x\,\mathscr{H} \tag{23}$$

where $\delta/\delta\Phi(r)$ is a functional derivative and Φ is the canonically conjugate field variable.

Using the methods of this note provides a new way of attacking problems that might be preferable to the path integral for certain discussions.

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